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Extending Geometric Discretisation

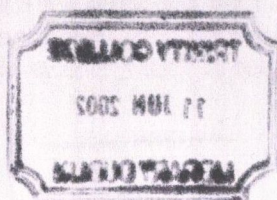
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Samik Sen

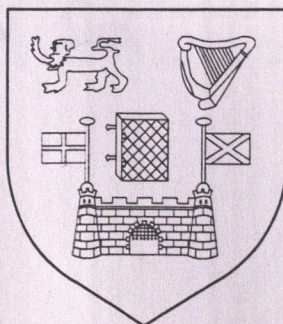
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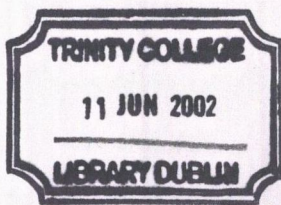
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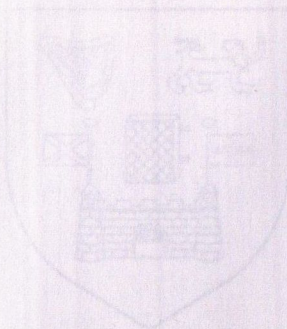
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October, 2001



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Summary

Geometric discretisation (GD) [1] is a novel approach capable of capturing topological properties, based on a correspondence between discrete objects and operations on a triangulation with continuum ones on a manifold. We felt that much work remained to be done to fulfill the potential it appeared to have and we were not wrong.

We began by trying to incorporate metric into the scheme where we found that a cubic formulation, which required the introduction of a non-trivial variation of the Whitney map [2], was well suited to the task. These were our initial goals.

Along the way we found an interesting space which is generated by the Whitney map. This is a finite dimensional space (FDS) which means that operators can be expressed as matrices and provides another discretisation scheme altogether: a variation of finite element methods in some sense. With this for example our discrete wedge product is associative which is not the case in GD. Unfortunately topology is lost in this process though.

In GD, we are trying to construct a discretisation scheme which captures differential geometry. From our point of view fermions provide an excellent laboratory in which to test what we have, since if we were able to reproduce the properties of continuum theory completely we would not have fermion doubling, which is after all an discretisation artifact.

Thus, we were interested in applying the insights we gained from our work to the Fermion doubling problem. The Dirac-Kähler [3] formulation puts the Dirac equation in terms of differential geometry which is what our scheme is based on too. We looked at this.

GD is too similar to standard Kogut-Susskind theory [4] and suffers from the same problem with constructing projection operators which leads to degeneracy due to being unable to separate the multiple Dirac fermions which arise. FDS, on the other hand, uses continuum operators and so can, but since it does not capture topology it suffers from spectrum doubling [5]. We have made some progress in identifying where the potential problem lies in our current work.

Acknowledgments

Thanks to Prof. Sexton for putting up with me and leaving me at it since I've never been the best at explaining to people what it is that I'm up to. Particularly for that time when I had this vague idea of FDS but just couldn't put my finger on it. I gave some kind of description of what I was going on about and he managed to spot that there was something there immediately!

Many thanks to Colm Connaughton too who worked on geometric discretisation for his masters and caught the bug. He really wanted to get it sorted out which was very helpful since he was someone else to discuss things with which provided an opportunity to mess around with the blackboard in the seminar room which can't be missed. His appearances always added a boost to things.

I'd also like to thank my parents for various reasons. My dad for I suppose coming up with the idea of geometric discretisation in the first place with David Adams(thanks to you too!). It has been a fun thing to work on. When I found out that the simplicial Whitney inner product calculation hit a dead end I might not have agreed but thank God for the cubic case! My mum for having to put up with yet another physicist in the house

Of course what fun would it have been without the people. Having been around the department for SO long there have been generations at this stage! — from my undergrad class to my G29 office mates. Then again if it wasn't for you maybe I would have been out of here a few years ago?

Contents

1	Introduction	1
2	Differential Geometry	7
2.1	Introduction	7
2.2	From manifolds to differential forms	7
2.2.1	Manifolds	7
2.2.2	The Tangent space - $T_p(M)$	9
2.2.3	The cotangent space - $T_p^*(M)$	9
2.2.4	The wedge product	10
2.3	Integration of differential forms	10
2.3.1	Orientations of manifolds	10
2.3.2	Partitions of unity	11
2.4	The Cartan exterior algebra	12
2.4.1	The exterior derivative	13
2.4.2	Hodge star	13
2.4.3	The adjoint of the exterior derivative	14
2.4.4	The Laplacian	14
2.5	Summary	14
3	Topology	15
3.1	Topological invariants	15
3.2	Simplicial complexes	16
3.3	Homology theory	17
3.4	Cohomology theory	19

3.5	Discretisation	20
3.5.1	Triangulations	20
3.5.2	Chains and cochains	22
3.5.3	Operations on the complex	24
3.5.4	An interpretation	24
4	Geometric discretisation	26
4.1	Introduction	26
4.2	The Simplicial Case	27
4.2.1	The de Rham map	27
4.2.2	The Whitney map	28
4.3	The Cubic Lattice and its Dual	34
4.3.1	Introduction	34
4.3.2	de Rham	35
4.3.3	Whitney	36
4.4	Wedge product	45
4.5	Hodge star	45
4.5.1	Barycentric subdivision and the Dual space	48
4.5.2	Simplicial	49
4.5.3	Cubic	51
4.6	A Generalised de Rham Map	51
4.6.1	Modifications to the exterior derivative	51
4.6.2	Modifications to the Whitney map	53
4.6.3	An interpretation	53
4.7	Computational GD	53
4.8	Convergence	54
4.8.1	Approximation	55
4.9	Summary	59
5	Incorporating metric	60
5.1	A heuristic	60
5.2	The inner product is the star	62

5.2.1	Basis lists	62
5.2.2	Determining *	63
5.3	S^1 example	65
5.3.1	Stage one	65
5.3.2	Whitney	68
5.3.3	Stage two	69
5.3.4	Stage three	70
5.4	Cubic Lattice case	73
6	Finite Dimensional Subspaces	80
6.1	Introduction	80
6.2	Back to function spaces	81
6.2.1	Review	82
6.3	FDS in practice	82
6.4	Topology	85
6.4.1	Nonconformal FDS	87
6.5	Electrostatics	88
6.6	Finite Element	89
6.7	Conclusions	90
7	Scalar field theory	92
8	The Dirac-Kähler Equation	95
8.1	The Dirac equation	95
8.2	The Dirac-Kähler equation	96
8.2.1	Becher and Joos	98
8.2.2	Geometric Discretisation	98
8.2.3	Finite Dimensional Subspaces	99
8.3	Topology and doubling	99
8.4	Fermion Doubling	101
8.5	Conclusions	102

9	Conclusions	104
9.1	Whitney	105
9.2	Metric	105
9.3	New discretisation schemes	106
9.4	Fermions on the lattice	106
9.5	Future work	107
A	Discrete Operator Approximations	109
A.1	Algebraic Topology	109
A.1.1	The Discrete Wedge	109
A.1.2	The Discrete Hodge Star	112
A.2	Dodziuk	113
B	Finite Element	118
B.1	Finite Element Method	118
B.1.1	Functional Analysis	118
B.1.2	Variational problem	120
B.1.3	Finite elements	124
B.2	Application to Field theory	125

Chapter 1

Introduction

QED has been spectacularly successful, with its determination of the Bohr magneton as 1.0011596522 compared to the experimental value of 1.0011596525, and inspired the Standard Model; one of the cornerstones of theoretical physics.

It is an Abelian theory with a small coupling constant which means that it is not easily generalised to other interactions where this is not the case. Due to the work of Yang and Mills [6] the first is no longer a problem but the coupling constant is. This is because we are unable to ignore higher order terms in expansions as we do in QED making analytical work very difficult; as a result we look at numerical methods.

In the early 70's Wilson used a lattice as a means for non-perturbative regularisation of QCD [7]. This enabled work involving strong interactions at long range where the coupling grows and analytic methods fail [8]-[19]. We can then evaluate path integrals using Monte Carlo methods to determine for example the string tension and mass gap.

Usually we work with perturbation theory expanding our action around the vacuum of the field, keeping highest order terms. Since the mid-70's though there has been growing interest in effects from extended field configurations which are stationary points of the action (instantons, for example) [20, 21, 22]. This effect is usually small though not in QCD and produces exotic effects in electroweak theory [23].

Standard discretisation involves taking a collection of points as the discrete space. Functions can then be approximated by their values at these points, interpolating in between. We can also implement finite difference as well as integration schemes

in this framework. We do not have any information about the connectivity of the underlying space (the topology) with the grid though and cannot recover it; we do not know whether there are holes in the regions between the points.

Finite element methods [24, 25, 26] on the other hand have a more complex discrete space. Here our discrete space is a triangulation as opposed to simply a collection of points and a triangulation can capture the topology of the space we are working with. We have a collection of cells with standard functions defined inside them, representing continuum functions with piecewise approximations.

In his work Wilson used a finite difference approach, for putting fermions on the lattice, losing the topological information now required, as well as leading to the fermion doubling problem [5]. A new approach is needed to deal with these effects computationally.

When we are dealing with topology in continuum theory we work with differential geometry and algebraic topology. Borrowing from these we can create a new form of discretisation where the topology is explicitly captured known as geometric discretisation. We work with a triangulation, which is topologically equivalent to the continuum space, and have discrete analogues of continuum objects and operations.

Geometric discretisation (GD) is a discrete analogue of differential geometry. A triangulation is used instead of a manifold with analogues for p -forms as well as various operators, including notably the Hodge star which was a significant development [1]. GD is a topological theory which we had used to compute invariants [27] and wanted to develop further. In particular we wanted to incorporate metric which would let us solve equations in more applied fields where the ability to capture properties which standard approaches are unable to might be fruitful. The theory has many exciting possibilities, including insights into field theory discretisation like the Dirac-Kähler formulation [3, 4, 28, 29, 30, 31] and fermion doubling as well as multi-equation solvers (meaning solving for a variable which must satisfy more than one differential equation simultaneously) to name but a few. So far geometric discretisation has used the tools of algebraic topology to construct a discretisation scheme but it remains too topological and the excitement associated with it is based more on potential than reality (though we hope this is changing). In this work we make four main contributions:

- We develop a cubic theory which is a non-trivial modification to the simplicial one.
- We incorporate metric demonstrating the convergence of $*$ as the complex is refined.
- We introduce a finite dimensional subspace (FDS) which provides a new discretisation scheme.
- We investigate Dirac-Kähler in both GD and FDS.

We begin by reviewing some differential geometry so that we can recall what the continuum theory, which we are trying to capture, is and what properties various objects and operators have. We would also like to make this accessible to an audience who might not have a theoretical physics background since ideally we would like to have a system which can be widely used.

We then look at topology. The basic notation and language we use comes from algebraic topology. Having looked at this we note the correspondence between the discrete structure we have here and the continuum one from differential geometry. Further development of this correspondence to GD. Note that cochains were not developed as discrete analogues of forms, this is just what we want to use them as.

We then move onto new work. Having noticed the potential correspondence between the discrete and the continuum, we develop it. We initially follow the work of Dodziuk [32] who used a pair of mappings: The Whitney (W^K), which maps discrete objects to continuous ones, and the de Rham (A^K), which is its left inverse. Taking the derivative before using either of these mappings gives the same result as taking it after. He proved that the various discrete operators converged to the correct continuum limit. Adams developed this further by introducing a new discrete Hodge star $*^K$ and wedge product, using which we were able to capture topological properties. In this work, we incorporate metric and show that in the new framework we also get the correct continuum limits.

We first note that we can do this by adding factors to our discrete $*^K$ but $*$ and the inner product are related since

$$(x, y) = \int_M x \wedge *y. \quad (1.1)$$

If we just introduce factors in an *ad hoc* manner to $*$ we break this relationship and therefore the discrete structure would no longer match the continuum one, which is our aim. That being the case we make a natural modification to our discrete inner product and see how this alters $*^K$. We find in doing this that our simplicial theory has problems but that for the cubic case we get exactly the factors which we had introduced previously in an *ad hoc* manner. This lets us show that $*^K$, the discrete coderivative and the discrete Laplacian all converge to the continuum cases.

In our work on $*^K$ in the simplicial case we needed to develop computational methods. We noticed that the W^K mapped onto linear functions which were finite dimensional, letting us deal with them computationally. We found that the space generated by W^K provided an interesting discretisation in itself. In this space, wedge is associative since we are no longer restricted to linear functions as we were in GD. If you wedge two linear functions you get a quadratic. This needed to be approximated in GD which is where the nonassociativity arose. Working in this finite dimensional space (FDS) we show that we can approximate functions as well as have operators which converge to the continuum results. This comes at a cost though since if we want to have an associative wedge we need a larger space which results in a nonconformal finite element method. This does not have the same topology as the continuum theory, though in the limit the topology is recovered. We see that the method is not too computationally expensive since even though the dimension of the spaces is very large, the operations which we perform on them are near linear. So FDS provides a practical scheme which is comparable to FE though with richer structure able to represent differential forms.

We then look briefly at how we can discretise scalar field theory, which follows from the fact that our discrete approximations converge to their continuum counterparts. Note that since our discrete derivative satisfies the Leibniz rule as well as Stokes' theorem, we can perform integration by parts discretely. So we have

$$\int \partial_\mu \phi \partial^\mu \phi = [\phi \partial_\mu \phi] - \int \phi \partial_\mu \partial^\mu \phi \quad (1.2)$$

$$= - \int \phi \partial_\mu \partial^\mu \phi. \quad (1.3)$$

Finally we look at the Dirac-Kähler (DK) formulation of the Dirac equation. Here we note the relationship of the Dirac equation to find the square root of the Laplacian.

In terms of differential geometry this is simply

$$d + \delta. \tag{1.4}$$

The Dirac fields can be represented by differential forms as shown in [31]. This leads to a 16-dimensional representation of the problem which in the continuum theory splits into 4 copies of the Dirac equation. In the discrete DK theory we cannot separate the spaces due to the non-locality of certain operators. We find that if we use FDS, instead of using GD, we can get around this problem since FDS works in the continuum space and so uses the local operators available. Unfortunately topology is not captured in FDS which from the work of Rabin [5] is related to spectrum degeneracy.

We have looked primarily at Becher and Joos [31] from which we can see that GD with its extra structure does not avoid the central problem of being unable to create a discrete projection operator. Rabin's analysis is perhaps more suited to our work since he shows that the degeneracy problem is fundamentally related to the lack of a proper discrete Hodge star operator, with the properties which we have in GD. This does not resolve the problem entirely though since in differential geometric terms chiral symmetry is invariance under the infinitesimal transformation $\omega^{(n-p)}$ to $\omega^{(n-p)} \pm i\epsilon * \omega^{(p)}$. In the discrete setting this involves a combination of elements on the original and dual space, but does this lead to a mixed solution which we cannot separate, as we found with Becher and Joos, or not? At worst we expect a single doubling, which is the case with Dirac-Kähler using continuous time, though degeneracy in a new form. Previously we have spectrum degeneracy from using an antisymmetric derivative and degenerate states which we are unable to separate in discrete Dirac-Kähler. Here the doubling, if it occurs, would be due to mixed states on the original and dual lattice.

Geometric discretisation aims to capture as much mathematical structure as we can and to isolate what the trade-offs are. The advantage of this is that we should be able to deal with fermions on a lattice, for example, with a generic system. Since we now have metric, this same system should also be applicable to problems related to gravity. It is still a theory in development, but we have most of the structure we set out to achieve. The specific objectives in this work have been reached in that

metric has been incorporated and we have generalised to a cubic lattice theory. We can now worry about how to apply what we have in various areas without having to be concerned about making new developments in GD.

We have four parts to this thesis:

1. We begin by reviewing differential geometry and algebraic topology, noting the relationships between their structures which leads to geometric discretisation.
2. We further develop GD, which is the main part of our work, generalising it to the cubic lattice case, demonstrating convergence and incorporating metric.
3. We investigated a finite dimensional space (FDS) that exists, associated with the image of the Whitney map.
4. We conclude by looking at applications of these ideas to scalar field theory and in particular the Dirac-Kähler approach to fermions.

2.2 From manifolds to differential forms

2.2.1 Manifolds

A manifold is a topological space which locally resembles Euclidean space near each point. It may or may not be connected, and it may or may not be compact. For example, the real line $\mathbb{R}$ is a manifold, as is the circle S^1 . A manifold is a space which is locally Euclidean, meaning that for every point p in the manifold, there is a neighborhood U of p which is homeomorphic to an open subset of $\mathbb{R}^n$.

We use the term n -manifold to mean a manifold of dimension n .

Chapter 2

Differential Geometry

2.1 Introduction

Differential geometry is calculus generalised to curved spaces. Since calculus is one of the pillars of mathematics, it appears in a wide range of applied and theoretical disciplines. Our objective is to create a discretisation scheme which captures the spirit of differential geometry, by creating a discrete analogue to the various objects, as well as operations, that appear in the continuum theory.

Note that we do not just want to capture features but to get the inter-relationships that exist, so that if we compute something in different ways the result will be the same. The classic example being Stokes' theorem which does not hold for most computational methods.

Before we create our discrete analogues we look at the continuum theory to see what it is that we are trying to capture.

2.2 From manifolds to differential forms

2.2.1 Manifolds

A manifold is a topological space which is locally Euclidean but not necessarily globally[33]. For example, the real line $\mathbb{R}$ is Euclidean globally, and hence a trivial manifold, whereas the circle, S^1 , is only locally.

We take the circle $x^2 + y^2 = 1$ in the xy -plane to demonstrate the structure of

manifolds explicitly. We parametrise it with one coordinate, θ and consider that case where we begin at $\theta = 0$ and keep moving away by constantly increasing θ . Even though the coordinate difference between $\theta = 0$ and θ is increasing we find that we end up back where we started which is not very satisfactory since points which are nearby should have coordinates which are close to each other. This can be remedied by splitting the space into regions each of which is Euclidean ; this is the key idea behind manifolds. Each region, with its associated coordinate function, is known as a *chart* and the collection of charts is known as an *atlas*. Continuing with our example, we need to determine an atlas for S^1 .

The initial problem we face is the selection of charts. It is reasonable to begin by looking at the simplest choice, that is using one chart with the region being the entire circle and the coordinate being θ , ranging from 0 to 2π . This has a problem though since points which are near each other do not necessarily have coordinates which are nearby. For example 0.01 and 2π appear to be distant but are not.

If, on the other hand, we choose two regions we can avoid this problem which is why manifolds are useful. For the first chart we can take the region $\theta \in (0, 2\pi)$ which covers all of S^1 except the point $(1, 0)$ and for the second the region $\theta \in (-\pi, +\pi)$ which covers all of S^1 except the point $(-1, 0)$. We could have chosen three, four or more charts if we wanted but two is sufficient in this case.

We need to introduce the idea of a *topological space* before we can provide a more precise description of what a manifold is. Let X be a set and $C = \{U_i \mid i \in I\}$ denote a collection of subsets of X . The pair (X, C) is a *topological space* if C satisfies the following requirements:

- $\emptyset, X \in C$.
- The union of any (may be infinite) collection of U_i 's is an element of C .
- The intersection of any finite collection of U_i 's is an element of C .

X is often called a topological space. The U_i 's are called open sets and C is said to give a topology to X .

So we can now say that M is an n -dimensional differentiable manifold if

1. M is a topological space.

2. M has a family of pairs $\{(U_i, \phi_i)\}$.
3. U_i is a family of open sets which covers M . ϕ_i is a homeomorphism from U_i to an open subset of $\mathbb{R}^n$.
4. Maps between coordinate systems in overlapping regions are infinitely differentiable.

2.2.2 The Tangent space - $T_p(M)$

Let M be an n -manifold with basis $(x_1, \dots, x_n)$ in each chart. The *tangent space* $T_p(M)$ is the vector space spanned by the tangents to all curves passing through p . $T_p(M)$ then is always an n -dimensional vector space at each point with basis vectors v_i given by

$$v_i = \frac{\partial}{\partial x_i} \quad (2.1)$$

evaluated at p . We have a vector field on M when the tangent vectors vary smoothly with p , as in

$$\vec{v} = a^i(\vec{x}) \frac{\partial}{\partial x_i} \quad (2.2)$$

with $a^i(\vec{x})$ some differentiable function of $\vec{x}$.

2.2.3 The cotangent space - $T_p^*(M)$

The cotangent space $T_p^*(M)$ is defined as the dual vector space to the tangent space $T_p(M)$, where a dual vector space V^* is defined as follows: Given an n -dimensional vector space V with basis E_i , $i = 1, \dots, n$, the basis e^i of the dual space V^* is determined by the scalar product

$$\langle E_i, e^j \rangle = \delta_i^j. \quad (2.3)$$

When we take the basis vectors $E_i = \frac{\partial}{\partial x^i}$ for $T_p(M)$, we write the basis vectors for $T_p^*(M)$ as the differential elements

$$e^i = dx^i. \quad (2.4)$$

Thus the scalar product is given by

$$\langle \frac{\partial}{\partial x^i}, dx^j \rangle = \delta_i^j. \quad (2.5)$$

Using the basis elements of $T_p(M)$ and $T_p^*(M)$ we can extend the concept of fields to include tensor fields with covariant and contravariant indices where each basis element is taken to act independently of the others. A tensor of type (p, q) has p contravariant indices and q covariant ones. For example,

$$w_{(q)}^{(p)} = w_{j_1 j_2 \dots j_q}^{i_1 i_2 \dots i_p} \frac{\partial}{\partial x^{i_1}} \otimes \dots \otimes \frac{\partial}{\partial x^{i_p}} \dots \otimes dx^{j_1} \otimes \dots \otimes dx^{j_q}. \quad (2.6)$$

Totally antisymmetric covariant tensor fields are known as differential forms. A p -form is of type $(0, p)$.

2.2.4 The wedge product

The wedge product of p 1-forms is defined as

$$dx^{\mu_1} \wedge dx^{\mu_2} \wedge \dots \wedge dx^{\mu_p} = \sum_{P \in S_p} \text{sgn}(P) dx^{\mu_{P(1)}} \otimes dx^{\mu_{P(2)}} \otimes \dots \otimes dx^{\mu_{P(p)}}, \quad (2.7)$$

where $\text{sgn}(P) = +1$ for even permutations and -1 for odd, and S_p is the symmetric group of order p . For example,

$$\begin{aligned} dx^p \wedge dx^q \wedge dx^r &= +dx^p \otimes dx^q \otimes dx^r - dx^p \otimes dx^r \otimes dx^q + dx^r \otimes dx^p \otimes dx^q \\ &\quad - dx^q \otimes dx^p \otimes dx^r + dx^q \otimes dx^r \otimes dx^p \\ &\quad - dx^r \otimes dx^q \otimes dx^p. \end{aligned} \quad (2.8)$$

It satisfies the following properties:

1. $dx^{i_1} \wedge \dots \wedge dx^{i_p} = 0$ if some i_q appears twice.
2. $dx^{i_1} \wedge \dots \wedge dx^{i_p} = \text{sgn}(P) dx^{i_{P(1)}} \wedge \dots \wedge dx^{i_{P(p)}}$.
3. $dx^{i_1} \wedge \dots \wedge dx^{i_p}$ is linear in each dx^{i_q} .

2.3 Integration of differential forms

2.3.1 Orientations of manifolds

Integration of forms can only be defined if M is orientable. This means that for any overlapping charts U_i and U_j there exist coordinates $\{x^\mu\}$ for U_i and $\{y^\alpha\}$ for U_j such

that

$$J = \det\left(\frac{\partial x^\mu}{\partial y^\alpha}\right) > 0. \quad (2.9)$$

If an m -dimensional manifold M is orientable then there exists an m -form, ω which vanishes nowhere, called the volume element. Two volume elements, ω_1 and ω_2 , are said to be equivalent if there exists a strictly positive function $h \in F(M)$ such that $\omega_1 = h\omega_2$.

2.3.2 Partitions of unity

Take an open covering $\{U_i\}$ of M such that each point of M is covered by a finite number of U_i . If this is always possible M is called *paracompact*, which we assume to be the case. If a family of differentiable functions $\epsilon_i(p)$ satisfies

- $0 \leq \epsilon_i(p) \leq 1$,
- $\epsilon_i(p) = 0$ if $p \notin U_i$,
- $\epsilon_1(p) + \epsilon_2(p) + \dots = 1$ for any point $p \in M$,

the family of functions is called a partition of unity subordinate to the covering $\{U_i\}$.

It follows that

$$f(p) = \sum_i f(p)\epsilon_i(p) = \sum_i f_i(p). \quad (2.10)$$

where $f_i(p) = f(p)\epsilon_i(p)$ vanishes outside of U_i . Hence given a point $p \in M$ there are only a finite number of terms in the summation over i due to paracompactness. For each $f_i(p)$ we can define the integral over U_i as

$$\int_{U_i} f_i \omega = \int_{\phi_i(U_i)} f_i(\phi_i^{-1}(x)) h(\phi_i^{-1}(x)) dx^1 \dots dx^m, \quad (2.11)$$

where the RHS is an ordinary multiple integration of a function of m variables.

The integral of f over M is then given by

$$\int_M f \omega = \sum_i \int_{U_i} f_i \omega. \quad (2.12)$$

Example: Let's evaluate $\int_0^{2\pi} \sin^2 \theta d\theta$. For simplicity we choose two charts $U_1 = S^1 - \{(1, 0)\}$ and $U_2 = S^1 - \{(-1, 0)\}$. We then need to get a partition of unity. So

take $\epsilon_1(\theta) = \sin^2(\theta/2)$ and $\epsilon_2(\theta) = \cos^2(\theta/2)$. Note that we use $\theta/2$ in order for the first condition, of being between 0 and 1, to hold. So we have

$$\int_{S^1} d\theta \sin^2(\theta) = \int_0^{2\pi} d\theta \sin^2(\theta/2) \sin^2(\theta) + \int_{-\pi}^{\pi} d\theta \cos^2(\theta/2) \sin^2(\theta) \quad (2.13)$$

$$= \frac{1}{2}\pi + \frac{1}{2}\pi = \pi, \quad (2.14)$$

which we know is the solution. We have left out h which we know is positive but otherwise arbitrary. We can not just set it to one since it depends on which coordinates are being used. This changes if the manifold has a metric, since then we get an invariant volume element which has a square root of the determinant of the metric term in it — so in the Euclidean case the factor is 1.

2.4 The Cartan exterior algebra

Let $\Lambda^p(x)$ be the set of anti-symmetric p -tensors at a point x . This is a vector space of dimension $\frac{n!}{p!(n-p)!}$. $C^\infty(\Lambda^p)$ is the space of smooth p -forms represented by anti-symmetric tensors $f_{ij\dots}(x)$ having p indices contracted with the wedge products of p differentials. The elements of $C^\infty(\Lambda^p)$ may then be written explicitly as follows:

$$C^\infty(\Lambda^0) = \{f(x)\}, \quad (2.15)$$

$$C^\infty(\Lambda^1) = \{f_i(x)dx^i\}, \quad (2.16)$$

$$C^\infty(\Lambda^2) = \{f_{ij}(x)dx^i \wedge dx^j\}, \quad (2.17)$$

$$C^\infty(\Lambda^n) = \{f_{i_1\dots i_n}dx^{i_1} \wedge \dots \wedge dx^{i_n}\}. \quad (2.18)$$

Note that Λ^p and Λ^{n-p} have the same dimension as vector spaces.

We can now introduce the Cartan exterior algebra (of differential forms) which is the space Λ^* of all possible antisymmetric covariant tensors. So we have

$$\Lambda^* = \Lambda^0 \otimes \Lambda^1 \otimes \Lambda^2 \otimes \dots \otimes \Lambda^n. \quad (2.19)$$

This space reproduces itself under the wedge product operation.

2.4.1 The exterior derivative

Another operation which can be applied to elements of this algebra is the exterior derivative which takes p -forms to $(p+1)$ -forms according to the rule

$$d : C^\infty(\Lambda^p) \rightarrow C^\infty(\Lambda^{p+1}), \quad (2.20)$$

$$d : f_{i_1 i_2 \dots i_p} dx_{i_1} \wedge \dots \wedge dx_{i_p} \rightarrow \sum_j \frac{\partial f_{i_1 i_2 \dots i_p}}{\partial x_j} dx_j \wedge dx_{i_1} \wedge \dots \wedge dx_{i_p}. \quad (2.21)$$

In the case of d acting on $C^\infty(\Lambda^1)$ explicitly, $d(f_j(x)dx^j) = \frac{\partial f_j}{\partial x^i} dx^i \wedge dx^j$. An important property of this is that $d^2 = 0$, which follows from the equality of mixed partial derivatives. For example

$$df = \partial_i f dx^i, \quad (2.22)$$

$$ddf = \partial_i \partial_j dx^i \wedge dx^j = \frac{1}{2}(\partial_i \partial_j f - \partial_j \partial_i f) dx^i \wedge dx^j = 0. \quad (2.23)$$

In 3D this operator is more familiarly known as grad, curl and div when acting on 0, 1 or 2 forms respectively:

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz = \text{grad } f, \quad (2.24)$$

$$d(f_1 dx + f_2 dy + f_3 dz) = \text{curl}(f_1 dx + f_2 dy + f_3 dz), \quad (2.25)$$

$$\omega = f_1 dx \wedge dy + f_2 dx \wedge dz + f_3 dy \wedge dz, \quad (2.26)$$

$$d\omega = \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} + \frac{\partial f_3}{\partial z} \right) dx \wedge dy \wedge dz = \text{div } \omega. \quad (2.27)$$

The exterior derivative naturally arises from Stokes' theorem

$$\int_M d\omega = \int_{\partial M} \omega. \quad (2.28)$$

2.4.2 Hodge star

The number of independent functions $C^\infty(\Lambda^p)$ is the same as that in $C^\infty(\Lambda^{n-p})$. Utilising this, the Hodge $*$ operator (or duality transformation) transforms p -forms into $(n-p)$ -forms. In a flat Euclidean space this operator is defined by

$$*(dx^{i_1} \wedge \dots \wedge dx^{i_p}) = \frac{1}{(n-p)!} \epsilon_{i_1 \dots i_p i_{p+1} \dots i_n} dx^{i_{p+1}} \wedge \dots \wedge dx^{i_n}. \quad (2.29)$$

Note that for a p -form ω_p we get

$$**\omega_p = (-1)^{p(n-p)} \omega_p. \quad (2.30)$$

2.4.3 The adjoint of the exterior derivative

We can now define the inner product of two p -forms, a_p and b_p , as

$$(a_p, b_p) = \int_M a_p \wedge (*b_p), \quad (2.31)$$

from which the adjoint of the derivative can be obtained since

$$(a_p, db_{p-1}) = (\delta a_p, b_{p-1}), \quad (2.32)$$

where

$$\delta = (-1)^{np+p+1} * d *. \quad (2.33)$$

2.4.4 The Laplacian

Once we have d and δ we can construct the Laplacian which is $(\delta + d)^2$. Using the fact that $d^2 = 0$ and $\delta^2 = 0$ we have

$$(d + \delta)^2 = d^2 + d\delta + \delta d + \delta^2 = d\delta + \delta d. \quad (2.34)$$

Note that d maps p -forms to $(p+1)$ -forms while δ maps from p -forms to $(p-1)$ -forms; so one followed by the other, maps from p -forms to p -forms.

2.5 Summary

In generalising calculus to deal with curved spaces we uncover a rich structure which we have only touched on in our brief review. We have p -forms, primitive operators $(d, \wedge, *)$ and the following properties:

1. $d^2 = 0$
2. $x^p \wedge y^q = (-1)^{pq} y^q \wedge x^p$
3. $d(x^p \wedge y^q) = dx^p \wedge y^q + (-1)^p x^p \wedge (dy^q)$
4. $(x \wedge y) \wedge z = x \wedge (y \wedge z)$
5. $** = (-1)^{p(n+1)} I$
6. $\delta = (-1)^{np+1} * d *$

There are many excellent texts on the subject, the following which I found to be particularly useful [33, 34, 35, 36, 37, 38].

Chapter 3

Topology

The vocabulary we use in our work was developed in topology for entirely different reasons. We begin by looking at some topology proper which is used to classify manifolds [34, 39, 40, 41, 42]. In so doing we notice that there is a correspondence between the objects we have found useful and the objects we have from differential geometry. This suggests that we can use them as the basis for a discrete differential geometry, which we go on to develop in subsequent chapters.

3.1 Topological invariants

A square and a triangle are topologically equivalent. This means that you can continuously deform a square into a triangle and vice versa. They are both 2-dimensional spaces without holes. We can see that their Euler characteristic, that is the difference between the number of even and odd dimensional pieces they are composed of, are equal. For a triangle we have 1 face and 3 vertices which add to give 4. We only have 3 edges so the Euler characteristic is $4 - 3 = 1$. For a square we have 1 face and 4 vertices which add to give 5 while we have 4 edges so the Euler characteristic is $5 - 4 = 1$ (See Fig. 3-1). As expected they are the same.

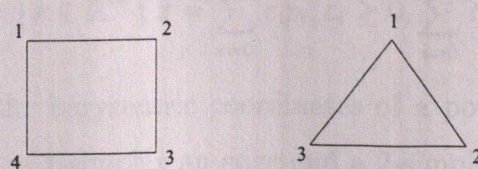


Figure 3-1: Triangulation of square and triangle.

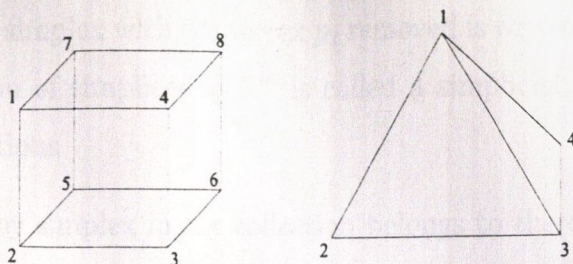


Figure 3-2: Triangulation of cube and tetrahedron.

Similarly in 3-dimensions we see that a cube and a tetrahedron have equal characteristics. For a tetrahedron we have 4 faces and 4 vertices which sum to give 8 while we have 1 volume element and 6 edges which add to give 7. The Euler characteristic is thus $8 - 7 = 1$. For a cube we have 8 vertices and 6 faces which add to 14 while we have 12 edges and 1 volume element which sum to 13 resulting in an Euler characteristic of $14 - 13 = 1$ (See Fig. 3-2). Again, they are the same.

The Euler characteristic is a topological invariant which means that two spaces which are topologically equivalent have the same values. Two spaces which have the same characteristic, though, are not necessarily topologically equivalent, for example a cube and a square.

This suggests that we can examine the properties of spaces of interest by analysing their triangulations. It is not known which spaces can be triangulated [39][40] but spaces which we will come across can (differentiable manifolds and/or 3D manifolds). Further development of this idea can lead to homology theory which in turn leads to cohomology theory which is our objective.

3.2 Simplicial complexes

Let $p_0, p_1, \dots, p_r$ be points geometrically independent in $\mathbb{R}^m$ where $m \geq r$. An r -simplex $\sigma_r = \langle p_0 \dots p_r \rangle$ can be written as

$$\sigma_r = \{x \in \mathbb{R}^m \mid x = \sum_{i=0}^r c_i p_i, c_i \geq 0, \sum_{i=0}^r c_i = 1\}. \quad (3.1)$$

$(c_0, \dots, c_r)$ are called the barycentric coordinates of a point on the simplex. A 0-simplex is thus a point, a 1-simplex an edge and a 2-simplex a triangle.

An $(r-1)$ -simplex formed from all the vertices of an r -simplex except one, is called

its face. The $(r-1)$ -simplex with the vertex p_2 removed is written as $\langle p_0 p_1 \hat{p}_2 \dots p_r \rangle$.

A finite collection of simplices in $\mathbb{R}^m$ is called a simplicial complex if it satisfies the following conditions

- The faces of any simplex in the collection belongs to the collection.
- Two simplices are joined only along common faces.

The dimension of a simplicial complex K is defined as the maximum dimension of simplexes in K . For example a triangle $\langle p_0 p_1 p_2 \rangle$ is part of a 2-dimensional simplicial complex consisting of

$$\langle p_0 p_1 p_2 \rangle, \langle p_0 p_1 \rangle, \langle p_0 p_2 \rangle, \langle p_1 p_2 \rangle, \langle p_0 \rangle, \langle p_1 \rangle, \langle p_2 \rangle. \quad (3.2)$$

We can assign orientations to simplices. Using the notation in [33] we say that

$$(p_0 p_1) = -(p_1 p_0), \quad (3.3)$$

where $(..)$ are used for oriented simplices while $\langle \dots \rangle$ are used for unoriented ones. We take the increasing order of vertices as being positively oriented. To determine whether a simplex is positively or negatively oriented determine the number of exchanges which are required to sort the vertices into increasing order. If an even (odd) number is needed then it is positively (negatively) oriented.

Let X be a topological space. If a homeomorphism $f : |K| \rightarrow X$ from a simplicial complex K to X exists then the pair (K, f) is called a triangulation of X . This triangulation is not unique.

3.3 Homology theory

Let K be an n -dimensional simplicial complex, its r -chain group $C_r(K)$ is a free Abelian group generated by the oriented r -simplices of K . If $r > \dim K$ then $C_r(K)$ is defined to be 0. An element of $C_r(K)$ is called an r -chain.

We introduce the boundary operator defined as

$$\partial_r(p_0 \dots p_r) = \sum_{i=0}^r (-1)^{(i)} (p_0 \dots \hat{p}_i \dots p_r). \quad (3.4)$$

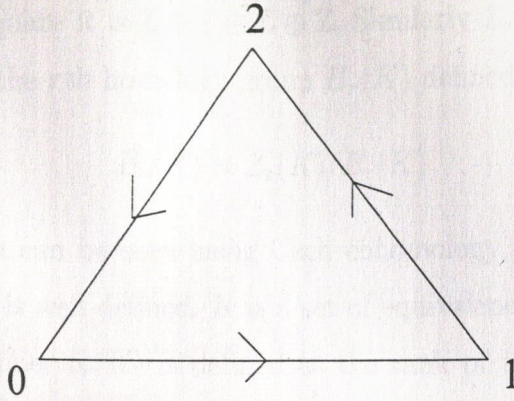


Figure 3-3: Oriented Triangle.

For example $\partial_2(p_0p_1p_2) = (p_1p_2) - (p_0p_2) + (p_0p_1)$ which gives the correct orientations for the various edges (See Fig. 3-3 whose boundary has an edge going from 2 to 0, hence $-< 0, 2 >$). The boundary operator defines a map $\partial_r : C_r(K) \rightarrow C_{r-1}(K)$.

If $c \in C_r(K)$ satisfies

$$\partial_r c = 0 \quad (3.5)$$

then it is called an r -cycle. The set of r -cycles $Z_r(K)$ is a subgroup of $C_r(K)$ called the r -cycle group. Note $Z_r(K) = \text{Ker} \partial_r$.

If $c \in C_r(K)$ with the property that there exists some $d \in C_{r+1}(K)$ such that

$$c = \partial_{r+1} d \quad (3.6)$$

then c is called an r -boundary. The set of r -boundaries $B_r(K)$ is also a subgroup of $C_r(K)$ and is called the r -boundary group. Note $B_r(K) = \text{Im} \partial_{r+1}$.

Since we know that the kernel and image of a homomorphism are subgroups we know that $Z_r(K)$ and $B_r(K)$ are subgroups of $C_r(K)$.

Theorem: $\partial_r(\partial_{r+1}\sigma) = 0$ [39].

Theorem: $B_r(K)$ is a subgroup of $Z_r(K)$.

Proof: Trivial consequence of the above theorem.

We now have three groups associated with the simplicial complex K and thus the topological space of which K is a triangulation. What topological properties do we have from this? Clearly $C_r(K)$ is not a topological invariant since it differs for a square and a triangle which are the same topologically ($C_1(K)$ is $\mathbb{Z} \oplus \mathbb{Z} \oplus \mathbb{Z}$ for a

triangle while for a square it is $\mathbb{Z} \oplus \mathbb{Z} \oplus \mathbb{Z} \oplus \mathbb{Z}$. Similarly $Z_r(K)$ and $B_r(K)$ are not invariants. However, the r th homology group $H_r(K)$ defined as

$$H_r(K) = Z_r(K)/B_r(K) \quad (3.7)$$

is an invariant (which can be seen using Čech cohomology [39]). Since $B_r(K)$ is a subgroup of $Z_r(K)$ it is well defined. It is a set of equivalence classes of r -cycles.

The r th Betti number $b_r(K)$ is defined as the rank of the free Abelian part of $H_r(K)$. This leads to the Euler-Poincaré theorem which defines the Euler characteristic, ξ , with which we began.

$$\xi(K) = \sum_{r=0}^n (-1)^r b_r(K). \quad (3.8)$$

Since the Betti numbers are topological invariants $\xi(K)$ is also an invariant.

3.4 Cohomology theory

We can define associated groups of forms. The set of closed forms is called the r th cocycle group, $Z^r(M)$. The set of exact r -forms is called the r th coboundary group $B^r(M)$. Since $d^2 = 0$ we again have $B^r(M) \subset Z^r(M)$ and can define the r th de Rham cohomology groups

$$H^r(M) = Z^r(M)/B^r(M). \quad (3.9)$$

Note that the vector spaces here have real rather than integral coefficients.

The duality between the cohomology and homology theory is due to de Rham's theorem. Given an r -form, ω , and an r -chain, c , we can define an inner product

$$(\omega, c) = \int_c \omega. \quad (3.10)$$

This provides an inner product between elements of $H^r(M)$ and $H_r(M)$. To show that $H^r(M)$ is the dual of $H_r(M)$ we need to show that their dimensions are the same which is a consequence of de Rham's theorem (the inner product is bilinear and non-degenerate).

3.5 Discretisation

Usually when working with differential equations, an approximation is made for the derivative which is

$$\frac{df}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}, \quad (3.11)$$

where instead of taking the limit as $h \rightarrow 0$ we set it to something small. This is called the finite difference approach.

As we noted in our introduction, the solution obtained using this approach does not have the physical properties of what it represents. For example if you were to integrate the energy density of an electric field inside a volume you would get a solution but this solution would not obey Stokes' theorem and so the flux at the surface of the volume would not be compatible with the charge inside.

In a way this is just a symptom of the underlying deficiency of taking a point wise discretisation of space. If we discretise a space with a collection of points we are unable to capture its topology. We have no knowledge of their connectivity which is essential to topology. What we can do instead is take a triangulation as our discrete space since we know it is topologically equivalent to the space it triangulates and so the topological information is not lost.

We can look at our discretisation as occurring at 3 layers. In the first we discretise the space (in the case of FD the collection of points), next we need to have a discrete representation of functions (the value of the function at the various points in FD) and finally a representation of operators like d (finite difference in FD). If we want to capture topology we can use a more elaborate discrete space (triangulations instead of just points). Note that the functions are built on top of the space we use which means that if we loose the topology at that level, as in FD, we are unable to regain it later.

3.5.1 Triangulations

We know that a triangulation captures topology so since a "triangulation" does not have to consist of triangles (the simplicial case) we look at the kind of triangulations we might consider as our discrete space (in 2D):

Simplicial case

Firstly, we have the simplicial case which consists of triangles, edges and vertices. This uses the standard notation, which we have been using so far, where triangles whose vertices are v_0 , v_1 and v_2 are denoted by $\langle v_0, v_1, v_2 \rangle$.

Cubic

The cubic case has squares, edges and vertices as its components. Here, we use the notation $[v_0, v_1, v_2, v_3]$ where the vertices are put in a specific order using what we call binary notation. Here we note that in binary $0 = 00$, $1 = 01$, $2 = 10$ and $3 = 11$. If we take the binary digits and use them as x and y coordinates we get that v_0 is the vertex in the bottom left, v_1 is the one on the bottom right, v_2 on the top left and v_3 on the top right.

This can easily be generalised to higher dimensions and has several advantages. For example in 3D we have $[0, 1, 2, 3, 4, 5, 6, 7]$. Here we can say that:

- Edges can only be in the x , y or z directions. This means that if we have an edge $[v_i, v_j]$ then $v_j - v_i$ must be either 1, 2 or 4 so we can tell immediately that $[0, 3]$ is not an edge while $[1, 3]$ is.
- We can look at the edge $[0, 4]$ and know that the edges parallel to it are $[1, 5]$ and $[2, 6]$ since we can shift both vertices in the 1 or 2 direction.

Dual

For every p -cell (not all complexes are simplicial, the generalisation of a simplex being a cell) there is an associated $(n - p)$ -cell. First though we need to subdivide the complex, after which we take the union of all the $(n - p)$ dimensional pieces which have p -cell as a face. This results in more exotic cells; for example we end up with polygons being associated with vertices, edges with edges and vertices with triangles. In the cubic case we end up associating squares with vertices, edges with edges and vertices with squares so we simply generate another cubic lattice. We discuss this in greater depth in Section 4.5.1.

In short we can discretise the space in various ways. We look at discrete functions and operators next.

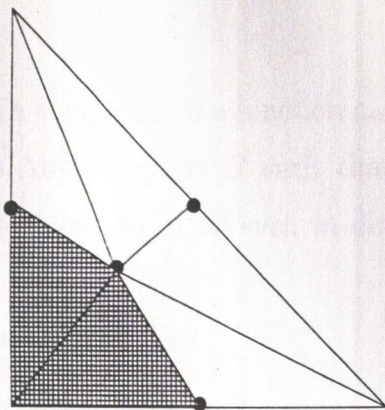


Figure 3-4: Dual of a vertex

3.5.2 Chains and cochains

Given a p -form, ϕ^p , we can integrate it over a p -dimensional volume. If the volume is composed of disjoint pieces then the integral can be expressed as the sum of many separate integrals, one for each piece. So

$$\int_V \phi^p = \int_{V_1 \cup V_2} \phi^p = \int_{V_1} \phi^p \pm \int_{V_2} \phi^p, \quad (3.12)$$

where $V = V_1 \cup V_2$. The $\pm$ is due to the fact that the orientations might be opposite.

If the volume is some complex K , with its associated simplices then we have many p dimensional volumes, σ_p^i . Because the simplices are disjoint, the integral over K can be written as the integral over $\cup_i c_i \sigma_p^i$ where the coefficients c_i are ± 1 . So we have that

$$\int_{\cup_i c_i \sigma_p^i} \phi^p = \sum_i c_i \int_{\sigma_p^i} \phi^p. \quad (3.13)$$

It is clear that this can be generalised by relaxing the restriction of c_i being ± 1 to say being a real number. Also note that the p -simplices are acting like basis elements of some vector space in the manner in which they are describing the p -volumes being integrated over. In this sense the differential forms — with the scalar product associated with integrating the forms over the simplices — are members of the dual vector space. This can be refined into the notion of chains (the basis elements of the vectors space) and cochains (their duals, which the forms can be expressed in terms of).

Chains

An m -dimensional chain on a complex K is a function c_m on the oriented m -simplices of K with values in some Abelian group G such that if $c_m(+\sigma_m) = g$, $g \in G$ then $c_m(-\sigma_m) = -g$. The collection of all such m -dimensional chains is denoted by $C_m(K, G)$.

Addition of m -chains can be defined as

$$(c_m^1 + c_m^2)(\sigma_m) = c_m^1(\sigma_m) + c_m^2(\sigma_m), \quad (3.14)$$

using the usual addition of the group.

Elementary m -chains have a close relationship to the simplices in that they map all of them to zero except one. They are denoted by the simplex which they are associated with, so the elementary m -chain σ_m^1 maps σ_m^1 to 1 and all other simplices to zero. An arbitrary m -chain c_m can be written as

$$\sum g_i \cdot \sigma_m^i, \quad (3.15)$$

where $g_i = c_m(+\sigma_m^i)$.

This means that if we take a collection of simplices — or their associated elementary chains — we can add them together to get another chain since the chains are a group and are thus closed.

Cochains

We can integrate a differential form over a given volume element to get a real number, which of course belongs to an Abelian group — the real numbers under addition. Now if the volume which is being integrated over is composed of several disjoint pieces then the integral can be broken into separate ones. So if the integral is being done over a collection of simplices belonging to a complex, it can be broken into one integral for each simplex since they are all disjoint, being members of a complex. In this way integration of a form maps the chains (since the collection of simplices corresponds to a member of the group of chains) to real numbers and can be seen as belonging to the dual space of the chains i.e. the cochains.

Cochains, as mentioned above, are the duals to chains. To every basis element of the chains there exists a cochain basis element which maps it to 1 and all the others

to zero. p -cochains have the p index raised, for instance σ^p , in contrast to p -chains which have lower indices. Once we have the dual basis elements we can write dual chains with respect to them. This is done for the differential forms using de Rham's theorem which says that the coefficient of dual basis element i is simply the integral of the form over the basis element i .

Example We take a simple example where our complex consists of the simplex $\sigma_1 = \langle 01 \rangle$. If we want to represent dx on it we evaluate the integral

$$\int_{\sigma_1} dx. \quad (3.16)$$

This is equal to $x([1]) - x([0])$, some real number c say. This means that the discrete analogue to dx is the cochain $c\sigma^1$.

3.5.3 Operations on the complex

Given a simplex, a natural operation on it is to obtain its boundary. So for example if we have a triangle $\langle v_0 v_1 v_2 \rangle$, its boundary is $\langle v_1 v_2 \rangle - \langle v_0 v_2 \rangle + \langle v_0 v_1 \rangle$. On an arbitrary p -simplex it is defined as

$$\partial \langle v_0 v_2 \cdots v_p \rangle = \sum_i (-1)^i \langle v_0 \cdots \hat{v}_i \cdots v_p \rangle, \quad (3.17)$$

where $\langle v_0 \cdots \hat{v}_i \cdots v_p \rangle$ is the face of the p -simplex with v_i removed.

We can similarly define the coboundary operator as

$$\delta \langle v_0 v_2 \cdots v_p \rangle = \sum_i (-1)^i \langle v_i v_0 \cdots v_p \rangle, \quad (3.18)$$

where the resulting $(p+1)$ -simplices must belong to the complex with which we are working. Also we have $\partial^2 = 0$ and $\delta^2 = 0$.

Finally with an inner product we can define the adjoint of the boundary which maps from p -cochains to $(p+1)$ -cochains.

3.5.4 An interpretation

This discrete structure is traditionally used to analyse manifolds in topology, as we did in the beginning of this chapter, but we are more interested in noting the overlap

Continuum	Discrete
Manifold	Complex
p -forms	p -cochains
d	Coboundary
δ	Boundary

Table 3.1: Analogues

between the discrete system which we have and differential geometry¹ (See Table 3.1). We will extend this analogy further next.

¹See Appendix A for further discussion on this topic

Chapter 4

Geometric discretisation

4.1 Introduction

Our aim is to build on the correspondence between the discrete structures associated with complexes and the continuum ones of differential geometry¹ which we observed in Sec.3.5.4, extending it as we go along:

Physics	Complex K	Manifold M
Fields	p -cochains: $C^p(K)$	p -forms: $\Omega^p(M)$
Operators	Coboundary: δ	Exterior derivative: d

Table 4.1: Objects in Physics and their Continuum/Discrete Analogues.

Essentially, we need to decide what features of the continuum theory we want to capture. Ideally we would like to have discrete objects which correspond to continuum ones. We would like to have analogous discrete operators on these objects and be able to switch from continuous to discrete and back again at will. Of course the discrete structure only has a finite amount of information, so we have to accept some loss of information in our discretisation, but we can expect convergence as we refine our triangulations? We set up the basic structures first, before moving on to convergence issues.

We begin by listing various properties of differential geometry before identifying discrete analogies. We have p -forms, primitive operators $(d, \wedge, *)$ and the following properties:

¹See Appendix A for a discussion on similar work

1. $d^2 = 0$
2. $x^p \wedge y^q = (-1)^p y^q \wedge x^p$
3. $d(x^p \wedge y^q) = dx^p \wedge y^q + (-1)^p x^p \wedge (dy^q)$
4. $(x \wedge y) \wedge z = z \wedge (y \wedge x)$
5. $** = (-1)^{p(n+1)} I$
6. $\delta = (-1)^{np+1} * d*$

This then is what we are aiming for. One of the key achievements of geometric discretisation (GD), as developed by Adams[1], is that it manages to do this (with the noticeable exception of an associative wedge). In our work, we extend this further by incorporating metric, as well as generalising to a cubic theory.

4.2 The Simplicial Case

4.2.1 The de Rham map

Our fundamental associations are those between p -cochains and δ on the complex K and p -forms and d on the manifold M . Here the de Rham map plays a vital role, specifying what the discrete analogue of a given p -form is. The idea is to simply integrate it over the p -chains. In this way we have a scalar product between p -forms and p -chains which means that we can describe the p -form in terms of p -cochains (since it belongs to the dual space of the chains).

The de Rham map A is a linear map from forms to cochains defined by

$$\langle A(\omega), \alpha \rangle = \int_{\alpha} \omega, \quad (4.1)$$

for each oriented p -simplex(chain) α in K .

Example: On the 1-simplex $[0, 1]$, we can see that the 1-form dx goes to:

$$\langle A(dx), [0, 1] \rangle = \int_{[0,1]} dx = x[1] - x[0]. \quad (4.2)$$

So that the associated cochain is $(x[1] - x[0])[0, 1]$.

An incidence number $[\sigma^p, \sigma^{p-1}]$ is defined as 0 if σ^{p-1} is not a face of σ^p or ± 1 if it is. If σ^{p-1} is a face then it contains all the vertices of σ^p except one. We get $\pm\sigma^{p-1}$ if we remove this vertex from σ^p which is what determines the sign. We can then define an incidence matrix I as

$$I_{ij} = [\sigma_i^p, \sigma_j^{p+1}]. \quad (4.3)$$

Using these we define

$$\partial\sigma_j^{p+1} = I_{ij}\sigma_i^p \quad (4.4)$$

and

$$d\sigma_i^p = I_{ij}\sigma_j^{p+1} \quad (4.5)$$

We have that for a p -form f

$$Adf = \int_{\sigma_j^{p+1}} df[\sigma_j^{p+1}]. \quad (4.6)$$

Using Stokes' theorem

$$= \int_{\partial\sigma_j^{p+1}} f[\sigma_j^{p+1}], \quad (4.7)$$

$$= \int_{I_{ij}\sigma_i^p} f[\sigma_j^{p+1}], \quad (4.8)$$

$$= \int_{\sigma_i^p} f I_{ij}[\sigma_j^{p+1}], \quad (4.9)$$

$$= \int_{\sigma_i^p} f d[\sigma_i^p], \quad (4.10)$$

$$= d\left(\int_{\sigma_i^p} f\right)[\sigma_i^p], \quad (4.11)$$

$$= dAf. \quad (4.12)$$

Thus

$$dA = Ad. \quad (4.13)$$

4.2.2 The Whitney map

Now with the de Rham map we can go from continuous objects to discrete ones but we would like to be able to go the other way too, which is where the Whitney map,

$W : C^p(K) \rightarrow \Omega^p(M)$, comes in. This has the remarkable property that $AW = I$ and $dW = Wd$ which provides the “commutative”² diagram below (Fig. 4-1):

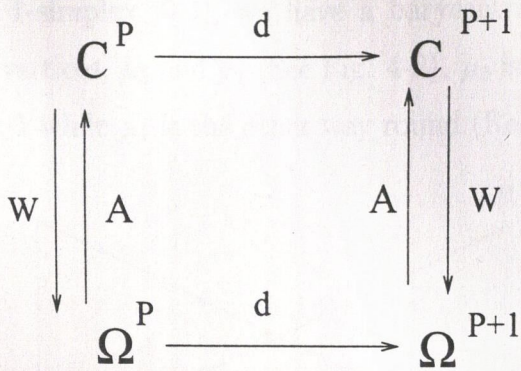


Figure 4-1: The interplay of W , A and d .

This is the heart of GD, where the equivalence between the discrete and the continuum is clear to see. It does not matter whether we take the derivative of something and then take its discrete approximation or make the approximation and then take its discrete derivative since both lead to that same result.

In order to define W though we first need to introduce an idea, the barycentric coordinates, which W is expressed in terms of.

Barycentric coordinates

The barycentric coordinates are a set of functions, $\mu_v:|K| \rightarrow A$, one for each vertex v of the complex K . These are equal to one at $v \in K$ and decrease linearly to zero at the boundary (and outside) of $St(v)$, where $St(v)$ is the union of the interiors of all the simplices in K containing v . They have the property that

$$\mu_v \in [0, 1] \tag{4.14}$$

and

$$\sum_{v \in \alpha} \mu_v(y) = 1, \quad \forall y \in |\alpha|, \tag{4.15}$$

where $\alpha \in K$ and are the discrete analogue of coordinates on a patch in manifolds. Note though that the number of coordinates is not equal to the dimension of the space and that the barycentric coordinates are not independent, since they satisfy

²It is not fully commutative since $WA \neq I$

the constraint that their sum must equal one.

Example: Given a 1-simplex $[0, 1]$, we have a barycentric coordinate associated with each of the two vertices, μ_0 and μ_1 (See Fig. 4-2). μ_0 is equal to 1 at the vertex 0 and 0 at the vertex 1 while μ_1 is the other way round (Recall $\mu_0 + \mu_1 = 1$).

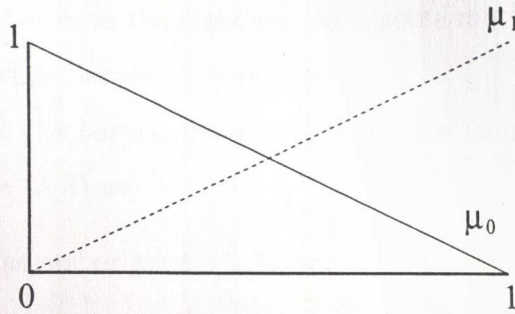


Figure 4-2: Barycentric coordinates

Determining barycentric coordinates for a triangle

For the standard triangle with coordinates

$$v_0 = (0, 0) \quad (4.16)$$

$$v_1 = (0, 1) \quad (4.17)$$

$$v_2 = (1, 0) \quad (4.18)$$

we have very simple barycentric coordinates:

$$\mu_0 = 1 - x - y \quad (4.19)$$

$$\mu_1 = y \quad (4.20)$$

$$\mu_2 = x \quad (4.21)$$

These satisfy the desired properties ($i = 0, 1, 2$):

$$\sum_i \mu_i = 1, \quad (4.22)$$

$$\mu_i \in [0, 1]. \quad (4.23)$$

In general we have that ($i = 1, \dots, D$)

$$\mu_i = x_i, \quad (4.24)$$

$$\mu_0 = 1 - \sum_i \mu_i. \quad (4.25)$$

But all triangles are not of this form. In general, we need to transform the particular triangle we are interested in to the standard, with some mapping which we can then use to get the appropriate barycentric coordinates.

For example to get the barycentric coordinates of a triangle with vertices $v_0 = (1, 2)$, $v_1 = (2, 4)$, $v_2 = (3, 3)$ we:

1. Choose a vertex as our origin b , $(1, 2)$ say.
2. Shift the others by this to get $(1, 2)$ and $(2, 1)$.
3. Determine the mapping from this shifted triangle to the standard one: to do this we note that we are looking for a 2×2 matrix which has 4 unknown components and say that A maps $(1, 2)$ to $(0, 1)$ and $(2, 1)$ to $(1, 0)$ which provides us with 4 equations. So A is

$$\begin{pmatrix} \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} \end{pmatrix}. \quad (4.26)$$

Then we have that $\mu_i = A(v_i - b)$ so that

$$\begin{aligned} \mu_1 &= \frac{1}{3}[2y - x - 3] \\ \mu_2 &= \frac{1}{3}[2x - y] \\ \mu_0 &= 1 - \mu_1 - \mu_2 = \frac{1}{3}[6 - x - y]. \end{aligned} \quad (4.27)$$

Note that these satisfy the properties that $\mu_i(v_j) = \delta_{ij}$ and $\sum_i \mu_i = 1$.

Now we can introduce the Whitney map [32, 2] which is the (right but not left) inverse of the de Rham map mapping from p -cochains to p -forms. It is a linear map, defined by

$$W(\alpha) = p! \sum_{i=0}^p (-1)^i \mu_i d\mu_0 \wedge \dots \wedge d\mu_{i-1} \wedge d\mu_{i+1} \wedge \dots \wedge d\mu_p, \quad (4.28)$$

where $\alpha = [v_0, \dots, v_p]$.

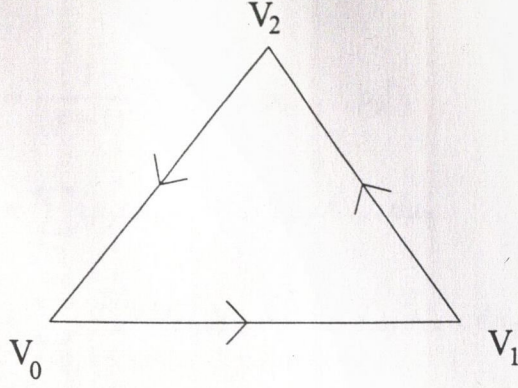


Figure 4-3: A triangulation of S^1 .

Example: Consider a triangulation of S^1 (Fig. 4-3) with $V_i = [i]$. We can act on the 1-simplex $[0, 1]$ to obtain

$$W^1([0, 1]) = \mu_0 d\mu_1 + \mu_1 d\mu_0, \quad (4.29)$$

but we know that $\mu_0 + \mu_1 = 1$ so that $d\mu_0 = -d\mu_1$. Using this we get

$$= (\mu_0 - \mu_1) d\mu_1 \quad (4.30)$$

$$= (\mu_0 - (1 - \mu_0)) d\mu_1 \quad (4.31)$$

$$= -d\mu_1 = d\mu_0. \quad (4.32)$$

W has the property that $dW = Wd$ as can be seen since if $\tau = [p_0, \dots, p_q]$ and $\sum'_p$ means the sum over all p such that $[p, p_0, \dots, p_q]$ belongs to K then we have that

$$\frac{1}{(q+1)!} W d\tau = \frac{1}{(q+1)!} W \left(\sum_p [p, p_0, \dots, p_q] \right), \quad (4.33)$$

$$= \sum_p (\mu_p d\mu_0 \wedge \dots \wedge \hat{d\mu}_p \wedge \dots d\mu_q) \quad (4.34)$$

$$+ \sum_{j=0}^q (-1)^{j+1} \mu_j d\mu_0 \wedge \dots \wedge \hat{d\mu}_j \wedge \dots d\mu_q, \quad (4.35)$$

$$= \sum_p (\mu_p d\mu_0 \wedge \dots \wedge \hat{d\mu}_p \wedge \dots d\mu_q), \quad (4.36)$$

$$+ \sum_{j=0}^q (-1)^{j+1} \mu_j \left(\sum_p \mu_p \right) d\mu_0 \wedge \dots \wedge \hat{d\mu}_j \wedge \dots d\mu_q, \quad (4.37)$$

$$= \sum_p (\mu_p d\mu_0 \wedge \dots \wedge \hat{d\mu}_p \wedge \dots d\mu_q) \quad (4.38)$$

$$+ \sum_{j=0}^q (-1)^j \mu_j \left(\sum_{j=0}^q \mu_j \right) d\mu_0 \wedge \dots \wedge \hat{d\mu}_j \wedge \dots d\mu_q, \quad (4.39)$$

$$= d\mu_0 \wedge d\mu_1 \wedge \dots \wedge d\mu_q, \quad (4.40)$$

and

$$dW\tau = d(q! \sum_{i=0}^q (-1)^i \mu_i d\mu_0 \wedge \dots \wedge \hat{d\mu}^i \wedge \dots \wedge d\mu_q), \quad (4.41)$$

$$= q! \sum_{i=0}^q d\mu_0 \wedge \dots \wedge d\mu_q = (q+1)! d\mu_0 \wedge \dots \wedge d\mu_q. \quad (4.42)$$

We also have that

$$AW = I, \quad (4.43)$$

or in other words

$$\int_{\beta} W(\alpha) = \langle \alpha, \beta \rangle. \quad (4.44)$$

With these two maps we can now transform between simplices and forms as we wish. This allows us to induce definitions onto cochains from forms, so that many results which hold on forms can nicely be carried over. Note that $WA \neq I$, which is reasonable since the discrete theory is cruder, so whilst forms capture faithfully all the details of the cochains the converse is not true.

4.3 The Cubic Lattice and its Dual

4.3.1 Introduction

We have been dealing with triangulations so far but can we generalise our scheme to deal with other complexes? The problem is that there is no systematic method to develop an appropriate Whitney map. We can see why the standard Whitney map works since we want $W[v_0, v_1]$ to give us a 1-form. A natural map would be to say that this gives terms involving $d\mu_0$ and $d\mu_1$. Now if we want $dW = Wd$, we need to have some function coefficient in front of the $d\mu_0$ which we can differentiate. This would have to involve a μ_1 which could be turned into a $d\mu_1$. So terms like $\mu_0 d\mu_1$ seem very natural. Then we want the mapping to have the same symmetry as the simplices so that $W[v_0, v_1] = -W[v_1, v_0]$ for example. This leads to the sign factors we have in the Whitney map and then with $AW = I$ we gain the normalisation. Of course this is easy to say when you know the answer but is it obvious that such a mapping should exist?

At first it seems that a cubic Whitney should be trivial since it is far closer to a Euclidean coordinate system. We would expect that W of the $x - y$ face of a 3D cube should simply be $dx dy$. We cannot get $dW = Wd$ using this though which is an essential property.

Notation is another problem. The simplicial setup can be very neatly expressed using a notation designed specifically for it. This means that initially things look far cruder in the cubic case simply because they are expressed in an unfamiliar language. The cubic system though has many advantages over the simplicial one as we will see.

We initially noted a natural way of describing cubes where the 8 vertices were labelled using their coordinates. We took a standard cube with vertices having x , y and z coordinates equal to either 0 or 1. Now each vertex has 3 numbers associated with it, as in its coordinates, and this combination is unique. This means that we can label the vertices by using these 3 coordinates, which we take as 3 binary digits. In other words the number 7, being 111 in binary, would have (1, 1, 1) as its coordinates.

This system has the advantage that it generalises to other dimensions and gives the relative positions of various vertices; so you know that vertex 7 is connected by an edge with vertex 6, 5 and 3 since there are edges in the $x(4)$, $y(2)$ and $z(1)$

direction. This seems to be quite a nice way of looking at things, but it did not lead to a Whitney map.

The spaces we are working with can be viewed as $\mathbb{R}^n$. This is just a collection of n real numbers in the interval $[0, 1]$. In 3D then we refer to a cube as $[x, y, z]$. This has the faces $[0, y, z]$, $[x, 0, z]$ and $[x, y, 0]$ as well as $[1, y, z]$, $[x, 1, z]$ and $[x, y, 1]$. The edges are of the form $[0, 0, z]$ as in it has one coordinate free and two set as constants 0 or 1. Note that $[x, y, 0]$ means that you have x and y ranging in the interval $[0, 1]$ while $z = 0$. In other words we can describe things as n -tuples $(a_1, \dots, a_n)$ where $a_i = x_i, 0$ or 1 . If there are p entries which are x_i 's then the object you are describing is a p dimensional face of the n -cube. There are 2^{n-p} parallel objects which are labelled by having 0 or 1 in the remaining $(n - p)$ slots. We look at a square to familiarise ourselves with the new language:

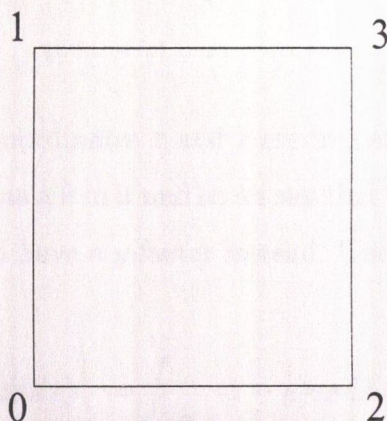


Figure 4-4: Labelling of vertices using binary convention.

We can then see how the various vertices, edges and faces of the figure above can be described (Table 4.2).

4.3.2 de Rham

The de Rham map can readily be applied to a cubic theory with no alterations needed with the cochains simply referring to cubes instead of simplices. Using incidence matrices we again get that $dA = Ad$ (this is covered in depth at the end of Sec. 4.3).

[0]	[0, 0]
[1]	[0, 1]
[2]	[1, 0]
[3]	[1, 1]
[0, 1]	[0, y]
[0, 2]	[x, 0]
[1, 3]	[x, 1]
[2, 3]	[1, y]
[0, 1, 2, 3]	[x, y]

Table 4.2: Cubic notation.

4.3.3 Whitney

We start with an example:

$$W[x, 0, z] = (1 - y)dx dz. \quad (4.45)$$

The idea here is that the coordinates x and z are free and so we have a dx and a dz factor. The y slot though has a 0 in it and so we say that we get a $(1 - y)$ contribution. If it had a 1 then we would have a y factor instead. The rational is simple since this is what gives us $AW = 1$.

$$AW[x, 0, z] = A((1 - y)dx dz) = \int_{[x, 0, z]} (1 - y)dx dz = \int_{[x, 0, z]} dx dz = 1, \quad (4.46)$$

since in the region $[x, 0, z]$ we have that $y = 0$ and so $(1 - y) = (1 - 0) = 1$. If we were working on the face $[x, 1, z]$ then we would have a factor y in a region where $y = 1$ and again get the same result.

An unfamiliar d ?

d does look quite odd but it is the d that you expect. It is given in the form which we constructed it though it can be viewed in a more algebraic manner. We want a d which has the property that $d^2 = 0$ and which is geometrically what we expect. We describe what it is operationally first since it is very simple then we can think about what it means.

$$D[x, 0, z] = -d[0, 2] = -[1, 0, 2] = [0, 1, 2] = [x, y, z]. \quad (4.47)$$

We call the new operator on the cube D to differentiate it from the familiar d . We associate with $[x, y, z]$, or $[x_0, x_1, x_2]$, the triangle $[0, 1, 2]$. We then act on the triangle with the familiar d and convert what we get back in terms of $[x, y, z]$. The only other thing is that if the constant factor being replaced by a coordinate is a 0 then we have an additional (-1) factor. This is because the face with a constant factor 1 is oppositely oriented to that with a constant factor 0 which needs to be taken into account. With this we get $Ad = DA$, $AW = I$ and $WD = dW$. In other words:

- Convert from $[x, y, z]$ language to $[0, 1, 2]$. This is done by ignoring the constant factors and replacing x_i by i . So $[x, 0, z] = [x_0, x_2] = [0, 2]$.
- Act on the resulting simplex with the traditional d operator. The only difference is that if we are joining vertex $[1]$ to the simplex we need to see what constant used to be in the x_1 slot. If the constant was 0 we insert a (-1) factor.
- Convert back from the the simplex language to the cubic one, putting in the constant factors that were there before into the available space.

We can look at the various examples below to see how it behaves in action.

Examples

$$dW = WD \quad (4.48)$$

$$dW[x, 0, z] = d(1 - y)dxdz = dxdydz \quad (4.49)$$

$$WD[x, 0, z] = W(-d[0, 2]) = W([0, 1, 2]) = dxdydz. \quad (4.50)$$

$$dW[x, 0, 0] = d(1 - y)(1 - z)dx = (1 - z)dxdy + (1 - y)dxdz \quad (4.51)$$

$$WD[x, 0, 0] = W(-d[0]) = W([0, 1] + [0, 2]) \quad (4.52)$$

$$= W([x, y, 0] + [x, 0, z]) = (1 - z)dxdy + (1 - y)dxdz. \quad (4.53)$$

$$dW[0, y, 0] = d(1 - x)(1 - z)dy = -(1 - z)dxdy + (1 - x)dydz \quad (4.54)$$

$$WD[0, y, 0] = W(-d[1]) = W(-[0, 1] + [1, 2]) \quad (4.55)$$

$$= W(-[x, y, 0] + [0, y, z]) = -(1 - z)dxdy + (1 - x)dydz. \quad (4.56)$$

$DA = Ad$ follows from Stokes' theorem as before.

Before providing a general proof we explicitly check that $WD = dW$ on all (28) possible cases for a 3D cube:

Cubes

$$[x, y, z]$$

$$D[x, y, z] = 0; WD = 0$$

$$W[x, y, z] = dxdydz, dW = 0$$

Faces

$$[x, y, 0]$$

$$D[x, y, 0] = -d[0, 1] = -[0, 1, 2] = -[x, y, z]; WD = -dxdydz$$

$$W[x, y, 0] = (1 - z)dxdy; dW = -dzdxdy = -dxdydz$$

$$[x, 0, z]$$

$$D[x, 0, z] = -d[0, 2] = [0, 1, 2]; WD = dxdydz$$

$$W[x, 0, z] = (1 - y)dxdz; dW = -dydxdz = dxdydz$$

$$[0, y, z]$$

$$D[0, y, z] = -d[1, 2] = -[0, 1, 2]; WD = -dxdydz$$

$$W[0, y, z] = (1 - x)dydz; dW = -dxdydz$$

$$[x, y, 1]$$

$$D[x, y, 1] = d[0, 1] = [0, 1, 2]; WD = dxdydz$$

$$W[x, y, 1] = zdxdy; dW = dzdxdy = dxdydz$$

$$[x, 1, z]$$

$$D[x, 1, z] = d[0, 2] = -[0, 1, 2]; WD = -dxdydz$$

$$W[x, 1, z] = ydxdz; dW = dydxdz = -dxdydz$$

$$[1, y, z]$$

$$D[1, y, z] = d[1, 2] = [0, 1, 2]; WD = dxdydz$$

$$W[1, y, z] = xdydz; dW = dxdydz$$

Edges

$$[x, 0, 0]$$

$$D[x, 0, 0] = d[0] = [0, 1] + [0, 2]; WD = (1 - z)dxdy + (1 - y)dxdz$$

$$W[x, 0, 0] = (1 - y)(1 - z)dx; dW = -(1 - z)dydx - (1 - y)dzdx = (1 - z)dxdy + (1 - y)dxdz$$

$$[x, 0, 1]$$

$$D[x, 0, 1] = d[0] = [0, 1] - [0, 2]; WD = zdxdy - (1 - y)dxdz$$

$$W[x, 0, 1] = (1 - y)zdx; dW = -zdydx + (1 - y)dzdx = zdxdy - (1 - y)dxdz$$

$$[x, 1, 0]$$

$$D[x, 1, 0] = d[0] = -[0, 1] + [0, 2]; WD = -(1 - z)dxdy + ydxdz$$

$$W[x, 1, 0] = y(1 - z)dx; dW = (1 - z)dydx - ydzdx = -(1 - z)dxdy + ydxdz$$

$$[x, 1, 1]$$

$$D[x, 1, 1] = d[0] = -[0, 1] - [0, 2]; WD = -zdxdy - ydxdz$$

$$W[x, 1, 1] = yzdx; dW = zdydx + ydzdx = -zdxdy - ydxdz$$

$$[0, y, 0]$$

$$D[0, y, 0] = d[1] = -[0, 1] - [2, 1]; WD = -(1 - z)dxdy + (1 - x)dydz$$

$$W[0, y, 0] = (1 - x)(1 - z)dy; dW = -(1 - z)dxdy - (1 - x)dzdy = -(1 - z)dxdy + (1 - x)dydz$$

$$[0, y, 1]$$

$$D[0, y, 1] = d[1] = -[0, 1] - [1, 2]; WD = -zdxdy - (1 - x)dydz$$

$$W[0, y, 1] = (1 - x)zdy; dW = -zdxdy - (1 - x)dydz$$

$$[1, y, 0]$$

$$D[1] = [0, 1] + [1, 2]; WD = (1 - z)dxdy + xdydz$$

$$W[1, y, 0] = x(1 - z)dy; dW = (1 - z)dxdy + xdydz$$

$$[1, y, 1]$$

$$D[1, y, 1] = d[1] = [0, 1] - [1, 2]; WD = zdxdy - xdydz$$

$$W[1, y, 1] = xzdy; dW = zdxdy - xdydz$$

$$[0, 0, z]$$

$$D[0, 0, z] = d[2] = -[0, 2] - [1, 2]; WD = -(1 - y)dxdz - (1 - x)dydz$$

$$W[0, 0, z] = (1 - x)(1 - y)dz; dW = -(1 - y)dxdz - (1 - x)dydz$$

Vertices

$$[0, 0, 0]$$

$$D[0, 0, 0] = -[0] - [1] - [2]; WD = -(1-y)(1-z)dx - (1-x)(1-z)dy \\ - (1-x)(1-y)dz$$

$$W[0, 0, 0] = (1-x)(1-y)(1-z); dW = -(1-y)(1-z)dx - (1-x)(1-z)dy \\ - (1-x)(1-y)dz$$

$$[0, 0, 1]$$

$$D[0, 0, 1] = -[0] - [1] + [2]; WD = -(1-y)zdx - (1-x)zdy + (1-x)(1-y)dz$$

$$W[0, 0, 1] = (1-x)(1-y)z; dW = -(1-y)zdx - (1-x)zdy + (1-x)(1-y)dz$$

$$[0, 1, 0]$$

$$D[0, 1, 0] = -[0] + [1] - [2]; WD = -y(1-z)dx + (1-x)(1-z)dy - (1-x)ydz$$

$$W[0, 1, 0] = (1-x)y(1-z); dW = -y(1-z)dx + (1-x)(1-z)dy - (1-x)ydz$$

$$[0, 1, 1]$$

$$D[0, 1, 1] = -[0] + [1] + [2]; WD = -yzdx + (1-x)zdy + (1-x)ydz$$

$$W[0, 1, 1] = (1-x)yz; dW = -yzdx + (1-x)zdy + (1-x)ydz$$

$$[1, 0, 0]$$

$$D[1, 0, 0] = [0] - [1] - [2]; WD = (1-y)(1-z)dx - x(1-z)dy - x(1-y)dz$$

$$W[1, 0, 0] = x(1-y)(1-z); dW = (1-y)(1-z)dx - x(1-z)dy - x(1-y)dz$$

$$[1, 0, 1]$$

$$D[1, 0, 1] = [0] - [1] + [2]; WD = (1-y)zdx - xzdy + x(1-y)dz$$

$$W[1, 0, 1] = x(1-y)z; dW = (1-y)zdx - xzdy + x(1-y)dz$$

$$[1, 1, 0]$$

$$D[1, 1, 0] = [0] + [1] - [2]; WD = y(1-z)dx + x(1-z)dy - xydz$$

$$W[1, 1, 0] = xy(1-z); dW = y(1-z)dx + x(1-z)dy - xydz$$

$$[1, 1, 1]$$

$$D[1, 1, 1] = [0] + [1] + [2]; WD = yzdx + xzdy + xydz$$

$$W[1, 1, 1] = xyz; dW = yzdx + xzdy + xydz$$

Finally we prove that $dW = WD$. To do this we first note that the cubic Whitney has a nice property whereby

$$W[a_0, a_1, \dots, a_n] = W[a_0]W[a_1] \dots W[a_n], \quad (4.57)$$

where $a_i = x_i$, 0 or 1. The only cases we need to know then are $W[a_i = 0] = (1 - x_i)$, $W[a_i = 1] = x_i$ and $W[a_i = x_i] = dx_i$ and d of these which are simply $dW[a_i = 0] = -dx_i$, $dW[a_i = 1] = dx_i$ and $dW[a_i = x_i] = 0$.

$$dW[a_0, a_1, \dots, a_n] = d(W[a_0]W[a_1] \dots W[a_n]) \quad (4.58)$$

$$= \sum_i (dW[a_i])W[a_0] \dots W[a_i] \dots W[a_n]. \quad (4.59)$$

Note that the only non-zero contributions come from those where $dW[a_i] \neq 0$ or in other words when $a_i \neq x_i$.

Let s_i equal +1 if $a_i = 1$, -1 if $a_i = 0$ and 0 otherwise. Using this s_i factor, we say that $dW[a_i]$ is equal to $s_i dx_i$ with no sign factor required. So

$$dW[a_0, \dots, a_n] = \sum_i s_i (dW[a_i])W[a_0] \dots W[a_i] \dots W[a_n]. \quad (4.60)$$

Now let n_i be the number of a_j 's which are x_j 's (as in not 0 or 1) for j less than i . As the $dW[a_i]$ factor is moved through n_i 1-forms to its proper place it generates a $p_i = (-1)^{(n_i)}$ factor. This means that

$$dW[a_0, \dots, a_n] = \sum_i s_i p_i W[a_0] \dots | dW[a_i] | \dots W[a_n] \quad (4.61)$$

which is exactly what we get from applying WD ; there is the $\pm$ factor depending on whether you have a 0 or a 1 and then a sign factor which arises when you move the dx_i into its rightful place.

So

$$D[a_0, \dots, a_n] = \sum_i s_i [a_i, a_0, \dots, \hat{a}_i, \dots, a_n] \quad (4.62)$$

$$= \sum_i s_i p_i [a_0, \dots, a_n], \quad (4.63)$$

which means that

$$WD[a_0, \dots, a_n] = \sum_i s_i p_i W[a_0] \dots W[a_n], \quad (4.64)$$

where the sum is over i where $a_i \neq x_i$. a_i is then converted to $s_i x_i$ which is how D is defined and then needs to be moved to the right place through various dx 's leading to the p_i term. This is what had for dW since $|dW[a_i]| = W[a_i = x_i] = dx_i$.

When determining dW , d gave non-zero terms if $a_i \neq x_i$. New terms in WD came by adding in vertices which corresponded to $a_i \neq x_i$ too. The s_i factors are identical which leaves the p_i factor. This is concerned with moving the new dx_i term to the proper place. When working with dW we needed n_i to count the number of dx 's it had to move through but with WD this is done automatically since while working with simplicial $[0, 1, 2]$ notation we discard the constant terms. It is the same factor and $dW = WD$.

A closer look at D

We have been using D as if it had the same properties as d_K (the discrete d acting on a simplicial complex K) without showing that this is the case. We can't just, for example, apply Stokes' theorem to determine that $AD = dA$ since we have yet to show that D is related to the incidence matrix in the appropriate manner.

We begin by looking at D^2 . The prescription here is to map our cubic object to a simplicial one to which we apply d_K . That being the case, when we use D^2 we apply d_K^2 and thereby automatically satisfy $D^2 = 0$. So at least D satisfies this basic property.

Next we introduce the boundary operator which we have yet to determine in the cubic case:

$$\partial : [a_0, \dots, a_n] = \sum_i p_i ([a_0, \dots, 1, \dots, a_n] - [a_0, \dots, 0, \dots, a_n]), \quad (4.65)$$

where we have replaced the i th slot with a 0 and a 1, the second one having opposite the orientation. p_i is the number of $a_j = x_j$'s with $j < i$. In other words

$$\partial[x] = [1] - [0] \quad (4.66)$$

and

$$\partial[x, y] = -[0, y] + [1, y] + [x, 0] - [x, 1] \quad (4.67)$$

which is what we expect the boundary operation to be. To test it more thoroughly we apply it to $[x, y, z]$:

$$\partial[x, y, z] = -[0, y, z] + [1, y, z] + [x, 0, z] - [x, 1, z] - [x, y, 0] + [x, y, 1] \quad (4.68)$$

$$\partial^2[x, y, z] = [0, 0, z] - [0, 1, z] + [0, y, 1] - [0, y, 0] + [1, 1, z] - [1, 0, z] + \quad (4.69)$$

$$\begin{aligned} & [1, y, 0] - [1, y, 1] + [1, 0, z] - [0, 0, z] + [x, 0, 0] - [x, 0, 1] \\ & - [1, 1, z] + [0, 1, z] + [x, 1, 1] - [x, 1, 0] - [1, y, 0] + [0, y, 0] \\ & + [x, 1, 0] - [x, 0, 0] + [1, y, 1] - [0, y, 1] - [x, 1, 1] + [x, 0, 1] \\ & = 0. \end{aligned} \quad (4.70)$$

The boundary map is clearly taking us to faces of the object it is acting on but from this we can see that the orientation of the various factors is being dealt with properly too.

We want to show that $\partial^2 = 0$ in general. We can see that this happens for various cases. When we determine the boundary of an edge $[0, 1]$, say, we end up with two vertices $[0]$ and $[1]$. The boundary of these is 0 since the boundary of a vertex is zero. The boundary of a square $[0, 1, 2, 3]$ results in four edges:

$$\partial[0, 1, 2, 3] = [0, 1] + [1, 3] - [2, 3] - [0, 2].$$

From this we get

$$\partial([0, 1] + [1, 3] - [2, 3] - [0, 2]) = [0] - [1] + [1] - [3] - [2] + [3] - [0] + [2] = 0.$$

So we find that the various vertices occur in pairs which cancel leading to the desired result. The same thing can be seen when we look at cubes, as in the edges which result, occur in oppositely oriented pairs and so cancel. Using this observation we can see how this occurs in general.

We have that the boundary, on an m -cell, maps it to two oppositely oriented pieces. We say that the first ∂ sets a_k to either 0 or 1. The second ∂ does the same to a_l . We denote this as

$$\partial\sigma^m = \sigma_0^{m-1} - \sigma_1^{m-1} \quad (4.71)$$

in short hand, where we mean sum over i where $a_i = 0$ by σ_0^{m-1} . Then

$$\partial^2\sigma^m = \sigma_{00}^{m-2} - \sigma_{01}^{m-2} - \sigma_{10}^{m-2} \sigma_{11}^{m-2}. \quad (4.72)$$

In fact we have two cases to consider, depending on whether $k < l$ or $k > l$. The idea is that if $k < l$ then we get the same sign factor if the first ∂ removes k or the second. This is not the case with l since the sign associated to this operation depends on whether l is odd or even. If l is odd and k has been removed before then l is now even which means that depending on whether k is removed first or second the sign changes. So we get two oppositely oriented versions of the same term which cancel. If $k > l$ then the same argument applies where the sign changes occur from the k term as opposed to the l one. Thus

- The sign from ∂ depends on the position of a_i . If it is the k th term then it depends on whether k is odd or even. Note that when we say k th here we are only counting the a_i 's which are equal to x_i since they are the only terms that contribute.
- If we are removing a_k and a_l where $k < l$ then our first ∂ could remove the k th term and the second one the l th or the other way round.
- The orientation is opposite, depending on which order things are done and so, since both versions occur, the net result is zero. In the continuum case, for example, we would have $dx \wedge dy = -dy \wedge dx$ and so a similar result.

We can define the incidence matrix and then use it to define ∂ and D or the other way round which is what we do here. These show how the pieces of various dimension fit together in a coherent manner.

The faces our D maps onto do contain the edges we act on but is the orientation correct? Since the incidence matrix is determined by the boundary operator we need only check to see whether the orientations determined by ∂ are compatible with the orientations determined by D . When ∂ maps a face to an edge we get an associated sign and when D acts on an edge we get a face with an associated sign. We need to show that they are the same.

Looking at ∂ we can see that the sign is determined by whether we introduce a 0 or a 1. This is also the case in D . We get a (-1) contribution if we introduce or remove a 0. The remaining factor is the p_i one which occurs in both ∂ and D . So the incidence matrix associated with ∂ induces a D which is the same as the one we have been using. Since D is compatible with the incidence matrix $AD = dA$ follows.

4.4 Wedge product

We can use W and A to induce a discrete wedge product³ on our cochains. So given a p -simplex, x^p , and a q -simplex, y^q , we define their wedge product, $\wedge^K : C^p(K) \times C^q(K) \rightarrow C^{p+q}(K)$ as

$$x^p \wedge^K y^q := A(W(x^p) \wedge W(y^q)). \quad (4.73)$$

Since $dA = Ad$ and $dW = Wd$ we have that

$$d^K(x^p \wedge^K y^q) = d^K x^p \wedge^K y^q + (-1)^p x^p \wedge^K d^K y^q, \quad (4.74)$$

and

$$x^p \wedge^K y^q = (-1)^{pq} y^q \wedge^K x^p. \quad (4.75)$$

Unfortunately our wedge is non-associative since

$$[v_0, \dots, v_p] \wedge^K [v_p, \dots, v_{p+q}] = \int_{|[v_0, \dots, v_{p+q}]|} W([v_0, \dots, v_p]) \wedge W([v_p, \dots, v_{p+q}]) \quad (4.76)$$

$$= \int p!q! \mu_p d\mu_1 \wedge \dots \wedge d\mu_{p+q} \quad (4.77)$$

$$= \frac{p!q!}{(p+q+1)!} [v_0, \dots, v_{p+q}] \quad (4.78)$$

which implies that

$$x^p \wedge^K (y^q \wedge^K z^r) = \left(\frac{p+q+1}{r+q+1} \right) (x^p \wedge^K y^q) \wedge^K z^r, \quad (4.79)$$

where x^p , y^q and z^r are p , q and r cochains respectively.

The wedge product also has these properties in the cubic case since $dW = Wd$ and $dA = Ad$ there too. The non-associativity follows from a similar calculation.

We can redefine our wedge product to make it associative by introducing a

$$\frac{(p+q+1)!}{p!q!} \quad (4.80)$$

term. This is not compatible with the Leibniz rule though.

4.5 Hodge star

The discrete star $*$ developed by Adams[1] is one of the cornerstones of geometric discretisation. The key observation was that:

³See appendix A.1.1 for further discussion on this issue.

1. The discrete Hodge star needs to map to a dual complex in order to satisfy

$$** = I. \tag{4.81}$$

2. We need to work in a subdivided space in order to satisfy

$$\delta = *d*. \tag{4.82}$$

With this we have extended our discrete analogy to near completion⁴.

First we note that if we do not use a dual space, we do not get $** = I$ type behaviour. If we act on a vertex of a triangle (See Fig. 4-5) with $*$, which must be mapped to a face in $2D$, the only option we have is to map it to the triangle. While if $*$ is applied to a triangle, which must be mapped to vertices in $2D$, it must mapped to all its vertices. As a result we end up with $**$ mapping a vertex of a triangle to all its vertices, as opposed to back to itself, which is not what we desire.

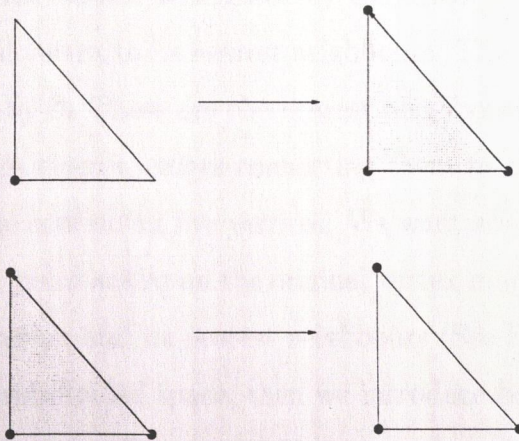


Figure 4-5: $**$ when there is no dual space.

With a dual space $*$ maps the vertex to the 2-cells in the dual space (See Fig. 4-6). When $*$ is applied to these there is only one vertex they can go to from the original complex and as a result we see $**$ mapping a vertex back to itself, as required.

⁴See Sec. A.1.2 for a discussion on other attempts to construct a discrete Hodge star.

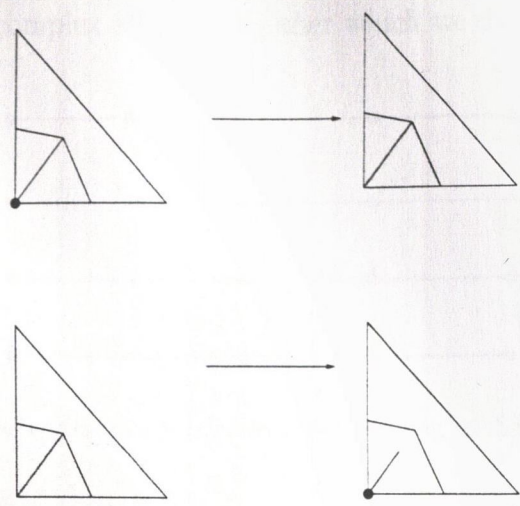


Figure 4-6: $**$ when there is a dual space.

In order to get the property $\delta = *\partial*$ we need to use a subdivided space. For example we look at a $1D$ complex (See Fig. 4-7) where we act on a vertex with $*\partial*$. We begin with the vertex highlighted by the arrow. $*$ maps this to an edge, connecting the original vertex to its nearest neighbours. This edge is then mapped to its boundary vertices by ∂ . These are the nearest neighbours of our original vertex. $*$ acting on these maps them to edges connecting them to their nearest neighbours which result in an edge containing five vertices. We want $*\partial*$ to correspond to δ , the coboundary operator, and δ acting on the original vertex maps to an edge containing just the the original vertex and its nearest neighbours (See Fig. 4-8).

If we work with a subdivided space, then we introduce barycentres at the centre of each of our original edges. Then $*$ would map to the original vertex to the edge between the two nearest neighbours which are both barycentres. ∂ would then take the boundary of this and $*$ of these would map to the nearest neighbours of the barycentres. The end result again being an edge containing five vertices but this time two of them are barycentres so we have exactly what δ maps to as desired. Note that here δ is the coboundary operator which lives in the original complex K and is not aware of the barycentres, whereas $*$ is.

The discrete Hodge operator maps to a different complex to the one it is acting on. Therefore we have two of them, $*^K$, which maps to the dual complex, and $*^L$, which maps back to the original complex. We need to introduce B , the barycentric subdivided complex in which both K and L can be embedded, to see how the original,

dual and subdivided complex all work together which we do next.

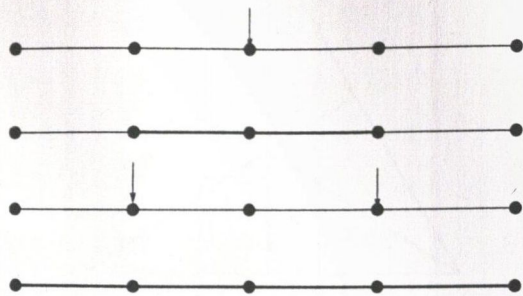


Figure 4-7: $\ast\partial\ast$ without a subdivided space, leading to the wrong result.

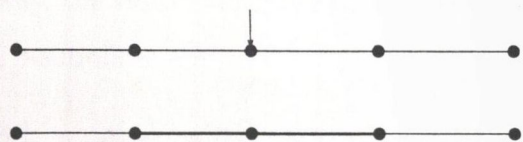


Figure 4-8: What $\ast\partial\ast$ should be.

4.5.1 Barycentric subdivision and the Dual space

Given a complex K , we can barycentric subdivide it to produce another complex, B . To do this we first add a new vertex to the middle of every simplex σ , called the barycentre $\tilde{\sigma}$ to determine the vertices and then connect them to nearest neighbours to create the new complex (See Fig. 4.5.1). The various barycentres for a triangle with vertices v_0, v_1 and v_2 are given in Table 4.3.

Geometrical object	Corresponding barycentre
$v_0 = \sigma_1^0 = [v_0]$	$\hat{v}_0 = v_0,$
$v_1 = \sigma_2^0 = [v_1]$	$\hat{v}_1 = v_1,$
$v_2 = \sigma_3^0 = [v_2]$	$\hat{v}_2 = v_2,$
$\sigma_1 = \sigma_1^{(1)} = [v_0, v_1]$	$\hat{\sigma}_3 = \frac{1}{2}(v_0 + v_1),$
$\sigma_2 = \sigma_2^{(1)} = [v_1, v_2]$	$\hat{\sigma}_4 = \frac{1}{2}(v_1 + v_2),$
$\sigma_3 = \sigma_3^{(1)} = [v_2, v_0]$	$\hat{\sigma}_5 = \frac{1}{2}(v_2 + v_0),$
$\sigma = \sigma^{(2)} = [v_0, v_1, v_2]$	$\hat{\sigma} = \frac{1}{3}(v_0 + v_1 + v_2).$

Table 4.3: The barycentres of a triangle.

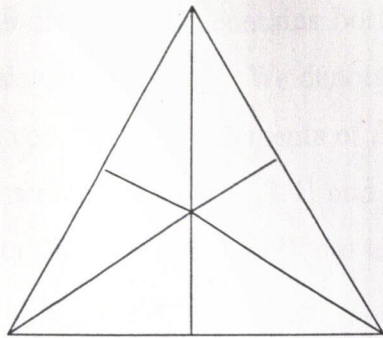


Figure 4-9: Barycentric subdivided triangle.

To put it another way, the vertices of B are the barycentre of the various simplices of K and its oriented p -simplices are

$$\{[\tilde{\alpha}^{(q_0)}, \dots, \tilde{\alpha}^{(q_p)} \mid \alpha^{(q_0)} \subset \alpha^{(q_1)} \subset \dots \subset \alpha^{(q_p)} \in K\}, \tag{4.83}$$

where $\alpha^1 \subset \alpha^2$ means that α^1 is a face of α^2 .

4.5.2 Simplicial

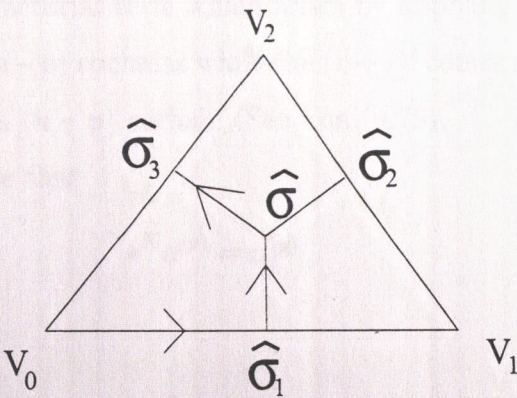


Figure 4-10: Dual complex.

The dual complex L is not composed of triangles but of general oriented p -cells. The dual to an oriented p -simplex $\alpha^{(p)}$ is denoted $\alpha^{(p)}$ and is an $(n - p)$ -cell. It is constructed by taking the union of all $(n - p)$ -simplices in B of the form $[\hat{\alpha}^{(p)}, \dots, \hat{\alpha}^{(n)}]$ where $\alpha^{(p)} \subset \alpha^{(p+1)} \subset \dots \subset \alpha^{(n)} \in K$. The orientation is uniquely determined by the orientation of $\alpha^{(p)}$ and M as follows: If $\alpha^{(0)} \subset \alpha^{(1)} \subset \dots \subset \alpha^{(n)} \in K$ such that $[\tilde{\alpha}^{(0)}, \dots, \tilde{\alpha}^{(p)}]$ is compatible with the orientation of M then the orientation of $\alpha^{(p)}$ is compatible with that of $[\tilde{\alpha}^{(p)}, \dots, \tilde{\alpha}^{(n)}]$ (See Fig. 4-10).

Since the barycentric subdivision of K contains both K and L , they can be described in terms of the basis elements of B . We denote x an element of K or L as Bx when expressing it as a combination of elements of B . For example an edge $[0, 1]$ with barycentre $[3]$ can be written as $[0, 3] + [3, 1]$ and for a $(p+1)$ -simplex α^p we end up with $N(\alpha^p) = p!$ bits. Following Adams [1] we use the convention

$$B\alpha^p := \frac{1}{N(\alpha^p)} \sum_{\alpha^p \subset \alpha^{p+1} \subset \dots \subset \alpha^n} \pm \tilde{\alpha}^p, \tilde{\alpha}^{p+1}, \dots, \tilde{\alpha}^n, \quad (4.84)$$

where the $\pm$ sign is chosen so that $[\tilde{\alpha}^p, \tilde{\alpha}^{p+1}, \dots, \tilde{\alpha}^n]$ has orientation compatible with α^p .

We then define the discrete Hodge star as

$$\langle *^K x, y \rangle := \frac{(n+1)!}{p!(n-p)!} \int_M W^B(Bx) \wedge W^B(By) \quad (4.85)$$

$$\langle *^L y, x \rangle := \frac{(n+1)!}{p!(n-p)!} \int_M W^B(By) \wedge W^B(Bx), \quad (4.86)$$

where $*^K : C^p(K) \rightarrow C^{n-p}(L)$ and $*^L : C^q(L) \rightarrow C^{n-q}(K)$.

The factors before the integrals are there for normalisation. The $p!$ and $(n-p)!$ are cancelled by the factorial term which arises by applying the Whitney map (See Eqn. 4.28) to p and $(n-p)$ cochains while the $(n+1)!$ comes from the wedge product of a p cochain with an $(n-p)$ cochain (See Eqn. 4.78).

With these we have that

$$*^K \alpha^{(p)} = \hat{\alpha}^{(p)} \quad (4.87)$$

and

$$*^L(\hat{\alpha}^{(p)}) = (-1)^{p(n+1)} \alpha^{(p)}, \quad (4.88)$$

where the $(-1)^{p(n+1)}$ factor is due to the fact that we have the x and y flipped in $W^B(y) \wedge W^B(x)$. This implies that

$$(*^K)^* = (*^K)^{-1} \quad \text{and} \quad (*^L)^* = (*^L)^{-1} \quad (4.89)$$

and

$$*_{n-p}^L *^K_p = (-1)^{p(n+1)} Id \quad \text{and} \quad *_{n-q}^K *^L_q = (-1)^{q(n+1)} Id. \quad (4.90)$$

Finally with some manipulation this implies that

$$(d_p^K)^* = (-1)^{np+1} *_{n-p}^L d_{n-p-1}^L *_{p+1}^K \quad \text{and} \quad (d_q^L)^* = (-1)^{nq+1} *_{n-q}^K d_{n-q}^K *_{q+1}^L. \quad (4.91)$$

4.5.3 Cubic

In the cubic case we have that the dual space is also a cubic complex, though a separate one. This means that we have a Whitney map on our dual space which was not the case before in the simplicial one. We can again in the same way generate a barycentric subdivided space and determine the same results, except instead of getting $p!$ terms we get 2^p .

4.6 A Generalised de Rham Map

We define the new de Rham map R — instead of A — by introducing a new factor, Z_i^p , as follows:

$$\langle R\omega^p, \sigma_i^p \rangle = \frac{1}{Z_i^p} \int_{\sigma_i^p} \omega^p. \quad (4.92)$$

4.6.1 Modifications to the exterior derivative

We have a natural definition for the boundary as

$$\partial : [v_0, \dots, v_n] = \sum_i (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_n], \quad (4.93)$$

where $[v_0, \dots, \hat{v}_i, \dots, v_n]$ means the n -simplex $[v_0, \dots, v_n]$ with v_i omitted. Similarly the coboundary can be defined as

$$\delta : [v_0, \dots, v_p] = \sum_k [v_k, v_0, \dots, v_n], \quad (4.94)$$

where $[v_k, v_0, \dots, v_p] \in K$. Both these operators act on chains. We refer to them as follows:

$$\begin{aligned} \partial S_{p,j} &= [\partial_p(K)]_j^k S_{p-1,k}, \\ \delta S_{p,j} &= [\delta_p(K)]_j^l S_{p+1,l}. \end{aligned}$$

We can now define the coboundary on cochains by setting

$$\langle \delta S^{p,j}, S_{p+1,n} \rangle = \langle S^{p,j}, \partial S_{p+1,n} \rangle. \quad (4.95)$$

We refer to this as

$$\delta S^{p,j} = [\delta^p(K)]_j^l S^{p+1,l}, \quad (4.96)$$

which tells us that

$$\langle [\delta^p(K)]_l^j S^{p+1,l}, S_{p+1,n} \rangle = \langle S^{p,j}, [\partial_{p+1}(K)]_n^k S_{p,k} \rangle, \quad (4.97)$$

$$[\delta^p(K)]_n^j = [\partial_{p+1}(K)]_n^j. \quad (4.98)$$

We want to check that $R[d\phi] = \delta R[\phi]$ using Stokes' theorem.

$$R[d\phi] = \langle R[d\phi], S_{p+1,k} \rangle S^{p+1,k} \quad (4.99)$$

$$= \frac{1}{Z_k^{p+1}} \int_{S_{p+1,k}} d\phi^p S^{p+1,k} \quad (4.100)$$

$$= \frac{1}{Z_k^{p+1}} \int_{\partial S_{p+1,k}} \phi^p S^{p+1,k} \quad (4.101)$$

$$= \frac{1}{Z_k^{p+1}} [\partial_{p+1}]_k^j \int_{S_{p,j}} \phi^p S^{p+1,k} \quad (4.102)$$

$$= \frac{Z_j^p}{Z_k^{p+1}} [\partial_{p+1}]_k^j \langle R[\phi], S_{p,j} \rangle S^{p+1,k} \quad (4.103)$$

$$= \frac{Z_j^p}{Z_k^{p+1}} [\delta^p]_k^j \langle R[\phi], S_{p,j} \rangle S^{p+1,k} \quad (4.104)$$

$$= \frac{Z_j^p}{Z_k^{p+1}} \langle R[\phi], S_{p,j} \rangle \delta S^{p,j} \quad (4.105)$$

$$= \frac{Z_j^p}{Z_k^{p+1}} \delta \langle R[\phi], S_{p,j} \rangle S^{p,j} \quad (4.106)$$

$$= \frac{Z_j^p}{Z_k^{p+1}} \delta R[\phi]. \quad (4.107)$$

So something has to be changed in order for this relationship to hold, to compensate for the changes made to R . The only option available is to modify δ with a $\frac{Z^p}{Z^{p+1}}$ factor so that

$$\delta S^{p,j} = \frac{Z_j^p}{Z_k^{p+1}} [\delta^p]_k^j S^{p+1,k}, \quad (4.108)$$

and Eqn. 4.105 becomes

$$= \langle R[\phi], S_{p,j} \rangle \delta S^{p,j}. \quad (4.109)$$

With this definition we have again that

$$R[d\phi] = \delta R[\phi]. \quad (4.110)$$

4.6.2 Modifications to the Whitney map

We have mentioned the generalisation of the de Rham map, next we look at the effect this has on W . We want

$$RW_{new} = I, \quad (4.111)$$

so we say that our new W simply has a Z_i^p multiplicative factor which cancels with the one we now have in R . So

$$W_{new}\sigma_i^p = Z_i^p W \sigma_i^p. \quad (4.112)$$

Using our new δ we also get $dW_{new} = W_{new}\delta_{new}$ since the LHS now has a Z_i^p factor as does the RHS as can be seen by doing the following calculation:

$$W_{new}\delta_{new}S^{p,i} = Z_j^{p+1}W \frac{Z_i^p}{Z_j^{p+1}}[\delta^p]_j^i S^{p+1,j} \quad (4.113)$$

$$= Z_i^p W [\delta^p]_j^i S^{p+1,j}. \quad (4.114)$$

So our new definitions are

$$\langle R\omega^p, \sigma_i^p \rangle = \frac{1}{Z_i^p} \int_{\sigma_i^p} \omega^p, \quad (4.115)$$

$$W_{new}\sigma_i^p = Z_i^p W \sigma_i^p, \quad (4.116)$$

$$\delta S^{p,j} = \frac{Z_j^p}{Z_k^{p+1}} [\delta^p]_k^j S^{p+1,k}. \quad (4.117)$$

4.6.3 An interpretation

Instead of looking at this freedom as something associated with R which filters through to W and d , we can for example say that we have a scale factor associated with d .

If we are working with a 3D complex and want to add a factor of 5 to d acting on vertices, 3 when acting on edges and 7 on faces then we can just set the Z 's on faces as being 3, Z 's on edges as $21 = 7 * 3$ and $Z = 105$ on vertices.

We have yet to find a use for this factor, though we know that this freedom exists.

4.7 Computational GD

To apply these ideas to perform calculations we define basis lists for the various complexes we are interested in. Using these we can then define matrices for operators

which we can happily work with. We start by creating a basis list for the complexes K and B , since they are both simplicial and can therefore be treated in the same way, leaving L for later.

A simplicial complex consists of vertices, edges, faces, $\dots$, n -simplices. Let n_p be the number of p -simplices then we say that the first n_0 basis list elements are the vertices, the next n_1 the edges and so on.

The dual complex, L , has to be treated differently since it is not simplicial. For example, say our original complex consisted of a single triangle $[0, 1, 2]$, then the dual to the vertex $[0]$ consists of two triangles in B . The basis list element which corresponds to this will have two entries which are the appropriate basis list elements of B . In other words the basis list elements of L are described in terms of basis list elements of B . The ordering is chosen so that the i th basis list element of L is the dual of the i th basis list element of K which means that the elements are arranged in decreasing as opposed to increasing dimension.

4.8 Convergence

We can map between a continuous and discrete theory with the use of W and A but we have yet to compare their behaviour. We know for example that $AW = I$ but what does this mean? How well do discrete objects approximate their continuum analogues? In fact, what do we mean by a discrete operator approximating a continuum one?

A natural way to proceed is to compare a continuous object with its image after WA has been applied to it. Ideally we would like to have

$$f - WAf = 0 \quad (4.118)$$

but we only have that $AW = I$ and not $WA = I$ so this is not the case. While we are unable to get perfect agreement, we do (as we will see) have that the discrete approximation converges to the continuum case as the triangulation is refined, which is what we would hope.

We will now go through the analysis, comparing discrete and continuum objects, where we find that p -form approximation converges, albeit only to $O(h)$ (which has

been shown before by Dodziuk [32]), as does the discrete d operator while there are problems with $*$. This is reasonable enough since our theory so far has been based on topological techniques which are of course metric independent whilst $*$ is not.

To deal with $*$ we use the insight gained from our analysis of discrete approximations to make a natural modification to our scheme and show that, with this change, $*$ too behaves properly (for the cubic case at least).

4.8.1 Approximation

We can compare discrete objects, X_{disc} , to continuous ones, X_{cont} by looking at the difference between X_{cont} and WX_{disc} . We start by looking at various p -forms before moving onto operators such as d and $*$.

Forms

The simplicial and cubic cases differ so we start with the simplicial and come back to the cubic.

If we look at a function (0-form) f , we can see how it behaves. First we need to map it to K using A . This results in assigning the value of f at each of the vertices to each vertex, since from the definition of the de Rham map you evaluate the integral of the function over the 0-cochain (vertex):

$$Af = \sum_i f_i[v_i], \quad (4.119)$$

where $f_i = f(v_i)$. Next, we use the Whitney map to take us back to the continuum space and compare the result with f . The Whitney map on vertices v_i gives us μ_i , which is one at the vertex and goes linearly to zero on other vertices (as well as outside the triangles which contain v_i). So we get

$$W Af = \sum_i f_i \mu_i, \quad (4.120)$$

which is a piecewise linear approximation of f . This agrees with the continuous case to $O(h^2)$ since

$$f_{cont}(x_i + h) = f_{cont}(x_i) + h \frac{\partial f_{cont} x_i}{\partial x} + O(h^2), \quad (4.121)$$

$$f_{disc}(x_i + h) = f_{disc}(x_i) + h \frac{\partial f_{disc} x_i}{\partial x}, \quad (4.122)$$

but

$$f_{disc}(x_i) = f_{cont}(x_i) \quad (4.123)$$

and

$$\frac{\partial f_{cont} x_i}{\partial x} = \frac{\partial f_{disc} x_i}{\partial x} + O(h), \quad (4.124)$$

since the slope of the approximation is the same to $O(h)$. So we have that

$$f_{cont}(x_i + h) - f_{disc}(x_i + h) = O(h^2). \quad (4.125)$$

Note that this is not a proper bound since we do not have a cap on the first derivative but working with Sobolev spaces, where this is not the case, is sufficiently general for our work. Next we look at a 1-form (on a 1D manifold) where A takes us to

$$A f dx = \int_{\sigma_i^1} f dx [\sigma_i^1], \quad (4.126)$$

and

$$W A f dx = \left(\int_{\sigma_i^1} f dx \right) W [\sigma_i^1]. \quad (4.127)$$

Now $[\sigma_i^1] = [v_i, v_j]$ which W maps to

$$\mu_i d\mu_j - \mu_j d\mu_i. \quad (4.128)$$

On the edge $[v_i, v_j]$ we know that $\mu_i + \mu_j = 1$, which implies that $d\mu_i = -d\mu_j$. Using this we get that

$$W[v_i, v_j] = (\mu_i + \mu_j) d\mu_j = d\mu_j. \quad (4.129)$$

We use the fact that we are on a 1D manifold here, since otherwise the edge might be a face of a triangle in that case $\mu_0 + \mu_1 \neq 1$ in general. Since

$$\mu_j = \frac{x - x_i}{x_j - x_i}, \quad (4.130)$$

we have

$$d\mu_j = \frac{dx}{x_j - x_i}, \quad (4.131)$$

which means that

$$W A f dx = \left(\int_{\sigma_i^1} f dx \right) \frac{dx}{x_j - x_i}. \quad (4.132)$$

This converges to the continuous result but only to $O(h)$ since it can be rewritten as

$$W A f dx = f_{average} dx, \quad (4.133)$$

because

$$f_{average} = \frac{\int_{[v_i, v_j]} f dx}{x_j - x_i}. \quad (4.134)$$

In other words, the discrete approximation is to simply take the average result. This in fact holds for p -forms in general which can be seen as follows. We assign the average value of the form to some point in the p -simplex, which we know due to the mean value theorem. Then the discrete function can be written as a Taylor expansion about this point which means that we get $f_{average} + O(h)$. The trick needed is to note that W of a p -simplex is equal to $d^p x$ when restricted to the p -simplex.

$$W[0, 1, \dots, p] = p! \sum_{i=0}^p (-1)^i \mu_i d\mu_0 \wedge \dots \wedge d\hat{\mu}_i \wedge \dots d\mu_p \quad (4.135)$$

$$= p! \mu_0 d\mu_1 \wedge \dots \wedge d\mu_p + p! d\mu_0 \wedge \left(\sum_{i=1}^p (-1)^i \mu_i d\mu_1 \wedge \dots \wedge d\hat{\mu}_i \wedge \dots d\mu_p \right) \quad (4.136)$$

Now using the fact that $\sum_i \mu_i = 1$ to replace $d\mu_0$ we get:

$$W[0, 1, \dots, p] = p! \mu_0 d\mu_1 \wedge \dots \wedge d\mu_p + p! \left(- \sum_{i=1}^p d\mu_i \right) \wedge \left(\sum_{i=1}^p (-1)^i \mu_i d\mu_1 \wedge \dots \wedge d\hat{\mu}_i \wedge \dots d\mu_p \right) \quad (4.137)$$

The $d\mu_i$ from this substitution fills in for the omitted $d\mu_i$ which ends up cancelling the $(-1)^i$ factor as it is moved to its proper place to give

$$= p! d\mu_1 \wedge \dots \wedge d\mu_p, \quad (4.138)$$

$$= \frac{1}{\text{Vol } \sigma^p} dx^1 \wedge \dots \wedge dx^p. \quad (4.139)$$

This works for the standard triangle but in general we are unable to convert to dx 's as easily as we did above. This means that we only have convergence results for the standard triangles case.

Now onto the cubic case where we have that

$$W[a_0, \dots, a_n] = \frac{1}{\text{Vol } \sigma^p} dx_0 \dots dx_p \quad (4.140)$$

on the p -face σ^p of the n -cube and so the result also holds. Note that this results from a sum of several terms of the form $[xdy + (1 - x)dy] = dy$.

The cubic theory has a product form, as in each dimension leads to a term which is independent of the others. The approximation in each is linear or average which leads to either $O(h^2)$ or $O(h)$ convergence respectively. If all the terms are linear, which is the case for functions, the overall approximation is $O(h^2)$, otherwise it is $O(h)$. So in that sense the result is the same as in the simplicial case.

We have demonstrated that our discrete objects converge to the continuous ones as the complexes are refined when the complex consists of cubes or regular triangles. Next we look at operators.

Operators

We begin with the exterior derivative. If we take the 1D case with vertices $[x_i]$ and edges $[x_i, x_{i+1}]$ we can look at the convergence of

$$df - Wd_K Af. \quad (4.141)$$

A acting on f assigns the value of f at each of the vertices to the vertices. So we have

$$Af = \sum_i f_i [x_i], \quad (4.142)$$

where $f_i = f(x_i)$ and that d_K acting on $[x_i]$ gives

$$[x_{i-1}, x_i] - [x_i, x_{i+1}]. \quad (4.143)$$

If we look at the $[x_i, x_{i+1}]$ term, it has an f_i coefficient, but there are two contributions to this, since d_K acting on $[x_{i+1}]$ also provides an $[x_i, x_{i+1}]$ term. This results in

$$d_K Af = \sum_i (f_{i+1} - f_i) [x_i, x_{i+1}]. \quad (4.144)$$

The Whitney map on this gives

$$Wd_K Af = \sum_i \frac{f_{i+1} - f_i}{x_{i+1} - x_i} dx, \quad (4.145)$$

which converges to the continuum result $O(h)$

$$df = \frac{df}{dx} dx. \quad (4.146)$$

Unfortunately this analysis is very specific so we are unable to say what happens for higher dimensional spaces. In general though the result follows from p -form approximation (which we only have for cubes and standard triangles) since $d_K A = Ad$:

$$df - Wd_K Af = df - [WA]df = O(h). \quad (4.147)$$

* requires metric which is the subject of the next chapter.

4.9 Summary

What then can our discrete theory do? Nearly everything. Looking at the table of properties from continuum theory we can say that our discrete theory has all of these with the only anomaly being the non-associativity of the wedge product. We have discrete forms with a discrete d , $*$ and $\wedge$ with the properties that:

1. $d^2 = 0$
2. $x^p \wedge y^q = (-1)^p y^q \wedge x^p$
3. $d(x^p \wedge y^q) = dx^p \wedge y^q + (-1)^p x^p \wedge (dy^q)$
4. $(x \wedge y) \wedge z \neq z \wedge (y \wedge x)$
5. $** = (-1)^{p(n+1)} I$
6. $\delta = (-1)^{np+1} * d*$

We have progressed considerably from our initial discrete system allowing us to capture most of the structure of differential geometry in a discrete setting (with the notable exception of the associativity of the wedge product). In particular we have developed a cubic lattice theory for the first time and demonstrated convergence of our discrete objects to their continuum analogies as we refine our triangulations. Since the dual space of a cubic lattice is also cubic, we finally have a Whitney map for our dual space too. This allows us to look at the convergence of our discrete Hodge star which we do next.

Chapter 5

Incorporating metric

5.1 A heuristic

$*$ is metric dependent while our theory is topological and hence metric independent. So, in order to truly have a discrete Hodge star, we need to deal with the metric. First we have to develop our understanding of our scheme to help us see what modifications can be made.

The idea is to note that p -forms are approximated by taking their averages; the de Rham map integrates the p -form over some volume element, σ^p , whilst the Whitney map replaces σ^p with a p -form divided by the volume of σ^p . Using this mechanism we have been able to prove the various convergence results so far though we have only been able to show that this is what actually happens in the regular triangle and cubic complexes.

This suggests why $*$ does not work. If we look at $W * A\omega$, where ω is some p -form, we can see that A integrates ω over some p -dimensional volume element. $*$ then maps the p -cochain to an $(n - p)$ -cochain, $\hat{\sigma}^{(n-p)}$, so W returns the wrong volume factor. Instead of getting the average value for the p -form over the space we get

$$W * A\omega = \frac{\int_{\sigma^p} \omega}{Vol(\hat{\sigma}^{(n-p)})} \hat{\omega} \quad (5.1)$$

where $\hat{\omega}$ is the $(n - p)$ -form which the Whitney map returns. A natural modification which can be made is to add a volume factor to $*$ so that we get

$$W * A\omega = \frac{\int_{\sigma^p} \omega}{Vol(\sigma^p)} \hat{\omega}, \quad (5.2)$$

which makes far more sense.

So the suggested change to $*$ is

$$*_K \sigma^p = \frac{\text{Vol}(\hat{\sigma}^{(n-p)})}{\text{Vol}(\sigma^p)} *, \quad (5.3)$$

where $*_K$ is the new $*$. A nice property of this is that when we take $**$, the volume factors introduced cancel and so we retain $** = 1$.

This means that we now have discrete forms converging to their continuous analogies as well as the operators d and $*$.

The coderivative and Laplacian

Note that

$$d_K = d_K A W = A d W, \quad (5.4)$$

so

$$W * d_K * A = W * A d W * A = (W * A) d (W * A). \quad (5.5)$$

Now each $W * A$ part converges properly since with the volume factors we know that $*$ makes sense and the d is the standard continuum exterior derivative. If we had not used this form of d_K , the convergence would not be so clear since the d_L would muddle things up by creating factors involving 4 different volumes which do not seem to make any sense:

$$\frac{\text{Vol}(\hat{\sigma}^{(n-p)})}{\text{Vol}(\sigma^p)} \frac{\text{Vol}(\sigma^{(p-1)})}{\text{Vol}(\hat{\sigma}^{(n-p+1)})}. \quad (5.6)$$

The convergence of the Laplacian follows from the convergence of the coderivative since d commutes with both A and W .

This seems to put things in good shape but again there is a problem since we have used W_L above which we know nothing about. As a result we are unable to apply the heuristic and so the whole argument falls. We do know what W_L is in the cubic case though since the dual space for a cube is also a cube and so the various convergence results do hold there.

So we have a natural modification which leads to a suitable $*$, but in a way that is too *ad hoc*. The various components of the theory are all related so you cannot just change one part without making appropriate changes elsewhere. For example if we use the generalised de Rham map we are unable to use our standard exterior

derivative if we want $dA = Ad$. In the case of $*$ we have a close relationship with $(,)$ which is destroyed if we only alter the former. That being the case we consider another way of introducing metric where we alter our inner product in a natural way and see what effect this has on $*$. We had in our original formulation that

$$(e^i, e^j) = \delta_{ij} \quad (5.7)$$

which means that the inner product of an edge with itself is 1 whilst we expect from the continuum case to get its length. This can be achieved by using a new inner product

$$(e^i, e^j) = \int W(e^i) \wedge *W(e^j) \quad (5.8)$$

as used by Dodziuk [32]. We want to investigate the effect this has on $*$. We have introduced metric information into our system which ideally should filter through the system in a nice way leaving all the properties which we are happy with whilst sorting out the metric dependence of $*$.

We begin by looking at how the inner product is related to the Hodge star after which we compute what $*$ results when we use our new $(,)$ for both the simplicial and cubic cases.

5.2 The inner product is the star

Any linear map on a vector space can be expressed in terms of the dual basis list elements. If we have any p -form λ we can wedge it to an $(n - p)$ -form, μ , to get an n -form $f d\sigma = \lambda \wedge \mu$. This is a linear map so f is uniquely determined. Since it is linear we can also express it as $(*\lambda, \mu) = f$ where $*\lambda$ belongs to the dual space. This $*$ is the Hodge star and we can see how closely it is related to $(,)$. We cannot change one without changing the other.

5.2.1 Basis lists

A complex consists of a collection of simplices of various dimensions. In our special case of S^1 we have just a triangle $[0, 1, 2]$. Each of these vertices have given coordinates so $v_i = (x_i, y_i)$ which we will use later. The basis list (see section 4.7) for this complex

is:

$$\begin{array}{ll}
 0 & [0] \\
 1 & [1] \\
 2 & [2] \\
 3 & [0, 1] \\
 4 & [0, 2] \\
 5 & [1, 2] \\
 6 & [0, 1, 2].
 \end{array} \tag{5.9}$$

Note that a basis list element e^i could refer to a simplex of any dimension but since we know how many elements of any given dimension there are we can easily pick whatever dimension we want.

Recall that we work with 3 complexes in general, the basic one, K , and two associated ones L and B which can be constructed from K . Their basis lists can also be determined though L is somewhat different since it is not a simplicial complex. B is just a subdivided complex and its basis list is written in the same way as the one above with the vertices first, then the edges and faces. In contrast the L basis list is ordered in reverse with the faces coming first, then the edges and finally the vertices. This is so that the dual of the i th basis element in K is the i th basis list element of L .

5.2.2 Determining *

Our inner product is given by

$$(e_B^i, e_B^j) = \int W^B(e_B^i) \wedge *W^B(e_B^j), \tag{5.10}$$

Note that e^i and e^j both need to be of the same dimension since we need an n -form on the *RHS* for it to be nonzero. We then define $*_K$ as follows:

$$(*_K e_K^l, e_L^m) = \int W^B(e_K^l) \wedge W^B(e_L^m), \tag{5.11}$$

where using the fact that e_K^l and e_L^m can be expressed in terms of elements of B .

Now we write

$$*_K e_K^l = h_m^l e_L^m. \tag{5.12}$$

We can use Eqn. (5.10) and Eqn. (5.11) to determine h_m^l , which determines the matrix for the Hodge star operator.

Firstly we define two more matrices A and B which allow us to move from basis elements of K and L to B respectively. So

$$e_K^l = A_i^l e_B^i, \quad (5.13)$$

$$e_L^m = B_j^m e_B^j. \quad (5.14)$$

So Eqn. (5.11) can be rewritten as

$$(*_K e_K^l, e_L^m) = (h_o^l e_B^o, e_B^m), \quad (5.15)$$

$$= h_o^l B_i^o B_j^m (e_B^i, e_B^j), \quad (5.16)$$

$$= h_o^l B_i^o B_j^m \int W(e_B^i) \wedge *W(e_B^j). \quad (5.17)$$

$$I^{ij} = \int W(e_B^i) \wedge *W(e_B^j). \quad (5.18)$$

$$(*_K e_K^l, e_L^m) = h_o^l B_i^o I^{ij} B_j^m, \quad (5.19)$$

$$= h_o^l X^{om}. \quad (5.20)$$

Also using Eqn. (5.11) we have that

$$(*_K e_K^l, e_L^m) = \int W(e_K^l) \wedge W(e_L^m), \quad (5.21)$$

$$= \int W(A_i^l e_B^i) \wedge W(B_j^m e_B^j), \quad (5.22)$$

$$= A_i^l B_j^m \int W(e_B^i) \wedge W(e_B^j). \quad (5.23)$$

$$J^{ij} = \int W(e_B^i) \wedge W(e_B^j). \quad (5.24)$$

$$(*_K e_K^l, e_L^m) = A_i^l J^{ij} B_j^m, \quad (5.25)$$

$$= S^{lm}. \quad (5.26)$$

We have that Eqn. (5.20)=Eqn. (5.26) so

$$h_o^l X^{om} = S^{lm}, \quad (5.27)$$

which is just a matrix equation. If we determine X^{-1} we can right multiply by this to get h which is $*_K$. We can get $*_L$ using a similar calculation.

We want to get h . To compute this we need to:

1. (a) Determine the basis list elements of B , L and K .
 - (b) Figure out what the barycentric coordinates are in the various simplices which we have.
 - (c) Evaluate what W acting on the various basis list elements are
2. Compute I and J , where we need to integrate expressions involving W .
3. (a) Compute X and S from I and J .
 - (b) Solve the matrix equation $hX = S$ to determine h .

We will now carry through this procedure for a single simplex triangulation of S^1 .

5.3 S^1 example

5.3.1 Stage one

We start with a triangulation. For the case of S^1 we use a single triangle $[0, 1, 2]$. We then get its basis list as well as the basis lists of L and B . We then determine the barycentric coordinates and the result of the Whitney map acting on the basis list elements. This gives us the basic objects we need to work with.

Basis list elements

The triangulation of S^1 which we use is $[0, 1, 2]$. So the basis list is

$$\begin{array}{ll}
 0 & [0] \\
 1 & [1] \\
 2 & [2] \\
 3 & [0, 1] \\
 4 & [0, 2] \\
 5 & [1, 2] \\
 6 & [0, 1, 2].
 \end{array} \tag{5.28}$$

To get B we just add the barycentres to the various simplices above. We name the barycentre of a simplex its basis list element number, so the barycentre of $[0, 1, 2]$

is 6 (see Eqn. 5.28). The basis list for B then is:

0 [0]

1 [1]

2 [2]

3 [3]

4 [4]

5 [5]

6 [6]

(5.29)

7 [0, 3]

8 [0, 4]

9 [0, 6]

10 [1, 3]

11 [1, 5]

12 [1, 6]

13 [2, 4]

14 [2, 5]

15 [2, 6]

16 [3, 6]

17 [4, 6]

18 [5, 6]

19 [0, 3, 6]

20 [0, 4, 6]

21 [1, 3, 6]

22 [1, 5, 6]

23 [2, 4, 6]

24 [2, 5, 6]

(5.30)

$[v_0, v_1, v_2]$	v_0	v_1	v_2
$[0, 3, 6]$	$(0,0)$	$(0.5,0)$	$(1/3,1/3)$
$[1, 3, 6]$	$(1,0)$	$(0.5,0)$	$(1/3,1/3)$
$[1, 5, 6]$	$(1,0)$	$(0.5,0.5)$	$(1/3,1/3)$
$[2, 5, 6]$	$(0,1)$	$(0.5,0.5)$	$(1/3,1/3)$
$[2, 4, 6]$	$(0,1)$	$(0,0.5)$	$(1/3,1/3)$
$[0, 4, 6]$	$(0,0)$	$(0,0.5)$	$(1/3,1/3)$

Table 5.1: Coordinates of triangles in B .

$[v_0, v_1, v_2]$	μ_0	μ_1	μ_2
$[0, 3, 6]$	$1-2x-y$	$2x-2y$	$3y$
$[1, 3, 6]$	$-1+2x+y$	$-2+2x-2y$	$3y$
$[1, 5, 6]$	$x-y$	$-2+2x-4y$	$3-3x-3y$
$[2, 5, 6]$	$y-x$	$-2+4x+2y$	$3-3x-3y$
$[2, 4, 6]$	$-1+x+2y$	$2-4x-2y$	$3x$
$[0, 4, 6]$	$1-x-2y$	$-2x+2y$	$3x$

Table 5.2: Barycentric coordinates associated with triangles in B .

Finally the dual basis list with its B basis list elements entries:

$$\begin{array}{rcl}
 0 & 19 & -20 \\
 1 & -21 & 22 \\
 2 & 23 & -24 \\
 3 & 16 & \\
 4 & 17 & \\
 5 & 18 & \\
 6 & 6 &
 \end{array} \tag{5.31}$$

Barycentric coordinates

From Sec. 4.2.2, we can determine the barycentric coordinates for the various triangles of our system. In particular, for S^1 we want the μ 's for the 6 triangles which $[0, 1, 2]$ is split into in forming B . These are given in Table 5.2 with the coordinates of the associated vertices in Table 5.1.

5.3.2 Whitney

Using these barycentres, which are of the form $a + bx + cy$, for a given triangle, we compute the Whitney map of the various simplices which belong to the triangle. So for the vertices we have

$$W[i] = \mu_i = a + bx + cy, \quad (5.32)$$

which is easily determined. Next for the edges

$$W[v_i, v_j] = \mu_i d\mu_j - \mu_j d\mu_i. \quad (5.33)$$

We say that

$$\mu_i = a + bx + cy, \quad (5.34)$$

$$\mu_j = p + qx + ry, \quad (5.35)$$

and

$$W[v_i, v_j] = (a + bx + cy)(qdx + rdy) - (p + qx + ry)(bdx + cdy) \quad (5.36)$$

$$= (aq + bq x + cq y - bp - bq x - br y)dx + (ar + br x + cr y \quad (5.37)$$

$$- pc - qc x - rc y)dy$$

$$= ((aq - bp) + (cq - br)y)dx + ((ar - pc) + (br - cq)x)dy. \quad (5.38)$$

Using this we can loop through the various vertices generating what the Whitney map of the various edges is. For the triangle we have that

$$W[v_i, v_j, v_k] = 2d\mu_i d\mu_j = 2(bdx + cdy)(qdx + rdy) = 2(br - cq). \quad (5.39)$$

So for $[0, 3, 6]$ we get

$$\begin{aligned} W[0] &= 1.000000 - 2.000000x - 1.000000y \\ W[3] &= 0.000000 + 2.000000x - 2.000000y \\ W[6] &= 0.000000 + 0.000000x + 3.000000y \\ W[0, 3] &= (2.000000 - 6.000000y)dx + (-2.000000 + 6.000000x)dy \\ W[0, 6] &= (0.000000 + 6.000000y)dx + (3.000000 - 6.000000x)dy \\ W[3, 6] &= (0.000000 - 6.000000y)dx + (0.000000 + 6.000000x)dy \\ W[0, 3, 6] &= 12.000000dxdy \end{aligned} \quad (5.40)$$

5.3.3 Stage two

Having determined what the Whitney map of the various basis list elements are we are now ready to enter the second stage of our computation of the discrete Hodge star, h , for S^1 . From sec. 5.2.2, we need to determine I and J in order to compute X and S before we can compute h .

$$I^{ij} = \int W(e^i) \wedge *W(e^j) \quad (5.41)$$

$$J^{ij} = \int W(e^i) \wedge W(e^j) \quad (5.42)$$

$$X = BIB \quad (5.43)$$

$$S = AJB. \quad (5.44)$$

Note that these are determined in each triangle of the triangulation since, for example, basis list element i exists in several triangles and $W(e^i)$ depends on which triangle you are in. The final result of the integrals for I is the sum over all the triangles with sign factors depending on the orientation of the triangle. So, a negatively oriented triangle's value for I^{ij} will be subtracted from the the total value.

Once we have X and S we can get h , from Eqn. 5.27, since

$$h = SX^{-1}. \quad (5.45)$$

I and J

To get I and J we need to integrate. The most general such integral being

$$\int (a + bx + cy + dx^2 + ey^2 + fxy) dx dy. \quad (5.46)$$

It is not simply $a + bx + cy$ since we take the product of two such objects which leads to second order terms. Integrating this over the standard triangle leads to

$$\int (a + bx + cy + dx^2 + ey^2 + fxy) dx dy = (1.0/24.0) * (12*a + 4*(b+c) + 2*(d+e) + f), \quad (5.47)$$

which was obtained using MuPad [43]. With this we can easily work out the matrices I and J though some further work is required since this integral formula is applicable when integrating over standard triangles while I and J involve integrals over the real triangles. We can perform a change of variable so that the integral is over standard

triangles using the transformation which we already have. If A maps from the actual triangle to the standard one, we know $A(x - b) = \hat{x}$ so that $x = A^{-1}(\hat{x}) + b$. We can then change from $a + bx + cy \rightarrow A + B\hat{x} + C\hat{y}$. So if we have an integral over the actual triangle with variables X and Y we say

$$x = A[0] * (X - b[0]) + A[1] * (Y - b[1]), \quad (5.48)$$

$$y = A[2] * (X - b[0]) + A[3] * (Y - b[1]). \quad (5.49)$$

Plugging this into the expression for the general function we get that

$$\begin{aligned} a + bx + cy + dx^2 + ey^2 + fxy = & (a + bXA[0] + dX^2A[0]^2 + \\ & bYA[1] + 2dXYA[0]A[1] + dY^2A[1]^2 + cXA[2] + fX^2A[0]A[2] + fXYA[1]A[2] + \\ & eX^2A[2]^2 + cYA[3] + fXYA[0]A[3] + fY^2A[1]A[3] + 2eXYA[2]A[3] + \\ & eY^2A[3]^2 - bA[0]b[0] - 2dXA[0]^2b[0] - 2dYA[0]A[1]b[0] - cA[2]b[0] - \\ & 2fXA[0]A[2]b[0] - fYA[1]A[2]b[0] - 2eXA[2]^2b[0] - fYA[0]A[3]b[0] - \\ & 2eYA[2]A[3]b[0] + dA[0]^2b[0]^2 + fA[0]A[2]b[0]^2 + eA[2]^2b[0]^2 - \\ & bA[1]b[1] - 2dXA[0]A[1]b[1] - 2dYA[1]^2b[1] - fXA[1]A[2]b[1] - cA[3]b[1] - \\ & fXA[0]A[3]b[1] - 2fYA[1]A[3]b[1] - 2eXA[2]A[3]b[1] - 2eYA[3]^2b[1] + \\ & 2dA[0]A[1]b[0]b[1] + fA[1]A[2]b[0]b[1] + fA[0]A[3]b[0]b[1] + \\ & 2eA[2]A[3]b[0]b[1] + dA[1]^2b[1]^2 + fA[1]A[3]b[1]^2 + eA[3]^2b[1]^2). \end{aligned} \quad (5.50)$$

We can then apply the integral formula since x and y are in the standard triangle. To determine A^{-1} we just determine A as before and invert.

Note that the solutions we get are locally based so we get I^k for the contribution to I from triangle k . To get the final value for I we need to sum these with appropriate sign factors taking into account how k is oriented with respect to the original triangle $[0, 1, 2]$. After this summation we have our desired matrices.

5.3.4 Stage three

Now we are ready to compute the discrete Hodge star matrix. Using the I 's and J 's which we have just computed to determine X and S , we just multiply by A 's and

B 's (see Eqn. 5.20 and Eqn. 5.26). This results in $X =$

$$\begin{array}{ccc} 0 & 0 & 216.021606 \\ 1 & 1 & 162.016205 \\ 2 & 2 & 54.005402 \\ 3 & 3 & -3.499199 \\ 4 & 4 & 9.501602 \\ 5 & 5 & -46.003204 \\ 6 & 6 & 50.505154 \end{array} \quad (5.51)$$

and $S =$

$$\begin{array}{ccc} 0 & 0 & 12.002400 \\ 1 & 1 & 8.000900 \\ 2 & 2 & 12.000601 \\ 3 & 3 & 10.001801 \\ 4 & 4 & -15.001502 \\ 5 & 5 & -78.007805 \\ 6 & 6 & 117.010803 \end{array} \quad (5.52)$$

We want to determine X^{-1} , once we have these, since the discrete Hodge is simply SX^{-1} . This leads to $h_K =$

$$\begin{array}{ccc} 0 & 0 & 5.555911e - 02 \\ 1 & 1 & 4.938155e - 02 \\ 2 & 2 & 2.222151e - 01 \\ 3 & 3 & -2.858315e + 00 \\ 4 & 4 & -1.578833e + 00 \\ 5 & 5 & 1.695734e + 00 \\ 6 & 6 & 2.316814e + 00 \end{array} \quad (5.53)$$

and $h_L =$

$$\begin{array}{ccc} 0 & 0 & 1.200000e + 01 \\ 1 & 1 & 7.784244e + 00 \\ 2 & 2 & -4.794487e + 01 \\ 3 & 3 & -2.001961e + 01 \\ 4 & 4 & -3.013560e + 01 \\ 5 & 5 & -2.999790e + 00 \\ 6 & 6 & 2.847700e - 01, \end{array} \quad (5.54)$$

which implies that $** =$:

$$\begin{array}{ccc} 0 & 0 & 6.667093e - 01 \\ 1 & 1 & 3.843980e - 01 \\ 2 & 2 & -1.065407e + 01 \\ 3 & 3 & 5.722235e + 01 \\ 4 & 4 & 4.757908e + 01 \\ 5 & 5 & -5.086846e + 00 \\ 6 & 6 & 6.597591e - 01, \end{array} \quad (5.55)$$

which is not proportional to the identity. Looking carefully at GD (Section 4.5.2) we see that essentially S is redefined to equal X there, in which case we trivially get $h = XX^{-1} = I$. In other words we have that $X_{ij} = \delta_{ij}$. This gives us $h_{ii} = S_{ii}$ which leads to h being diagonal but not $** = \pm I$. To remedy the situation we normalise S_{ij} to $\pm\delta_{ij}$ by using the $\frac{(p+q+1)!}{p!q!}$ factor which gives us $h_{ij} = \pm\delta_{ij}$.

Now we have a different X , due to our new inner product, but it is unclear what we should do with it. We might normalise S and then compare the results we get with the heuristic, though we do not even know whether the heuristic holds in general¹. If we normalise S , to $\pm\delta_{ij}$, this does not ensure that h will be too since the new X is no longer $\pm\delta_{ij}$. There is a temptation to over normalise in which case we factor out all the changes due to the inner product and so end up throwing away the metric information we set out to capture. We have been able to compute h using the simplicial case but the results are unsatisfactory since have been unable to see whether the new inner product leads to a discrete Hodge star which converges to the continuum one.

¹we only know it works for the standard triangles.

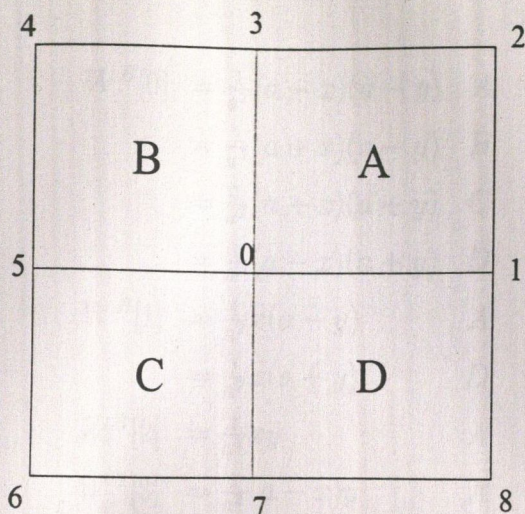


Figure 5-1: The reference square

5.4 Cubic Lattice case

In contrast to the simplicial case, the cubic lattice is more amenable to analysis and can, in fact, be dealt with by hand. We take a simple one square system which is subdivided as our reference system.

As for the simplicial case we define $*_K$ and $*_L$ using our basic equations:

$$(x_B^p, y_B^p)_B = \int W^B(x_B^p) \wedge *W^B(y_B^p), \quad (5.56)$$

$$(*_K u_K^p, v_L^{n-p})_L = \int W^B(u_K^p) \wedge W^B(v_L^{n-p}) \quad (5.57)$$

$$(*_L u_L^p, v_K^{n-p})_K = \int W^B(u_L^p) \wedge W^B(v_K^{n-p}). \quad (5.58)$$

We only need to determine what the Whitney map is when applied to various components of a single cube to know the answer in general since the only free factor is the length scale "a". Of course this is also true for the standard triangle case so is not the main point but the fact that it is the case is important and worth mentioning. Also, the integrals being performed are all basically the same, which means that it is far easier to get what we want than one would expect.

We focus our attention on the example shown in Fig. 5 – 1. We need to know what W^B acting on the various components of the reference square is to proceed so

we do this next:

$$\begin{aligned}
 W^B[0] &= \frac{1}{a^2}(a-x)(a-y) & A \\
 &= \frac{1}{a^2}(a+x)(a-y) & B \\
 &= \frac{1}{a^2}(a+x)(a+y) & C \\
 &= \frac{1}{a^2}(a-x)(a+y) & D \\
 W^B[1] &= \frac{1}{a^2}x(a-y) & A \\
 &= \frac{1}{a^2}x(a+y) & D \\
 W^B[2] &= \frac{1}{a^2}xy & A \\
 W^B[3] &= \frac{1}{a^2}(a-x)y & A \\
 &= \frac{1}{a^2}(a+x)y & B \\
 W^B[4] &= -\frac{1}{a^2}xy & B \\
 W^B[5] &= -\frac{1}{a^2}x(a-y) & B \\
 &= -\frac{1}{a^2}x(a+y) & C \\
 W^B[6] &= \frac{1}{a^2}xy & C \\
 W^B[7] &= -\frac{1}{a^2}(a+x)y & C \\
 &= -\frac{1}{a^2}(a-x)y & D \\
 W^B[8] &= -\frac{1}{a^2}xy & D \\
 W^B[01] &= \frac{1}{a^2}(a-y)dx & A \\
 &= \frac{1}{a^2}(a+y)dx & D \\
 W^B[12] &= \frac{1}{a^2}xdy & A \\
 W^B[23] &= -\frac{1}{a^2}ydx & A \\
 W^B[30] &= -\frac{1}{a^2}(a-x)dy & A \\
 &= -\frac{1}{a^2}(a+x)dy & B \\
 W^B[34] &= -\frac{1}{a^2}ydx & B \\
 W^B[45] &= -\frac{1}{a^2}(-x)dy & B \\
 W^B[50] &= \frac{1}{a^2}(a-y)dx & B \\
 &= \frac{1}{a^2}(a+y)dx & C \\
 W^B[56] &= -\frac{1}{a^2}(-x)dy & C \\
 W^B[67] &= \frac{1}{a^2}(-y)dx & C \\
 W^B[70] &= \frac{1}{a^2}(a+x)dy & C \\
 &= \frac{1}{a^2}(a-x)dy & D
 \end{aligned} \tag{5.59}$$

$$W^B[78] = \frac{1}{a^2}(-y)dx \quad D \quad (5.60)$$

$$W^B[81] = \frac{1}{a^2}xdy \quad D$$

$$W^B[0123] = \frac{1}{a^2}dx \wedge dy$$

We next use the fact that K can be embedded in the subdivided space B so that if x belongs to K its image in B is Bx to get

$$(x_K^p, y_K^p)_K = \int W^B[Bx_K^p] \wedge *W^B[By_K^p] \quad (5.61)$$

where the component on the RHS are known. Let $x = e^i$ and $y = e^j$ be basis list elements of the complex K then we define

$$I^{ij} = (e_K^i, e_K^j)_K = (x_K^p, y_K^p)_K. \quad (5.62)$$

Note that:

1. I is diagonal since x and y are in different squares of B and so their images after W do not overlap.
2. The various integrals that appear are the same since we are integrating either x^2 from 0 to a or something which can be expressed as this with a change of variable.
3. The dx and dy integrals are independent and both of the form mentioned above.

The three possible cases are:

$$\int_0^a x^2 dx = \left[\frac{x^3}{3}\right]_0^a = \frac{a^3}{3} \quad (5.63)$$

$$\int_0^a (a-x)^2 dx = \int_a^0 y^2(-dy) = \frac{a^3}{3} \quad (5.64)$$

$$\int_0^a (x-a)^2 dx = \int_0^a y^2 dy = \frac{a^3}{3}. \quad (5.65)$$

So any of the integrals which we have is equal to $\frac{a^3}{3}$. In the case of vertices we have two such integrals leading to $\frac{F*a^6}{9}$ factors with a symmetry term F to specify how often a term occurs. For edges we only have one integral since we do not get x^2y^2 terms but x^2dy instead. For the faces we get no such terms since the integral is

simply $dx dy$. Finally W also has a $\frac{1}{a^2}$ term associated with it so for vertices we get

$$\frac{Fa^6}{9a^4}, \quad (5.66)$$

for edges

$$\frac{Fa^4}{3a^4} \quad (5.67)$$

and for faces

$$\frac{a^2}{a^4}. \quad (5.68)$$

For L we similarly get

$$([\hat{0}], [\hat{0}])_L = \frac{1}{a^2} \quad (5.69)$$

$$([\hat{01}], [\hat{01}])_L = \frac{F}{3} \quad (5.70)$$

$$([\hat{0123}], [\hat{0123}])_L = \frac{Fa^2}{9} \quad (5.71)$$

We only mention the results for particular vertices, edges and faces but they are all the same except for the F factors and so the above is enough. In fact we are interested in complexes without boundary in which case every vertex has $F = 4$ and every edge has $F = 2$.

To determine $*_K$ we use

$$(*_K x_K^p, y_L^{n-p})_L = \int W^B(Bx_K^p) \wedge W^B(By_L^{n-p}). \quad (5.72)$$

We have the LHS except $*_K$ so need the RHS next. Note that since both $(,)_K$ and $(,)_L$ are diagonal, we only get contributions when $y = \hat{x}$. Again we look at the various cases.

Performing the RHS integral for the vertices, if we have $x = [0]$ then $y = [\hat{0}]$, we get:

$$= 4 \int_A \frac{1}{a^4} (a-x)(a-y) dx \wedge dy \quad (5.73)$$

$$= 4 \frac{1}{a^4} \frac{a^2}{2} \frac{a^2}{2} \quad (5.74)$$

$$= 1. \quad (5.75)$$

For the edges we get:

$$= 4 \int_A W^B[01] \wedge W^B[03] \quad (5.76)$$

$$= 4 \int_A \frac{1}{a^4} \frac{a^2}{2} \frac{a^2}{2} \quad (5.77)$$

$$= 1. \quad (5.78)$$

And for the faces:

$$= \int W^B[0123] \wedge W^B[0] \quad (5.79)$$

$$= 4 \int_A \frac{1}{a^4} \frac{a^2}{2} \frac{a^2}{2} \quad (5.80)$$

$$= 1. \quad (5.81)$$

The dual calculations are the same apart from sign factors which arise when the $W(x)$ and $W(y)$ terms are flipped. So for the edges case we get a (-1) sign.

Determining $*_K$ is now trivial since both sides of the equation are diagonal. The i th diagonal element of $*_K$ is simply the i th diagonal element of the RHS (which are all just ± 1) divided by the i th diagonal element of $(\cdot)_L$ which only depends on whether we are dealing with vertices, edges or faces. So on 0-cochains we have

$$*_K[0] = a^2[\hat{0}] \quad (5.82)$$

on edges we have

$$*_K[01] = \frac{3}{2}[\hat{01}] \quad (5.83)$$

and for faces we have

$$*_K[0123] = \frac{9}{4a^2}[0\hat{1}23]. \quad (5.84)$$

We can get $*_L$ in the same way:

$$*_L[\hat{0}] = \frac{9}{4a^2}[0] \quad (5.85)$$

$$*_L[\hat{01}] = -\frac{3}{2}[01] \quad (5.86)$$

$$*_L[0\hat{1}23] = a^2[0123] \quad (5.87)$$

With this we get

$$** = \pm \frac{9}{64}I, \quad (5.88)$$

which is not only diagonal but proportional to the identity. We can then introduce a normalisation factor to Eqn. 5.72:

$$(*_K x_K^p, y_L^{n-p})_L = \frac{8}{3} \int W^B(Bx_K^p) \wedge W^B(By_L^{n-p}). \quad (5.89)$$

We can then determine convergence results, since we can see how the length scale a appears in the various operators. In short they appear as you would expect them to using the heuristic which means that δ and the Laplacian converge to the continuum case.

Firstly we look explicitly at what happens in 2D. In the continuum we know that:

$$*d * f = *df dx dy = 0, \quad (5.90)$$

$$*d * f dx = *df dy = * \frac{\partial f}{\partial x} dx \wedge dy = \frac{\partial f}{\partial x}, \quad (5.91)$$

$$*d * f dx dy = *df = * \left(\frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy \right) = \frac{\partial f}{\partial x} dy - \frac{\partial f}{\partial y} dx. \quad (5.92)$$

We can now look at what happens in the cubic case. We want to compare $W^K *_L d_L *_K A^K$ with the above.

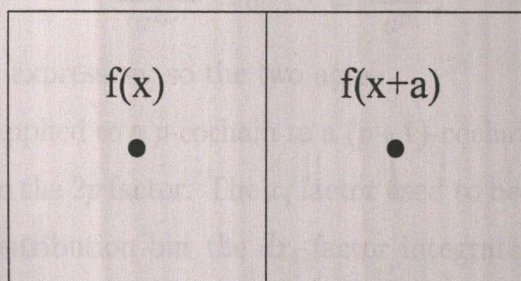


Figure 5-2: Oppositely oriented adjacent regions lead to $f(x+a) - f(x)$ terms.

Note that $\partial = *d*$, with some sign factor. This means that $*d*$ applied to $[xy]$ gives us its boundary. Since we have a manifold without boundary every edge has an oppositely oriented pair in an adjacent face. So a face is mapped onto the edges which are its boundary. For example if we take the edge $[0, y]$ we map $-f_i$ onto it where f_i is $f dx dy$ integrated over the face i . The adjacent face will also contribute to this edge with a $+f_j$ term. Face i is a away in the x direction from face j and so we effectively get an $f(x+a) - f(x)$ term, which after Whitney will give (See Fig. 5-2)

$$\frac{f(x+a) - f(x)}{a} dy. \quad (5.93)$$

In this way we can see that we agree with the continuum result. The 1-form case follows similarly with the boundary now vertices and the 0-form case is trivial since $*$ maps to a 2-form which d takes to zero.

The volume factors which arise are precisely those which we required from our heuristic (Sec. 5.1) so this result can be generalised to higher dimensions. First we note that this is the case in $2D$ since $*$ applied to vertices leads to an a^2 which is the volume of the cell mapped to, divided by that of the cell acted on. For edges we get a factor independent of a which again agrees with this picture as does the $\frac{1}{a^2}$ factor for faces.

In general we have a^{3D-2p}/a^{2D} for p -cochains. In two dimensions this means that we have a^{6-2p}/a^4 so a^2 for vertices, 1 for edges and a^{-2} for faces. Similarly in three dimensions we have a^{9-2p}/a^6 or a^3 for vertices, a for edges, a^{-1} for faces and a^{-3} for cubes. In general the heuristic expression is the volume of the space mapped to, a^{D-p} , divided by the volume of the object acted on, a^p . Our general expression above was

$$\frac{a^{3D-2p}}{a^{2D}} = a^{D-2p} = \frac{a^{D-p}}{a^p}, \quad (5.94)$$

which is our heuristic expression; so the two agree.

As we go from W applied to a p -cochain to a $(p+1)$ -cochain, an x_i term becomes a dx_i one, which leads to the $2p$ factor. The x_i factor used to be squared and integrated, contributing an a^3 contribution but the dx_i factor integrated only contributes an a factor which is a^2 less.

We had already seen that the heuristic suggested a modification² that could be made to $*^K$ so that it, along with the coderivative and Laplacian, would converge to the continuum result. The problem with this was that it broke the relationship between the inner product and $*$ which we have in differential geometry. In order to retain this we made a natural modification to the discrete inner product to see what effect this had on $*^K$. We have found that this resulted in adding precisely the factors which we wanted from the heuristic. As a result we can use the various convergence results which we had before except of course the relationship of $*^K$ and the inner product is now preserved.

²See Sec. 5.1.

6.2 Back to function spaces

We have been using a complex space for space we noted the relationship between the objects on the complex with the objects on manifolds. This provided us with a more general framework which we can use to look at things from an applied perspective. It is not as nice as topology. The finite dimensional space of functions, which W maps to provides an alternate approach to capturing differential

Chapter 6

Finite Dimensional Subspaces

6.1 Introduction

We now move on to a new phase of our work. Finite dimensional subspaces (FDS) provides a discrete representation of DG in a slightly different manner to GD. It has an associative wedge product at the expense of topology which can be an acceptable trade off as we will see later on.

When we were trying to determine the Hodge star associated with our new choice of inner product (See Chap.5) in the simplicial case, we required computational methods. In this work we noticed that W of a cochain mapped to a function of the following form in D dimensions:

$$f = a_0 + \sum_{i=1}^D a_i x_i. \quad (6.1)$$

In other words **W maps to linear functions**. This is a far simpler system to work with since the space of functions has a finite dimensional basis list. So we need only a finite dimensional subspace of the original function space. For example in $2D$ our general function is $a + bx + cy$ which means that 3 numbers (a, b, c) parametrise the entire space of functions of interest.

W having this form is also interesting from a theoretical point of view since it offers a different style of discretisation where, instead of mapping onto a triangulation, we map onto a subspace of our original function space much like in finite element methods (FE).

6.2 Back to function spaces

We have been using a complex since originally we noted the relationship between the objects on the complex with the objects on manifolds. This provided us with a ready made language which we used but we are looking at things from an applied point of view or at least not as algebraic topologists. The finite dimensional space of functions, which W maps, to provides an alternate approach to capturing differential geometry computationally which has several advantages.

Since $AW = I$ we can map back from FDS to GD without loss of information so in some sense they are the same BUT we can chose to use the standard continuum operations on the forms we have and extend the subspace too. So FDS is a generalisation of GD.

Firstly note that since the forms we use are equivalent to the GD picture we know that they converge to the continuum case. In fact that is how we compared the two in the first place, by mapping the GD objects to differential forms using Whitney.

We also know that d acting on them gives the same result as if WA was applied to df since it commutes with both W and A . This means that the topology appears to be captured since we reproduce the homology classes. We will look at this more closely in Sec. 6.4. Next we note that we get different finite dimensional subspaces in the cubic and simplicial case.

In $2D$ we have that fdx is mapped to $Fdx + Gdy$, in the simplicial theory, since the de Rham map maps onto two edges, one of which has a dy component when acted on by the simplicial Whitney. So we get dx going to $dx + hdy$ which converges to dx as we take finer triangulations but is not as good as in the cubic case.

The cubic version is far neater since dx is mapped cleanly only onto edges which are parallel to the x -axis and are mapped back to dx by the cubic Whitney. The functions are not linear ones but higher order polynomials, but this is not a problem, since the polynomial can approximate linear functions exactly. So the cubic theory is our theory of choice.

So we get that $WAffdx = f_a dx$, in the cubic case. If we apply the continuum $*$ to the result we get $f_a dy$ instead of $f dy$ and since f_a converges to f , $*$ converges to the continuum operator.

Wedge works this way too since we get $f_a \wedge g_a$, instead of $f \wedge g$. This is at least the same as in GD, where we are always restricted to linear functions which is a problem. If we wedge 2 linear functions together, the result is not linear, while in GD we are forced to make it linear by taking an approximation; this is why the wedge is non-associative. If we have $p \wedge q \wedge r$ then taking the linear approximation of $p \wedge q$ and wedging it to r is not the same as taking the linear approximation of $q \wedge r$ and then wedging it to p . In contrast, we can extend our basis list of functions in FDS to make enough room to avoid this. Of course in the cubic theory our functions are not linear but a similar extension can be made.

We could define our operations to be compatible with those from GD with $*$ defined as $W * A$ say, but this would be more complex and not even as good with, for example, a non-associative wedge. So it seems preferable to use the continuum operators with an extended space.

6.2.1 Review

To summarize:

- WA maps forms to a subspace.
- This subspace has a finite dimensional basis list.
- It can be extended so that it is closed under the wedge product.
- We apply the usual continuum operators.
- We get the correct continuum limit as our triangulation is refined, for our objects and operators.
- No dual space is required.
- $f dx$ is mapped cleanly to $F dx$ in the cubic, but not the simplicial, case.

6.3 FDS in practice

We now look at some examples of FDS in action, starting in 1D, which is a very simple system, before moving onto 2D where the whole scheme becomes clear.

We use the cubic theory since there $f dx$ is mapped to $F dx$, with no dy components as in the simplicial case. This is because A maps dx only to edges parallel to x which results in a cleaner theory.

In the 1D continuum theory we have functions $f(x)$ and 1-forms $f dx$. The FDS analogies are f_{pl} and $f_{average} dx$, since functions are approximated using piecewise linear functions and 1-forms by averages. We look at these a little closer. In 1D the complex consists of edges. On the edge $[v_0, v_1]$ we have that the function is mapped to the vertices using the de Rham map resulting in $f(x_0)[v_0] + f(x_1)[v_1]$. Whitney on this gives

$$f(x_0) \frac{(h-x)}{h} + f(x_1) \frac{x}{h} \quad (6.2)$$

where x ranges from 0 to the length of the edge, h . This is simply a linear function, from $f(x_0)$, at the vertex v_0 located at x_0 , to $f(x_1)$, at the vertex v_1 located at x_1 . So we have a linear approximation f_{pl} to our original function f .

The one form approximation is also simple. A maps $f dx$ to $(\int f dx)[v_0, v_1]$ which W maps to

$$\frac{\int f dx}{h} dx = f_{average} dx. \quad (6.3)$$

So we approximate a function on an edge with its average value on it.

We can then act on our discrete objects with $*$ which maps f_{pl} to $f_{pl} dx$ or $*f_{average} dx = f_{average}$, both of which converge to the correct continuum limit. We also know that d is treated properly since d can go through A and W . Since we are in 1D we have nothing to wedge dx to. This then is FDS in 1D. We have discrete approximations to the various continuum objects and which we can apply continuum operators to. The approximations are also made such that the topology is captured. Next we move up a dimension and repeat the process.

In 2D we can have either functions, 1-forms or 2-forms. As above we look at each in turn. Our space consists of a collection of squares. In each square we have $f(x, y)$ mapped to a polynomial approximation. We can see that again linear functions are captured exactly.

We take our standard square $[0, 1, 2, 3]$ as in Fig.6-1. WA applied to f results in

$$(1-y)[f_0(1-x) + f_1x] + y[f_2(1-x) + f_3x], \quad (6.4)$$

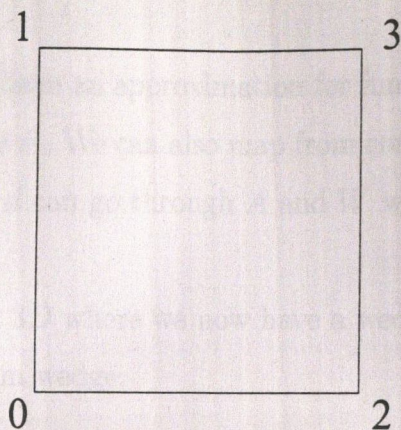


Figure 6-1: Labelling of vertices using binary convention.

where we are taking the unit square for simplicity. Then if the function is linear we have $f(x, y) = a + bx + cy$. Substituting this into the expression above we get

$$(1 - y)[(a + bx_0 + cy_0)(1 - x) + (a + b(x_0 + 1) + cy_0)x] + y[(a + bx_0 + c(y_0 + 1))(1 - x) + (a + b(x_0 + 1) + c(y_0 + 1))x] \quad (6.5)$$

$$= (1 - y + y)a + (1 - y)[bx_0 + cy_0 + bx] + y[bx_0 + c(y_0 + 1) + bx] \quad (6.6)$$

$$= a + bx_0 + cy_0 + bx + cy. \quad (6.7)$$

The linear function $f = a + bx + cy = a + b(x_0 + x) + c(y_0 + y)$ is captured perfectly so we have at least a linear approximation.

2-forms are mapped to an average while 1-forms are part average and part linear approximations. This is because in the cubic theory the various dimensions are multiplied together so in the 1-form case we have one dimension averaged and the other approximated by a linear function. This results in something like an average since the product of an $O(h)$ times an $O(h^2)$ approximation leads to an $O(h)$ one.

* and d are as before. A product of two linear functions in x leads to a quadratic one so when we wedge polynomial functions together, we end up with higher order polynomials than we started with. As a result in order to have a closed space we need to expand it. In 2D we can, at most, have second order terms in each variable so we say our basis list is the complete set of polynomials in $\{1, x, y\}$ up to second order in any given variable; in other words $\{1, x, y, x^2, y^2, xy\}$. This expanded basis list of functions is closed under wedge for the various objects we get from W . If W maps to $f dx$, then f has no x factor in it so we only need variables to the $(D - 1)$ th

order in D dimensions.

With this basis list we have an approximation for functions and the various forms. We have $*$ and d as well as $\wedge$. We can also map from continuum objects to this space preserving topology since d can go through A and W which is what is special about our system.

We can do the same in $3D$ where we now have a wedge which is associative since we are using the continuum wedge.

6.4 Topology

We know that $d(WA) = (WA)d$ which suggests that the homology classes are captured. We have to check.

We begin by looking at continuum theory, where we can see how results are determined before reproducing them in FDS; ideally leading to the same set of results being established there.

We can integrate forms over chains as we noted in Sec.3.5.2. So we can define the inner product $(\cdot, \cdot) : C_r(K) \times \Omega^r(M) \rightarrow \mathbb{R}$ as

$$c, \omega \rightarrow (c, \omega) \equiv \int_c \omega. \quad (6.8)$$

In this language Stokes' theorem can be expressed as

$$(cd\omega) = (\partial c, \omega) \quad (6.9)$$

which we use next.

This then induces an inner product, Λ , between elements of $H_r(K)$ and $H^r(M)$. Note that these are homology classes and not just chains and forms. For this to be well defined we need

$$(c + \partial c', \omega) = (c, \omega) + (c', d\omega) = (c, \omega), \quad (6.10)$$

since $d\omega = 0$ follows from ω being an element of $H^r(M)$. Similarly

$$(c, \omega + d\phi) = (c, \omega) + (\partial c, \phi) = (c, \omega), \quad (6.11)$$

since $\partial c = 0$.

To prove the duality of H_r and H^r we need to show that their dimensions are the same. This is achieved by de Rham's theorem which states that the inner product on a compact manifold is bilinear and non-degenerate. If we can perform the same procedure with FDS then we are done.

This involves

1. Defining an inner product between forms and chains.
2. Defining an inner product on elements of the homology groups.
3. Showing with use of Stokes' theorem that this is well defined.
4. Applying de Rham's theorem to show that H^r is dual to H^r .

We can define the inner products, since we have forms in FDS which we can integrate over chains. We do not, however, have Stokes' theorem.

If we take a differential form, which is defined over the manifold, it is mapped to a form defined over the triangulation. This has internal boundaries which do not exist in the continuum object and leads to non-zero terms.

This is not a problem in GD since the internal boundaries occur in oppositely oriented pairs, which cancel. For example if we take an edge, the value on it is determined by integrating the form over it. This results in the same value on both oppositely oriented edges which cancel. In FDS, we have a function associated to each cell and these need not agree. If they do not agree, they do not cancel. If they do not cancel we do not get Stokes' theorem.

If we do not have Stokes' theorem we do not have the inner product on the homology classes being well defined and cannot apply de Rham's theorem to show that they are dual to each other. Thus their topologies are not the same.

Note that the functions need not agree. This does not mean that they have to disagree. The question then is how can we ensure that they agree? We basically need conformal elements. If they do agree we have Stokes' theorem and topology.

If we have an edge then how do we ensure that the functions agree along it?, by using linear functions. Then knowing the value of the functions on the vertices fixes the value everywhere along the edge uniquely which is not the case with higher order

polynomials. In fact this is what the Whitney map does in GD. The problem then is that we are back to using linear functions and a non-associative wedge.

We can use polynomials and sacrifice topology but then we might as well use FE or other standard methods? The only advantage to using an FDS without topology is that it captures the structure of differential geometry, in that we have functions and various dimensional differential forms, which we can act on using d , $*$ and $\wedge$ and this is non-trivial.

6.4.1 Nonconformal FDS

If we sacrifice topology, this means that we use approximations which do not agree in regions that overlap. In other words this involves using nonconformal methods, for which we need to demonstrate convergence to agreeing in overlap regions.

Since our discrete theory approximates the continuum one we know that as we refine the triangulation, our objects converge to their continuum counterparts. As a result, since various versions of an object converge to the same continuum value, they must converge to each other as required.

In particular we have $Mx = y$. We map y to y_a , an approximation using WA . Do we have that x_a , the solution to the FDS equation, converges to x , the continuum solution? Note that x_a belongs to a different space to y_a . If y_a is a linear function, we need x_a to be one power higher. This is to ensure existence of our solutions since $df = a + bx$ means that f has to have an x^2 term. y_a is contained in a subspace of the bigger space (which is the image of WA extended, in order to have an associative wedge as well as existence of solutions to equations), containing x_a , in which we work.

The operators we are interested in are linear and the the FDS operator is the same as the continuum one. Subtracting the FDS equation from the continuum one we have:

$$Mx - Mx_a = y - y_a. \quad (6.12)$$

Since M is a linear operator this is the same as

$$M(x - x_a) = y - y_a \quad (6.13)$$

which means

$$M(x - x_a) = O(h) \quad (6.14)$$

because y_a is an approximation of y . So x_a converges to x .

For example we can look at $\frac{df}{dx} = f$ in FDS. Here the RHS is $1 + x$ since we are in 1D. Then f on the LHS equals $x + \frac{x^2}{2}$ which approximately equals e^x . The constant term is fixed as one in order to agree with the one on the RHS. If we have a complex consisting of two edges A and B then on each the solution above would be $1 + x + \frac{x^2}{2}$. We have x ranging from 0 to a on each locally but globally x_B ranges from a to $2a$. On the vertex where A and B meet the function agrees since $x_A = a = x_B$, and they have the same functional form.

So with nonconformal FDS we have the structure of differential geometry and convergence to agreement on overlap regions.

6.5 Electrostatics

GD and FDS capture much of differential geometry. As a result they are better suited to deal with electromagnetism which is naturally formulated in this language. In other words if we use GD to solve an electrostatics problem we get physical solutions. If we have an electric field $E = E_1 dx \wedge dy + E_2 dx \wedge dz + E_3 dy \wedge dz$ then

$$\int \nabla \cdot E dV = \int E \cdot dS, \quad (6.15)$$

is Gauss' law which is a special case of Stokes' theorem.

If we use a finite difference approach then ∇ , which is simply d acting on 2-forms in 3D, would only converge to the continuum result, as would non-conformal FDS. This means that E would converge to the case where Gauss' law held but the law, being exact, would not hold; so our discrete electric field would be quite unphysical. At least with FDS we automatically have $d^2 = 0$.

Mathematically electromagnetic theory in its proper form is expressed in terms of differential forms [36], computationally this means GD/FDS.

Some work has been done along these lines by Bossavit [44, 45], where Whitney forms are associated with FE, which we have only recently come across. He introduces

a mixture of elements to capture various dimensional differential forms so that he has $d^2 = 0$ too.

6.6 Finite Element

There are many similarities between FDS and FE. Both are based on a triangulation and involve finite dimensional subspaces in each cell. In fact FE usually means a triplet of the triangulation, the function space and a basis list for the finite dimensional space.

We used to call this approach FDS, since it emphasises the shift from the triangulation to the function spaces but then read in Braess [25] that when we say finite elements we mean polynomials which are finite dimensional; suggesting that finite element is the appropriate term for what we are doing. That is not the case though since FE is quite different in nature.

Finite element is based on the following logic¹. We begin with a differential equation. We replace this with a variational one which in turn can be expressed as a matrix equation. We can then show that the solution exists within this framework and that the solution of the matrix equation is a solution of the differential equation we began with.

In FDS we begin with a differential equation and then map it to a matrix equation by analogy. We do not convert it to a variational equation. We do not prove existence via the Lax-Milgram² theorem. We have existence since the space which we work with is closed. We know that if $df = a$, then $f = ax + b$ and $ax + b$ belongs to our space. We know that the operator is the continuum operator and that everything of interest converges to the relevant continuum analogy.

So in some sense FDS is a finite element method, but FE is based on the variational principle which FDS is not. Courant [46] is generally regarded to be the inventor of FE theory in 1943 though, again from Braess [25], Schellback's work [47] had been done nearly a century before and FE also appeared in some work of Euler depending on how we define FE. In other words, FDS can be classified as being a finite element method though, since it is not a variational method, it is not standard finite element.

¹See Appendix B for a more detailed description of the foundations of FE.

²See Sec.B.1.2 for further details.

The central calculation in FE involves inverting matrices. You reduce the problem to the form $Ax = y$ and invert A to determine the solution you are looking for. This is made easier since the matrix in general is near diagonal which simplifies things considerably. In contrast the matrix inversions are simpler still in FDS. If we are looking for $df = a + bx$, we know that the solution is $ax + bx^2/2 + \text{const}$. We can invert the matrices theoretically which means that finding the solution is simply a matter of matrix multiplication. The problem is also easily parallelisable since each region is solved independently.

We also need to do some work setting up the problem. In FDS, M can be computed once and for all, as well as M^{-1} . It depends on the dimension of the space and is the same in all cells. In comparison, computing M in FE requires integrals to be evaluated. x is determined once we know M^{-1} in the same way for both approaches. y in FDS requires applying WA which involves a simple integral. This is also required in FE so all in all FDS requires less work.

FE has the advantage that we can move down Pascal's triangle and have $O(h^3)$ accuracy for example, which is not so easily done in FDS. It might be possible to use some other method to project continuum forms to our subspace instead of WA which we have not considered yet.

At the moment it appears that not only is FDS feasible to work with but surprisingly fast. That would be the case if the dimensions of the matrices were similar, which they are not. Each 3D cell in FDS has a 256D basis list associated with it which is far larger than is usually the case in FE. This swings the advantage speed-wise back to FE. At the same time, even though the matrices are large they are very easy to work with. If we had needed to say invert many 256D general matrices it would have made things practically impossible.

6.7 Conclusions

The Whitney map projects onto a finite dimensional space. Looking at this we can see why the wedge in GD is non-associative (see Sec. 6.2). We can avoid this problem by extending the function space but this results in losing the topology.

This is quite similar to FE in that we have many regions, with finite dimensional

spaces in each. FE though is based on a variational principle and the existence of its solutions are shown with a different set of results (see Appendix B).

We have yet to determine how boundary conditions are handled, though this will be done when the method is implemented in future work. We should be able to treat this in the same way as it is done in standard FE.

Finally, we note that our basic objects are differential forms. This means that we can represent Clifford algebras and Grassman variables which is not the case in FE. Otherwise FDS is just a numerical technique to solve differential equations akin to FE.

Chapter 7

Scalar field theory

We have in scalar field theory that

$$S = \int \partial_\mu \phi \partial^\mu \phi + \frac{1}{2} m \phi^2 \quad (7.1)$$

$$= \int [d\phi \wedge *d\phi] + [\frac{1}{2} m \phi \wedge *\phi] \quad (7.2)$$

$$= (d\phi, d\phi) + \frac{1}{2} m(\phi, \phi), \quad (7.3)$$

since we have $dW = Wd$ and $dR = Rd$ we need only look at the second term since the first one follows.

To begin with we need a complex which we take as being cubic without boundary. We know that the discrete analogue of p -forms are p -cochains so we have objects of the form

$$M_{i,j} = \int W(\sigma_i) \wedge *W(\sigma_j), \quad (7.4)$$

where σ_i and σ_j are p -cochains. Our discrete analogue of $(\cdot, \cdot)$ is then

$$\int \phi \wedge *\phi = \int W[A\phi] \wedge *W[A\phi] \quad (7.5)$$

$$= \int \sum_i a_i W[\sigma_i] \wedge * \sum_j a_j W[\sigma_j] \quad (7.6)$$

$$= \sum_{i,j} a_i a_j M_{i,j}. \quad (7.7)$$

The field is a 0-form, so the discrete analogy is defined on the vertices. We have two factors that contribute to M :

$$X = \int \frac{1}{a^2} x^2 dx = \frac{a}{3} \quad (7.8)$$

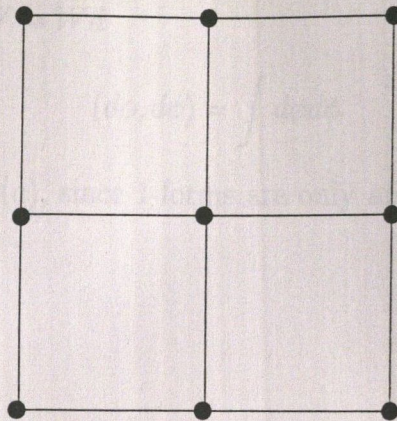


Figure 7-1: Neighbours of a vertex in a cubic complex

and

$$Y = \int \frac{1}{a^2} (a - x) x dx = \frac{1}{a^2} \int (ax - \frac{x^2}{2}) = \frac{a}{6}. \quad (7.9)$$

From Fig. 7-1 we can see we have 3 types of terms in M .

1. XX which come from a vertex interacting with itself.
2. XY which comes from a vertex interacting with a vertex which is directly above, below, to the left or to the right of it.
3. YY which comes from a vertex interacting with a vertex which is diagonally positions: top right, top left, bottom left or bottom right.

This leads to

$$M_{i,j} = XX\delta_{i,j} + 2XY[\delta_{i+\hat{x},j} + \delta_{i+\hat{y},j}] + YY\delta_{i+\hat{x}+\hat{y},j} \quad (7.10)$$

$$\int M_{ij} f(i) f(j) = \left(\frac{a^2}{9} + \frac{4a^2}{18} + \frac{4a^2}{36} + O(a^2) \right) f_i^2 = f(i)^2 \frac{4a^2}{9} + O(a^2), \quad (7.11)$$

where $i + \hat{x}$ refers to the vertex which is above or below vertex i . We then absorb the $\frac{4}{9}$ factor into our definition of $(\cdot, \cdot)_K$ for 0-cochains.

We have Taylor expanded terms like $f(i + \delta)$ and $f(i - \delta)$ to get $2f(i) + O(a^2)$.

$$\sum M_{i,j} f(i) f(j) = \sum_{i=1}^{N^2} a^2 f(i)^2 + O(a^2), \quad (7.12)$$

which clearly converges to the expected continuum result

$$(\phi, \phi) = \int \phi^2.$$

Since $dR = Rd$ and $dW = Wd$

$$(d\phi, d\phi) = \int d\phi d\phi$$

follows, though only to $O(a)$, since 1-forms are only approximated to this accuracy in GD.

Chapter 8

The Dirac-Kähler Equation

8.1 The Dirac equation

Dirac noted that the non-relativistic Schrödinger equation did not have negative probabilities since it was linear in time, while the Klein-Gordon, being quadratic, did. So he tried to find a wave equation that was linear in time but still retained the mass shell constraint.

$$\gamma_\mu p^\mu = \delta \quad \gamma^2 = -1 \quad \gamma^0 = \gamma^3$$

He took the first order equation (assuming the square root of the Klein-Gordon)

$$\frac{\partial \psi}{\partial t} = -i(\alpha \cdot \nabla + \beta m)\psi$$

where α_i and β are constant matrices acting on ψ . We want to get the mass shell condition by squaring the operator in front of ψ :

$$\frac{\partial^2 \psi}{\partial t^2} = (-i(\alpha \cdot \nabla + \beta m))^2 \psi$$

$$= (-\nabla^2 + m^2)\psi$$

This implies that we must have

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

$$\{\alpha_i, \beta\} = 0$$

$$\alpha_i^2 = \beta^2 = 1$$

We can define $\gamma^0 = \beta$ and $\gamma^i = i\alpha_i$. Multiplying both sides by γ^0 we get the Dirac equation (DE):

$$(\gamma^\mu \partial_\mu + m)\psi = 0$$

Chapter 8

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8.1 The Dirac equation

Dirac noted that the non-relativistic Schrödinger equation did not have negative probabilities since it was linear in time, while the Klein-Gordon, being quadratic, did. So he tried to find a wave equation that was linear in time but still satisfied the mass-shell constraint:

$$p_\mu p^\mu = E^2 - \vec{p} \cdot \vec{p} = m^2. \quad (8.1)$$

He took the first-order equation (involving the square root of the Laplacian):

$$i \frac{\partial \psi}{\partial t} = (-\alpha_i \nabla^i + \beta m) \psi, \quad (8.2)$$

where α_i and β are constant matrices acting on ψ . We want to get the mass-shell condition by squaring the operator in front of ψ :

$$-\frac{\partial^2}{\partial t^2} \psi = (-i\alpha \cdot \nabla + \beta m)^2 \psi \quad (8.3)$$

$$= (-\nabla^2 + m^2) \psi. \quad (8.4)$$

This means that we must have:

$$\{\alpha_i, \alpha_k\} = 2\delta_{ik}, \quad (8.5)$$

$$\{\alpha_i, \beta\} = 0, \quad (8.6)$$

$$\alpha_i^2 = \beta^2 = 1. \quad (8.7)$$

We can define $\gamma^0 = \beta$ and $\gamma^i = \alpha^i$. Multiplying Eqn.8.3 by β we get the Dirac equation (DE):

$$(i\gamma^\mu \partial_\mu - m)\psi = 0, \quad (8.8)$$

where

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \quad (8.9)$$

8.2 The Dirac-Kähler equation

The Dirac equation involved determining the square root of the Laplacian. In differential geometric terms this is simply

$$d - \delta. \quad (8.10)$$

This leads to the Dirac-Kähler equation (DKE)

$$(d - \delta + m)\phi = 0, \quad (8.11)$$

where the Dirac field is an inhomogeneous differential form. For example in 2D we have

$$\phi = \psi(x) + \psi_\mu(x)dx^\mu + \frac{1}{2!}\psi_{\mu\nu}(x)dx^\mu \wedge dx^\nu. \quad (8.12)$$

Following Becher and Joos (BJ) [31] we have that

$$d\phi = dx^\mu \wedge \partial_\mu \phi. \quad (8.13)$$

In a similar manner we can define the Clifford product $\vee$ to get

$$(d - \delta)\phi = dx^\mu \vee \partial_\mu \phi. \quad (8.14)$$

This product of forms, which is distributive and associative, is defined as:

$$1 \vee 1 = 1 \quad 1 \vee dx^\mu = dx^\mu \vee 1 = dx^\mu \quad (8.15)$$

$$dx^\mu \vee dx^\nu = g^{\mu\nu} \cdot 1 + dx^\mu \wedge dx^\nu. \quad (8.16)$$

These relations are those of the γ matrices:

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}. \quad (8.17)$$

So $dx^\mu \vee$ in 4D defines a representation of the algebra of γ -matrices in the 16D space of complex differential forms. Now, all representations of the complex Clifford algebra of 4D Euclidean space can be decomposed into 4D irreducibles, equivalent to those

generated by the γ -matrices, so we can decompose the space of differential forms into 4D invariant subspaces [48] on which, the DKE implies the Dirac equation

$$(d - \delta + m)\phi = (dx^\mu \vee \partial_\mu + m)\phi = 0 \quad (8.18)$$

$$= (\gamma^\mu \partial_\mu + m)\Psi = 0, \quad (8.19)$$

where Ψ belongs to one of the invariant subspaces.

We would like to actually be able to compute with these differential form fields and separate them into the four subspaces which we know they can be split into. This can be done using techniques from representation theory [49] where we introduce a new basis with the property

$$dx^\alpha \vee (Z_{ab}) = \left(\sum_c (\gamma^{\alpha T})_{ac} Z_{cb} \right) \equiv \gamma^{\alpha T} Z. \quad (8.20)$$

This allows the decomposition of the Clifford algebra, which the Dirac fields are a representation of, into subspaces as desired.

The Dirac field in this new basis is given by

$$\begin{aligned} Z = & 1 + \gamma_\mu^T dx^\mu + \frac{1}{2!} \gamma_\mu^T \gamma_\nu^T dx^\mu \wedge dx^\nu + \frac{1}{3!} \gamma_\mu^T \gamma_\nu^T \gamma_\rho^T dx^\mu \wedge dx^\nu \wedge dx^\rho \\ & + \frac{1}{4!} \gamma_\mu^T \gamma_\nu^T \gamma_\rho^T \gamma_\sigma^T dx^\mu \wedge dx^\nu \wedge dx^\rho \wedge dx^\sigma. \end{aligned} \quad (8.21)$$

This can be inverted to give the dx 's in terms of the Z 's so that we can say

$$\Phi = \sum_H \phi(x, H) dx^H = \sum_{a,b} \psi_a^{(b)}(x) Z_{ab} \quad (8.22)$$

or

$$\Phi^{(b)} = \sum_a \psi_a^{(b)}(x) Z_{ab} \in \mathcal{D}^b, \quad (8.23)$$

with b fixed. The dx^H here is just a sum over the various differential forms which is used by BJ. Then DKE for Φ implies DE for $\psi^{(b)}(x)$ which is an explicit representation of Eqn.8.18.

BJ create a projection operator to separate the various solutions using right $\vee$ -multiplication. Using this they have a subsidiary condition, that a projection operator maps the field back to itself, which used in conjunction with the Dirac-Kähler equation is equivalent to the Dirac equation.

Continuum	Discrete
dx^p	σ^p
d	d_K
δ	δ_K
$x \wedge y$	$x_K \cup y_K$

Table 8.1:

With the DKE, we now have a formulation of the DE based on differential geometry, which we can deal with computationally. We look at 3 approaches. The first is that followed by BJ themselves, which is similar to our GD work in many ways since they see cochains as the discrete analogue of differential forms. Then we have GD where we have the Whitney and de Rham map allowing us to map to and from the continuum. Finally we have FDS, where we live in the continuum and not the complex, which is ideally suited for Dirac-Kähler.

8.2.1 Becher and Joos

We can work on a discrete form of this theory using cochains on complexes instead of forms on manifolds, which was done by BJ. They used the following correspondences:

This (see Table 8.1) is quite similar to what we use in GD, although they use the cup product as their wedge. This is associative but not anti-symmetric. The DKE calculation above can be reproduced using this scheme but we have no projection operator to select one subspace from the four leaving us with a degenerate theory; the Susskind method [4, 28, 29] in fact . This is due to the non-locality of the discrete Clifford product. BJ show that, in the continuum limit, this leads to the continuum result.

8.2.2 Geometric Discretisation

This is very similar to what BJ did and so has the same problem. We do have a different $*$ and wedge and can define a different Clifford product but it would be non-local too.

8.2.3 Finite Dimensional Subspaces

We can use FDS instead of GD since then we simply have continuum functions on which we use the continuum operators. That being the case we can simply use the continuum projection operator to pick out the subspaces and no longer suffer from degeneracy. That is for nonconformal FDS where we have the algebra but not the topology.

Recall that in cubic FDS we have the same forms as in the continuum theory (see Sec. 6.2). By this we mean that $f dx$ is mapped to $F dx$ where F is an approximation of the continuum function f BUT the dx part is the same. That being the case the whole DK analysis carries through since all our operations are defined on the “form” part. We can use the same change of basis list, the same Clifford product and projection operator since the only difference in our theory is that we have $F dx$ instead of $f dx$ with F converging to f as we refine the triangulation.

Nonconformal FDS does not capture topology though which can be a source of spectral degeneracy as shown by Rabin [5]. We take a brief look at his work next.

8.3 Topology and doubling

In [5], Rabin points out that the essential problem in dealing with chirality in a discrete theory is related to $*$. We need to have

$$** = I \tag{8.24}$$

$$\delta = *d*, \tag{8.25}$$

which was not available to him, but we have this in GD.

He points out two sources of degeneracy. One is from discretising without respecting the geometry of the problem. If we use a symmetric difference for our discrete Laplacian we inevitably introduce degeneracy since the topology is distorted. This is not only the case for the Dirac equation but even for the Klein-Gordon equation where we know there is no degeneracy problem. This is related to the harmonic forms, which are forms which are mapped to zero by the Laplacian. There is one harmonic form in each homology class ; apart from linear combinations of these. From this

we can show that no doubling can occur for topological reasons. Therefore spectrum degeneracy is forbidden.

When dealing with the Dirac equation, we need to use the Dirac-Kähler formulation. Here though the antisymmetric derivatives do not lead to 4 copies of the Dirac equation but into 4 decoupled Dirac spinors. Note we have no spectrum degeneracy due to the topological reasons mentioned above but degeneracy of a different kind.

In this formalism chiral symmetry corresponds, upto sign, to $*$:

$$\psi \rightarrow \gamma^5 \psi \iff \omega^{(4-p)} \rightarrow \pm *_K \omega^{(p)}. \quad (8.26)$$

The Dirac equation is then invariant under the continuous chiral symmetry

$$\omega^{(4-p)} \rightarrow \omega^{(4-p)} \pm i\epsilon *_K \omega^{(p)}. \quad (8.27)$$

This makes no sense in the traditional discrete setting since $*_K \omega^{(p)}$ is defined on the dual space. In GD though we can imagine both the dual space and the original space being in the subdivided space. He also notes that “In a real sense both the spectrum and chiral problems are due to the existence of the dual lattice and the consequent difference in properties of $*$ and $\star$ ¹”. Fermion doubling is thus intimately related to the discrete Hodge star. We should either be able to represent fermions without doubling or pin point why a problem arises.

Note the SLAC derivative [50] can also be understood within the Rabin analysis. There, even though a symmetric difference is used, the extra “harmonic” functions associated do not correspond to particles in the continuum limit.

Other attempts have also been made to work with fermions. Some even using FE methods [51, 52, 53, 54, 55], though very different in style to what we have done. There they developed a scheme which manages to capture the canonical commutation² relations though with problems regarding locality. Work has also been done involving non-commutative geometry [56, 57, 58, 59, 60] which is similar in that this provides a discrete differential geometry too but in a fundamentally different way. This does not appear to suffer from any problem, though it has yet to be computationally implemented.

¹The discrete star.

²See Sec. B.2 for a more detailed description of this.

8.4 Fermion Doubling

If we put scalars on the lattice we can make the substitution

$$\partial_\mu \phi \rightarrow \frac{1}{a}(\phi_{n+\hat{\mu}} - \phi_n). \quad (8.28)$$

We can then calculate the propagator to find

$$k^2 + m^2 \rightarrow m^2 + \sum_\mu \frac{4}{a^2} \sin^2(ak_\mu/2). \quad (8.29)$$

In the limit as $a \rightarrow 0$ we find that the two expressions are identical, for small k . They do differ for large k , but large k values are cut-off by being placed on the lattice.

If we try to do the same for fermions though we find

$$k^2 + m^2 \rightarrow \frac{1}{a^2} \sin^2 ak_\mu + m^2. \quad (8.30)$$

Unfortunately this has bad behaviour as we take the continuum limit. As before we have a minimum at $k = 0$, but we now also have a minimum located at $k = \pm\pi/a$. Therefore we have an unphysical doubling problem for each space-time dimension.

This can be avoided by adding the following Wilson term to our discrete action

$$\frac{1}{2a} \bar{\psi}_n (\psi_{n+\hat{\mu}} + \psi_{n-\hat{\mu}} - 2\psi_n). \quad (8.31)$$

This preserves the minimum at $k = 0$ and eliminates the unwanted ones, but at a cost.

On the lattice, chiral symmetry is exact for massless fermions. This means that there can be no anomaly. Fermion doubling is the price we pay for the absence of the anomaly. If we calculate the the chiralities of the two types of fermions we find that they are opposite and hence produce no anomaly. The fermions doubling problem is thus deeply connected with the problem of chiral symmetry breaking on the lattice. For example, adding the Wilson correction term violates chiral symmetry.

This inability to avoid degeneracy, whilst capturing chiral symmetry, on the lattice is known as the fermion doubling problem and led to the Nielsen-Ninomiya [61, 62] no-go theorem³ which states that it is not possible to solve the problem of Dirac

³there are other related no-go theorems including Karsten and Smit [63, 64], for example, though Nielsen-Ninomiya is more general.

fermion degeneracy on a lattice in a chirally invariant way for a general class of fermion theories.

This constraint has been circumvented by slightly generalising it, so that we replace the chiral symmetry condition γ_5 commutes with D , the lattice Dirac operator, with

$$\gamma_5 D + D \gamma_5 = a D \gamma_5 D, \quad (8.32)$$

which was done by Ginsparg and Wilson [68].

This can be traced back to Callan and Harvey [65] and to two subsequent papers. One by Kaplan [66] and the other by Frolov and Slavnov [67]. Based on these papers a generalised way to realize chiral symmetry on the lattice was devised known as the “overlap”.

Once this was completed it was realized that this could have been arrived at starting from an older work of Ginsparg and Wilson [68]. See [69] and [70] for a review of these developments [71]-[89]. Note that the overlap operator is a special case of Ginsparg-Wilson.

An alternative, and mathematically equivalent version exists, known as the domain wall formulation, which has the advantage that its local action has the same form as traditional lattice work which means that tested numerical methods can be applied.

This means that the fermion doubling problem has effectively been resolved with the main difficulty being computational cost since Ginsparg-Wilson involves of the order of 100 times more work.

8.5 Conclusions

We attempted to discretise fermions without doubling using the Dirac-Kähler approach but were unable to do so. This is because using GD we suffer from the same problem as previous attempts using discrete Dirac-Kähler, the lack of a discrete projection operator. Using FDS this is not a problem, but since we lose topology we suffer from doubling too. We know this from Rabin’s work which suggests that our discrete Hodge star operator is good enough to capture chirality and avoid degeneracy of the standard kinds. Further investigation is needed to see whether doubling arises due to having the original and dual space, or not, which is our main topic of

current research.

The advantage of our approach is naturality. We have a discretisation scheme which captures mathematical structure more richly. As a result we aim to be able to reproduce continuum theory in our discrete one. Since we have topology we know we cannot have spectral degeneracy. Since we have a discrete $*$ we know we can represent chiral symmetry. If we are able to do this without doubling, and we do not know whether we can or not yet, then we would be dealing with fermions on the lattice with a generic structure. It would work because it captures the continuum structures sufficiently well that the theory could be transferred to the discretisation without serious difficulties.

We began with geometric ideas, linking $\mathbb{R}^4$ to $\mathbb{C}P^1$ via the Hopf fibration and wedge product, which we then generalised to $\mathbb{R}^n$ via the $\mathbb{R}^n$ to $\mathbb{C}P^{n/2}$ fibration. This is a topological invariant and we used it to develop a correspondence between objects and operators on a type III_1 von Neumann algebra. We arrived at a natural invariant in this space and we have now further refined the invariant.

Our initial objectives were to:

1. See whether we could show a relationship with Witten's index
2. Incorporate statistics
3. Develop a new discretisation scheme with no other operators to be introduced as well as the fermion physics using the boson we defined from our work
4. Look at how the method developed would deal with fermions on the lattice

We made considerable progress in all of these.

Now that our approach has been laid out on $\mathbb{C}P^1$ primarily, before looking at other areas, since we felt that we needed to develop the foundations of the theory further before we could have anything concrete to say in other areas. Now $\mathbb{C}P^1$ is sufficiently mature that we are aware of what the theory is, that we have a fully developed picture of what we should be able to translate continuum theory to, e.g. to physics and that should be effortless, while the discrete structure is supposed to capture all the continuum physics which we require. For example, when working with fermions, since we have a discrete Hilbert space we can capture chiral symmetry automatically. Of

Chapter 9

Conclusions

We began with geometric discretisation (GD), with its discrete Hodge star and wedge product, which we had previously used to compute the Ray-Singer torsion [27], a topological invariant on 3-manifolds. The idea being to develop a correspondence between objects and operations on a complex and a manifold. We set out to continue in this spirit and see how much further we could go.

Our initial objectives were to:

1. See whether we could develop a variation of the Whitney map.
2. Incorporate metric.
3. Develop a new discretisation scheme with potential applications to engineering as well as theoretical physics using the insights we gained from our work.
4. Look at how the method developed would deal with fermions on the lattice.

We made considerable progress in all of these.

Note that our approach has been to develop GD primarily, before looking at other areas, since we felt that we needed to develop the foundations of the theory further before we could have anything concrete to say in other areas. Now GD is sufficiently mature that we are aware of what the issues are. Once we have it fully developed we should be able to translate continuum theory to it by analogy and this should be effortless, since the discrete structure is supposed to capture all the continuum ones which we require. For example, when working with fermions, since we have a discrete Hodge star, we can capture chirality without degeneracy automatically. Of

course in this case we have yet to demonstrate that no doubling occurs, but it is also interesting to isolate why if it does?

GD captures the properties of operators as well as just the basic continuum objects. As a result we have many constraints on our system. This means that we have little freedom to change any one part since to do so would change other parts too. For example we would like to have an associative wedge, we can do so by redefining it by adding a factor, but if we do this then we lose the Leibniz rule property which we would also like (see Sec. 4.4). This is the beauty of the approach since we are unable to brush a problem under the carpet.

We begin by looking at how we have dealt with our initial objectives before considering our current status.

9.1 Whitney

We did not know whether it was possible to create a new Whitney map and made several attempts at doing so, with little success. We then developed a new notation for the cubic case using which it quite naturally emerged. We showed that this cubic formulation had all the desired properties. Since the dual space of a cubic lattice is also cubic this meant that we also had a dual Whitney map too which was not the case before. We still do not have a systematic method to develop Whitney maps on say hexagons or other objects of interest and do not even know whether that is possible but the cubic case was number one on our list (See Chap. 4).

9.2 Metric

Initially we noted that GD approximates things by taking averages. The de Rham map integrates continuum things over the associated discrete space and the Whitney map divides by a volume factor, and hence the average. When $*$ is taken though the discrete space we are working with is changed and so W divides by the wrong volume. In order to correct this we can put in a correction term by hand using which we can show that $*$ converges to the continuum limit as well as δ and the Laplacian.

This is unsatisfactory though since there is a relationship between the inner prod-

uct and $*$. If we put in terms by hand then this is no longer that case. As a result we made a natural modification to our inner product and looked at what effect this had on the discrete Hodge (See Chap. 5).

We had some difficulties with this in the simplicial case but in the cubic case we could compute things by hand and show that we ended up with exactly the volume factors which we had previously put in by hand. As a result we could show that everything converged to their continuum counterparts as desired.

9.3 New discretisation schemes

When computing the discrete Hodge star, associated with our new inner product we needed to develop computational methods in order to perform the many calculations needed. Doing so we noted that the Whitney map, mapped onto a finite dimensional space and began to look more closely at it. We could think of this finite dimensional space as our discretisation instead of our complex and we could use our continuum operations on it. We could then express our theories within this space with the benefit, for example, of having an associative wedge, at the cost of topology (See Chap. 6).

We made some comparisons with the finite element method which is a variational formulation as opposed to an analogue method, which we use.

Since this scheme is a discrete differential geometry of sorts our basic objects are differential forms which can be used to represent Clifford algebras and Grassman variables.

9.4 Fermions on the lattice

GD suffers from the same problems as Becher and Joos when implementing Dirac-Kähler fermions, in that we are unable to construct a discrete projection operator to separate the mixed copies of the Dirac equation which we have. FDS does not suffer from this problem, but since we lose topology in nonconformal FDS we might have a degenerate spectrum (see Sec. 8.3). If we use conformal FDS though, we have a projection operator and the topology is captured so the situation is not so clear.

Doubling might occur due to having two lattices, the original and the dual. Note that in comparison Becher and Joos only have a single doubling if continuous time is used.

9.5 Future work

We have developed geometric discretisation further, as planned, but we have only began applying it to our areas of interest. From Rabin [5] it appears that we should be able to work with fermions without doubling unless we get a mixed solution on the original and dual lattice which we are unable to deal with properly. This needs to be investigated further.

FDS is a natural evolution of GD. From the FDS perspective it is clear why the wedge in GD is non-associative since GD is restricted to linear functions and when we wedge linear functions we do not get another linear function (see Sec. 6.2). FDS is also close to FE and formulating differential equations can easily be done. It requires further development to sort out how boundary conditions should be handled, for example, but this should not be a problem since it is very similar to FE in this regard.

GD is still restricted to only being able to deal with Abelian theory. This is a non-trivial problem which needs a key idea in order to be resolved. As things stand it is very hard to see how this could be done.

Now that we have incorporated metric into GD, we can consider applying it to gravity problems and look at the relationship with Regge calculus [90, 91, 92, 93], which, as with FE, has similarities.

The main questions which we now face then are:

1. Do we suffer from degeneracy in the Rabin approach? At worst we suffer from a single doubling due to a mixed solution on the original and dual lattice, but at best we have none.
2. What the relative computational costs are for problems using FDS and FE? FDS needs little development for application. More detailed comparisons with FE need to be made.

3. Can GD deal with Non-Abelian theory? This is something we have not yet looked at but something that would expand that applicability of GD enormously.
4. With metric incorporated into GD, applications to gravity problems can now be considered.

Appendix A

Discrete Operator Approximations

A.1 Algebraic Topology

We have already discussed the similarities between the discrete structures from algebraic topology and the continuous structures from geometry in Sec. 3.5. The two have been and still are more similar than different. We will restrict ourselves to looking at the problem of defining a discrete wedge and edge structure as well as what the wedge operation is.

A.1.1 The Discrete Wedge

In the continuous we can wedge a p -form α to a q -form β to make a $(p+q)$ -form. We begin with a list of properties which this product has so that we have something to compare our discrete theory's definition with. Let α^p denote a p -form.

1. $\alpha^p \wedge \alpha^p = 0$, antisymmetry
2. $\alpha^p \wedge \beta^q = (-1)^{pq} \beta^q \wedge \alpha^p$, anticommutativity
3. $(d\alpha^p) \wedge \beta^q = d(\alpha^p \wedge \beta^q) - \alpha^p \wedge d\beta^q$, Leibniz rule
4. $(\alpha^p \wedge \beta^q) \wedge \gamma^r = \alpha^p \wedge (\beta^q \wedge \gamma^r)$, associativity

In GD we have the first three of these but not associativity. We next look at the discrete discrete wedge, the exterior or cup product.

If an oriented complex has vertices $v_1, \dots, v_n$ and $v_1 < v_2 < \dots < v_n$ it is implied that $v_1 < v_2 < \dots < v_n$ is the ordering. The cup product is defined on vertices

ω^p and ω^q as follows:

$$\omega^p \wedge \omega^q = \omega^{p+q}, \quad \omega^p \wedge \omega^q = (-1)^p \omega^q \wedge \omega^p, \quad d(\omega^p \wedge \omega^q) = (d\omega^p) \wedge \omega^q + (-1)^p \omega^p \wedge (d\omega^q),$$

It satisfies the following properties:

Appendix A

Discrete Operator Approximations

A.1 Algebraic Topology

We have already discussed the similarities between the discrete structures from algebraic topology and the continuum ones in differential geometry in Sec. 3.5.2. There have been and still are many attempts to build on this interplay. We will restrict ourselves to looking at the problem of finding a discrete wedge and Hodge star as well as what the goal of this effort is.

A.1.1 The Discrete Wedge

In the continuum we can wedge a p form with a q form to obtain a $(p+q)$ form. We begin with a list of properties which this product has so that we have something to compare our prospective discrete candidates with. Let ω^p denote a p -form.

1. $\omega^p \wedge \omega^q = \omega^{p+q}$, basic property.
2. $\omega^p \wedge \omega^q = (-1)^p \omega^q \wedge \omega^p$, antisymmetry.
3. $d(\omega^p \wedge \omega^q) = (d\omega^p) \wedge \omega^q + (-1)^p \omega^p \wedge (d\omega^q)$, Leibniz rule.
4. $(\omega^p \wedge \omega^q) \wedge \omega^r = \omega^p \wedge (\omega^q \wedge \omega^r)$, associativity.

In GD we have the first three of these but not associativity. We next look at the classic discrete wedge, the cohomology or cup product.

In an oriented complex the vertices when we write $\sigma^p = \langle v_0, \dots, v_p \rangle$ it is implied that $v_0 < v_1 < \dots < v_p$ in that ordering. The cup product $\cup$ is defined on cochains

c^p and c^q as follows

$$c^p \cup c^q (< v_0, v_1, \dots, v_{p+q} >) = c^p (< v_0, v_1, \dots, v_p >) \cdot c^q (< v_p, v_{p+1}, \dots, v_{p+q} >). \quad (\text{A.1})$$

It satisfies the following properties:

1. $c^p \cup c^q$ is a bilinear function.
2. $c^p \cup c^q = c^{p+q}$.
3. $(c^p \cup c^q) \cup c^r = c^p \cup (c^q \cup c^r)$.
4. $\delta(c^p \cup c^q) = \delta c^p \cup c^q + (-1)^p c^p \cup \delta c^q$.

Note that in contrast to the wedge product on forms, this is not anti-symmetric.

The cup product on cochains was defined in terms of a particular ordering of the vertices of the complex. We can though induce a cup product on cohomology classes which is independent of ordering and hence the cohomology ring is well defined (See [39] p308 for details of the proof which involves showing that two cohomology rings associated with different orderings are in fact isomorphic which means that they must be independent of the ordering). Using this we have

$$a^p \cup b^q = (-1)^{pq} b^q \cup a^p, \quad (\text{A.2})$$

and obtain a ring which is not quite commutative as we can see from Eq. (A.2) above which is known as the Grassman property; note that in GD the wedge product has this property (Sec. 4.4) on cochains and not just cohomology classes.

We can see why this is the case by considering two cup products, $\cup$ and $\cup'$, which are associated with oppositely oriented vertices. Let $\sigma^{p+q} = < v_0, \dots, v_{p+q} >$ be a $(p+q)$ -simplex in the first ordering. For the second we write, $< v_{p+q}, \dots, v_0 >'$, the prime being used merely to denote that the simplex is ordered in the opposite of the given ordering. By definition we have

$$z^q \cup' z^p (< v_{p+q}, \dots, v_0 >') = z^q (< v_{p+q}, \dots, v_p >') \cdot z^p (< v_p, \dots, v_0 >'). \quad (\text{A.3})$$

We also know that

$$< v_{p+q}, \dots, v_0 >' = (-1)^{\frac{1}{2}(p+q)(p+q+1)} < v_0, \dots, v_{p+q} > \quad (\text{A.4})$$

since it will take exactly $\frac{1}{2}(p+q)(p+q+1)$ interchanges of the $p+q$ vertices to reverse their order. Similarly

$$\langle v_{p+q}, \dots, v_p \rangle' = (-1)^{\frac{1}{2}(q)(q+1)} \langle v_p, \dots, v_{p+q} \rangle \quad (\text{A.5})$$

and

$$\langle v_p, \dots, v_0 \rangle' = (-1)^{\frac{1}{2}(p)(p+1)} \langle v_0, \dots, v_p \rangle \quad (\text{A.6})$$

Hence we may simply compute the result. First

$$z^q \cup' z^p (\langle v_{p+q}, \dots, v_0 \rangle') = (-1)^{\frac{1}{2}(p+q)(p+q+1)} z^q \cup' z^p (\langle v_0, \dots, v_{p+q} \rangle), \quad (\text{A.7})$$

$$z^q (\langle v_{p+q}, \dots, v_p \rangle') = (-1)^{\frac{1}{2}(q)(q+1)} z^q (\langle v_p, \dots, v_{p+q} \rangle), \quad (\text{A.8})$$

and

$$z^p (\langle v_p, \dots, v_0 \rangle') = (-1)^{\frac{1}{2}(p)(p+1)} z^p (\langle v_0, \dots, v_p \rangle), \quad (\text{A.9})$$

This implies that

$$(-1)^{\frac{1}{2}(p+q)(p+q+1)} z^q \cup' z^p (\langle v_0, \dots, v_{p+q} \rangle) = (-1)^{\frac{1}{2}(q)(q+1)} z^q (\langle v_p, \dots, v_{p+q} \rangle) \cdot \quad (\text{A.10})$$

$$(-1)^{\frac{1}{2}(p)(p+1)} z^p (\langle v_0, \dots, v_p \rangle), \quad (\text{A.11})$$

or

$$z^q \cup' z^p (\langle v_0, \dots, v_{p+q} \rangle) = (-1)^{pq} z^q (\langle v_p, \dots, v_{p+q} \rangle) \cdot z^p (\langle v_0, \dots, v_p \rangle), \quad (\text{A.12})$$

and, using the commutativity of the coefficient ring R , we next find that

$$z^q \cup' z^p (\langle v_0, \dots, v_{p+q} \rangle) = (-1)^{pq} z^q (\langle v_0, \dots, v_p \rangle) \cdot z^p (\langle v_p, \dots, v_{p+q} \rangle), \quad (\text{A.13})$$

Finally, since $z^q \cup z^p$ is the same as $z^q \cup' z^p$ for cohomology classes, since the cup product is independent of ordering and therefore $\cup$ and $\cup'$ are the same, we have

$$z^q \cup z^p \approx z^q \cup' z^p = (-1)^{pq} z^p \cup z^q. \quad (\text{A.14})$$

This then implies that, for cohomology classes,

$$[z^q \cup z^p] = (-1)^{pq} [z^p \cup z^q], \quad (\text{A.15})$$

and the Grassman property of the cohomology ring is established, as required.

We next consider a variant of the cup product known as the star product [94] which is somewhat closer to what we use in GD in that they are both an antisymmetrisation¹ of the usual cup product.

Let P denote one of the $(p+q+1)!$ permutations of a set of vertices $\{v_0, v_1, \dots, v_{p+q}\}$ which span some $(p+q)$ -simplex and Pv_i be the value of that permutation on v_i . We define $\star : C^p(K) \times C^q(K) \rightarrow C^{p+q}(K)$ by

$$\langle c^p \star c^q, [v_0, v_1, \dots, v_{p+q}] \rangle = \frac{1}{(p+q+1)!} \sum_p (-1)^{|p|} \quad (\text{A.16})$$

$$\times \langle c^p, [Pv_0, \dots, Pv_p] \rangle \cdot \langle c^q, [Pv_{p+1}, \dots, Pv_{p+q}] \rangle, \quad (\text{A.17})$$

when the order $v_0, v_1, \dots, v_{p+q}$ is in the equivalence class of the orientations of the simplices $[v_0, v_1, \dots, v_{p+q}]$ and where the sum is over all permutations of the vertices.

The number of independent terms in this sum is given by the number of ways we can partition the set of vertices into two parts which contain one vertex in common.

In other words

$$\frac{(p+q+1)!}{p!q!}. \quad (\text{A.18})$$

Note that we are explicitly dividing by integers in the normalisation which means that we can only deal with coefficient rings which include rational numbers and so we do not have the same generality as we had with the cup product.

This product is graded commutative in that we have

$$c^p \star c^q = (-1)^{pq} c^q \star c^p \quad (\text{A.19})$$

and also captures the derivation property

$$\delta(c^p \star c^q) = (\delta c^p) \star c^q + (-1)^p c^p \star (\delta c^q) \quad (\text{A.20})$$

but, as in GD, is non-associative.

A.1.2 The Discrete Hodge Star

A discrete analogue of the Hodge star can be developed via some dual lattice [5] aside from what we have done in GD, where the metric becomes an issue.

¹This is also the case in [95].

The problem is that we need a $\star$ with

$$\delta = \star d \star \quad (\text{A.21})$$

and

$$\star \star = 1. \quad (\text{A.22})$$

Attempts to develop a discrete Hodge star are usually of the following kind:

1. Given the value of $\star \omega^p$ on a $(4-p)$ -cell $\star C_{4-p}$ of the dual lattice let $\star \omega^p$ take the same value on the $(4-p)$ cell on the original lattice reached from $\star C_{4-p}$ by translation of $\frac{1}{2}$ in all lattice directions. This is unsatisfactory though because $\star \star$ leads to a translation of $+1$ in all lattice directions and $\delta \neq \star d \star$.
2. Given the value of $\star \omega^p$ on a $(4-p)$ -cell $\star C_{4-p}$ of the dual lattice let $\star \omega^p$ take the same value on the $(4-p)$ -cell of the original lattice. This obeys $\star \star = 1$ but not $\delta = \star d \star$. All similar attempts fail as well.

The problem with a discrete $\star$ is related to the existence of the dual lattice and its relationship to the original lattice which is at the heart of GD.

Topological field theories have produced many exact [96, 97, 98, 99], non-perturbative, results and can be considered as natural testing grounds for computational techniques which are applied to conventional theories. In order to do so it is vital to have suitable discrete formulations on arbitrary manifolds with effective treatment of fundamental continuum operations such as the wedge product and the Hodge star operator.

A.2 Dodziuk

Dodziuk [32] worked with a complex and used both the Whitney and the de Rham map, as we do in GD, as well as the inner product

$$(x, y) = \int W(x) \wedge \star W(y) \quad (\text{A.23})$$

which we used to incorporate metric. He did not however have a dual space and a discrete wedge or $\star$.

He showed that WRf converged to f and that the Hodge decomposition theorem which states that a form can be written as the sum of an exact, coexact and harmonic

pieces is faithfully translated, meaning that the exact piece is mapped to an exact piece, the coexact to a coexact and the harmonic to a harmonic. He also showed that the eigenvalues of the Laplacian acting on functions and 1-forms converged to their continuum values. We'll focus on his central result which is the Hodge decomposition theorem.

Let $\sigma = [p_0, p_1, \dots, p_m]$ be an m -simplex in $\mathbb{R}^k$, $k \geq m$. The vertices of $S\sigma$, the standard subdivision of σ are the points

$$p_{ij} = \frac{1}{2}(p_i + p_j), \quad i \leq j. \quad (\text{A.24})$$

We define partial ordering of the vertices of $S\sigma$ by setting

$$p_{ij} \leq p_{kl} \text{ if } i \geq k \text{ and } j \leq l. \quad (\text{A.25})$$

The simplices of $S\sigma$ are the increasing sequences of vertices with respect to the above ordering.

If τ is a face of σ then the simplices of $S\sigma$ which are contained in τ form a subdivision of τ which is precisely the standard subdivision of τ . This observation allows us to define the standard subdivision of any simplicial complex L since we can subdivide each simplex of L separately and to get SL .

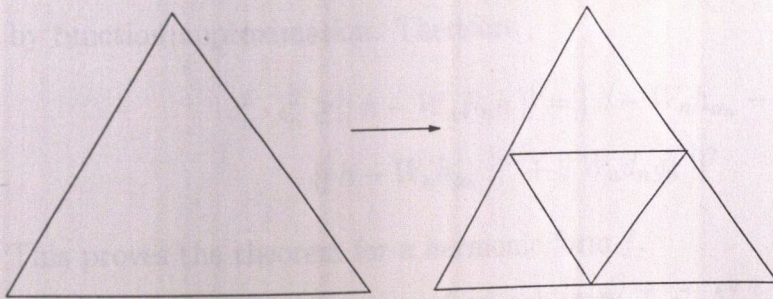


Figure A-1: Standard subdivision

Using this subdivision we can generate a series of complexes from our original one L , with $S_0L = L$ and $S_{n+1}L = S(S_nL)$. In this framework we can define R_n as being the de Rham map onto the n th subdivision of our original complex and W_n being the associated Whitney map. Using the mean value theorem Dodziuk showed function approximation for large n as we have done also.

The Hodge decomposition theorem: Let $f \in \Lambda_1^q$ so that R_nf is an element of C^q . Let

$$R_nf = d_ng_n + h_n + \delta_n k_n \quad (\text{A.26})$$

be the Hodge decomposition of R_nf . If

$$f = dg + h + \delta k \quad (\text{A.27})$$

is the Hodge decomposition of f then

$$\lim_{n \rightarrow \infty} W_n h_n = h \quad (\text{A.28})$$

$$\lim_{n \rightarrow \infty} W_n d_n g_n = g \quad (\text{A.29})$$

$$\lim_{n \rightarrow \infty} W_n \delta_n k_n = \delta k \quad (\text{A.30})$$

where the limits are in the norm of $L^2 \Lambda^q$.

Proof: We prove that this holds for when $f = h$ is harmonic. $R_n h$ is a cocycle by Stokes' theorem. It represents the same cohomology class α as h . Therefore

$$R_n h = h_{\alpha_n} + d_n g_n \quad (\text{A.31})$$

with $h_{\alpha_n} \in H_q^n$ representing α . We have

$$(W_n d_n g_n, h) = (d W_n g_n, h) = (W_n g_n, \delta h) = 0. \quad (\text{A.32})$$

On the other hand

$$\|h - W_n R_n h\| \leq c_h \cdot \iota_n \quad (\text{A.33})$$

by function approximation. Therefore

$$c_n^2 \cdot \iota_n^2 \geq \|h - W_n R_n h\|^2 = \|h - W_n h_{\alpha_n} - W_n d_n g_n\|^2 \quad (\text{A.34})$$

$$\|h - W_n h_{\alpha_n}\|^2 + \|W_n d_n g_n\|^2 \quad (\text{A.35})$$

This proves the theorem for a harmonic form f .

Now we consider the case of an arbitrary $f \in \Lambda_1^q$. Let P_n be the orthogonal projection of C^q onto the subspace of cocycles. We first estimate the norm of $P_n R_n \delta k$. let $c \in C^q$ be a cocycle. Then

$$|(P_n R_n \delta k, c)| = |(R_n \delta k, c)| = |(W_n R_n \delta k, W_n c)| \quad (\text{A.36})$$

$$= |(W_n R_n \delta k - \delta k, W_n c)| \quad (\text{A.37})$$

because $(\delta k, W_n c) = 0$. So

$$|(P_n R_n \delta k, c)| \leq \|W_n R_n \delta k - \delta k\| \cdot \|c\| \quad (\text{A.38})$$

$$\leq c_{\delta k} \cdot \iota_n \cdot \|c\|. \quad (\text{A.39})$$

This implies that

$$\| P_n R_n \delta k \| \leq c_{\delta k} \cdot \iota_n. \quad (\text{A.40})$$

Now we can complete the proof. We have

$$W_n R_n f = W_n R_n dg + W_n R_n h + W_n R_n \delta k \quad (\text{A.41})$$

and

$$\| W_n R_n dg - dg \| \leq c_{dg} \cdot \iota_n \quad (\text{A.42})$$

$$\| W_n R_n h - h \| \leq c_h \cdot \iota_n \quad (\text{A.43})$$

$$\| W_n R_n \delta k - \delta k \| \leq c_{\delta k} \cdot \iota_n \quad (\text{A.44})$$

By first part of the proof we know that

$$R_n h = h'_n + \epsilon_1 \quad (\text{A.45})$$

where $h'_n \in H_n^q$ and $\| \epsilon_1 \| \leq c_h \cdot \iota_n$. Moreover

$$R_n \delta j = P_n R_n \delta k + R_n \delta k - P_n R_n \delta k \quad (\text{A.46})$$

where $R_n \delta k - P_n R_n \delta k = \delta_n k'_n$ and $\| P_n R_n \delta k \| \leq c_{\delta k} \cdot \iota_n$. We write $\epsilon_2 = P_n R_n \delta k$. So we get

$$R_n f = R_n dg + h'_n + \delta_n k'_n + \epsilon_1 + \epsilon_2. \quad (\text{A.47})$$

Subtracting this from the Hodge decomposition of $R_n f$ we see that

$$(\epsilon_1 + \epsilon_2) = (h_n - h'_n) + (\delta_n k_n - \delta_n k'_n) + (d_n g_n - R_n dg) \quad (\text{A.48})$$

which implies that

$$\| h_n - h'_n \| \leq c_1 \iota_n \quad (\text{A.49})$$

$$\| \delta_n k_n - \delta_n k'_n \| \leq c_2 \iota_n \quad (\text{A.50})$$

$$\| d_n g_n - R_n dg \| \leq c_3 \iota_n \quad (\text{A.51})$$

for some constants $c_1, c_2, c_3 > 0$.

Finally

$$\| h - W_n h_n \| \leq \| h - W_n R_n h \| + \| W_n R_n h - W_n h_n \| \quad (\text{A.52})$$

$$= \| h - W_n R_n h \| + \| R_n h - h_n \| \quad (\text{A.53})$$

$$\leq \| h - W_n R_n h \| + \| h'_n - h_n \| + \| \epsilon_1 \| \leq c' \cdot \iota_n. \quad (\text{A.54})$$

Similarly

$$\| dg - W_n d_n g_n \| \leq \| dg - W_n R_n dg \| + \| W_n R_n dg - W_n d_n g_n \| \quad (\text{A.55})$$

$$= \| dg - W_n R_n dg \| + \| R_n dg - d_n g_n \| \leq c'' \cdot \iota_n \quad (\text{A.56})$$

and

$$\| \delta k - W_n \delta_n k_n \| \leq \| \delta k - W_n R_n \delta k \| + \| W_n R_n \delta k - W_n \delta_n k_n \| \quad (\text{A.57})$$

$$\leq \| \delta k - W_n R_n \delta k \| + \| R_n \delta k - \delta_n k_n \| \quad (\text{A.58})$$

$$\leq \| \delta k - W_n R_n \delta k \| + \| \delta_n k'_n - \delta_n k_n \| + \| \epsilon_2 \| \quad (\text{A.59})$$

$$\leq c''' \cdot \iota_n, \quad (\text{A.60})$$

as required.

Our work is closely related to that of Dodziuk. We both use the de Rham and Whitney map as well as the same inner product. We also show that our Laplacian converges to the continuum one. At the same time our space is more complex, containing both the original and its dual space, in order to incorporate our discrete Hodge star operator which is our central extension. This enables us to work in a closed discrete space with a rich set of operators and a novel variation for the discrete wedge product. We have also developed a cubic theory.

Appendix B

Finite Element

B.1 Finite Element Method

We take a brief look at some of the main components behind the finite element method in three phases:

1. Functional analysis which provides the basic framework in which the theory is established.
2. The Variational formulation which links the partial differential equations which we want to solve to the spaces established above.
3. Finite elements, where we express the problem as a matrix equation and establish error bounds.

This is just an outline of a huge field and we make no claims of completeness. Fortunately there is no shortage of excellent texts for comprehensive treatment of this area; see for example [24, 25].

B.1.1 Functional Analysis

Let Ω be an open subset of $\mathbb{R}^n$ with piecewise smooth boundary. $L_2(\Omega)$ consists of all functions u which are square integrable over Ω in the sense of Lebesgue. We identify two functions u and v whenever $u(x) = v(x)$ for all $x \in \Omega$ except on a set of measure zero. $L_2(\Omega)$ becomes a Hilbert space with the scalar product

$$(u, v)_0 := (u, v)_{L_2} = \int_{\Omega} u(x)v(x)dx \quad (\text{B.1})$$

and corresponding norm

$$\|u\|_0 = \sqrt{(u, u)_0}. \quad (\text{B.2})$$

$u \in L_2(\Omega)$ possesses the (weak) derivative $v = \partial^\alpha u$ in $L_2(\Omega)$ provided that $v \in L_2(\Omega)$ and

$$(\phi, v)_0 = (-1)^{|\alpha|} (\partial^\alpha \phi, u)_0 \text{ for all } \phi \in C_0^\infty(\Omega), \quad (\text{B.3})$$

where $C^\infty(\Omega)$ denotes the space of infinitely differentiable functions and $C_0^\infty(\Omega)$ denotes the subspace of such functions which are nonzero only on a compact subset of Ω .

Given an integer $m \geq 0$ let $H^m(\Omega)$, a Sobolev space, be the set of all functions u in $L_2(\Omega)$ which possess weak derivatives $\partial^\alpha u$ for all $|\alpha| \leq m$. We can define a scalar product on $H^m(\Omega)$ by

$$(u, v)_m := \sum_{|\alpha| \leq m} (\partial^\alpha u, \partial^\alpha v)_0 \quad (\text{B.4})$$

with the associated norm

$$\|u\|_m := \sqrt{(u, u)_m} = \sqrt{\sum_{|\alpha| \leq m} \|\partial^\alpha u\|_{L_2(\Omega)}^2} \quad (\text{B.5})$$

and semi-norm

$$|u|_m := \sqrt{\sum_{|\alpha|=m} \|\partial^\alpha u\|_{L_2(\Omega)}^2}. \quad (\text{B.6})$$

$H^m(\Omega)$ is complete with respect to the norm $\|\cdot\|_m$ and is thus a Hilbert space.

Poincare-Friedrich's Inequality: Suppose Ω is contained within an n -dimensional cube with side length s . Then

$$\|v\|_0 \leq s |v|_1 \text{ for all } v \in H_0^1(\Omega). \quad (\text{B.7})$$

Proof: Since $C_0^\infty(\Omega)$ is dense in $H_0^1(\Omega)$ it suffices to establish the inequality for $v \in C_0^\infty(\Omega)$. We may assume that $\Omega \subset W := \{(x_1, x_2, \dots, x_n); 0 < x_i < s\}$, and set $v = 0$ for all $x \in W \setminus \Omega$. Then

$$v(x_1, x_2, \dots, x_n) = v(0, x_2, \dots, x_n) + \int_0^{x_1} \partial_1 v(t, x_2, \dots, x_n) dt. \quad (\text{B.8})$$

The boundary term vanishes and using the Cauchy-Schwarz inequality gives

$$|v(x)|^2 \leq \int_0^{x_0} 1^2 dt \int_0^{x_1} |\partial_1 v(t, x_2, \dots, x_n)|^2 dt \quad (\text{B.9})$$

$$\leq s \int_0^s |\partial_1 v(t, x_2, \dots, x_n)|^2 dt. \quad (\text{B.10})$$

Since the right-hand side is independent of x_1 it follows that

$$\int_0^s |v(x)|^2 dx_1 \leq s^2 \int_0^s |\partial_1 v(x)|^2 dx_1. \quad (\text{B.11})$$

To complete the proof we integrate over the other coordinates to obtain

$$\int_W |v|^2 dx \leq s^2 \int_W |\partial_1 v|^2 dx \leq s^2 |v|_1^2. \quad (\text{B.12})$$

See [100, 101] for more on functional analysis¹ in general as opposed to standard finite element material.

B.1.2 Variational problem

Partial differential equations can be re-expressed as variational problems which the finite element method is based on. We work our way through a selection of the key theorems which are required to do this.

Characterisation Theorem: Let V be a linear space, and suppose

$$a : V \times V \rightarrow \mathbb{R} \quad (\text{B.13})$$

is a symmetric positive bilinear form. In addition let

$$l : V \rightarrow \mathbb{R} \quad (\text{B.14})$$

be a linear functional. Then the quantity

$$J(v) := \frac{1}{2}a(v, v) - \langle l, v \rangle \quad (\text{B.15})$$

attains its minimum over V at u if and only if

$$a(u, v) = \langle l, v \rangle \quad (\text{B.16})$$

for all $v \in V$. Moreover there is at most one solution to Eq. (B.16).

¹“... It is impossible to imagine the theory of computations with no Banach spaces, as well as with no computers.” - S. Sobolev.

Proof: For $u, v \in V$ and $t \in \mathbb{R}$ we have

$$J(u + tv) = \frac{1}{2}a(u + tv, u + tv) - \langle l, u + tv \rangle \quad (\text{B.17})$$

$$= J(u) + t[a(u, v) - \langle l, v \rangle] + \frac{1}{2}t^2a(v, v). \quad (\text{B.18})$$

If $u \in V$ satisfies Eq. (B.16) then Eq. (B.18) with $t = 1$ implies

$$J(u + v) = J(u) + \frac{1}{2}a(v, v) \text{ for all } v \in V \quad (\text{B.19})$$

$$> J(u) \text{ if } v \neq 0. \quad (\text{B.20})$$

Thus u is a unique minimal point. Conversely if J has a minimum at u then for every $v \in V$ the derivative of the function $t \rightarrow J(u + tv)$ must vanish at $t = 0$, By Eq. (B.18) the derivative is $a(u, v) - \langle l, v \rangle$ and Eq. (B.16) follows.

Minimal Property: Every classical solution of the boundary-value problem

$$-\sum_{i,k} \partial_i(a_{ik} \partial_k u) + a_0 u = f \text{ in } \Omega \quad (\text{B.21})$$

$$u = 0 \text{ on } \partial\Omega \quad (\text{B.22})$$

is a solution of the variational problem

$$J(v) := \int_{\Omega} \left[\frac{1}{2} \sum_{i,k} a_{ik} \partial_i v \partial_k v + \frac{1}{2} a_0 v^2 - f v \right] dx \rightarrow \min! \quad (\text{B.23})$$

among all functions $C^2(\Omega) \cap C^0(\bar{\Omega})$ with zero boundary values.

Proof: The proof proceeds with the help of Green's formula

$$\int_{\Omega} v \partial_i w dx = - \int_{\Omega} \partial_i v dx + \int_{\partial\Omega} v w v_i ds. \quad (\text{B.24})$$

Here v and w are assume to be C^1 functions and v_i is the i -th component of the outward pointing normal v . Inserting $w := a_{ik} \partial_k u$ in Eq. (B.24) we have

$$\int_{\Omega} v \partial_i (a_{ik} \partial_k u) dx = - \int_{\Omega} a_{ik} \partial_i v \partial_k u dx \quad (\text{B.25})$$

provided $v = 0$ on $\partial\Omega$. Let

$$a(u, v) := \int_{\Omega} \left[\sum_{i,k} a_{ik} \partial_i u \partial_k v + a_0 uv \right] dx, \quad (\text{B.26})$$

$$\langle l, v \rangle := \int_{\Omega} f v dx. \quad (\text{B.27})$$

Summing Eq. (B.25) over i and k gives that for every $v \in C^1(\Omega) \cap C(\bar{\Omega})$ with $v = 0$ on $\partial\Omega$,

$$a(u, v) - \langle l, v \rangle = \int_{\Omega} v \left[- \sum_{i,k} \partial_i (a_{ik} \partial_k u) + a_0 u - f \right] dx \quad (\text{B.28})$$

$$= \int_{\Omega} v [Lu - f] dx = 0, \quad (\text{B.29})$$

provided $Lu = f$. This is true if u is a classical solution. Now the characterisation theorem implies the minimal property.

Lax-Milgram Theorem(for Convex Sets). Let V be a closed convex set in a Hilbert space H and let $a : H \times H \rightarrow \mathbb{R}$ be an elliptic bilinear form. Then for every $l \in H'$, the variational problem

$$J(v) := \frac{1}{2} a(v, v) - \langle l, v \rangle \rightarrow \min! \quad (\text{B.30})$$

has a unique solution in V .

Proof: J is bounded from below since

$$\begin{aligned} J(v) &\geq \frac{1}{2} \alpha \|v\|^2 - \|l\| \|v\| \quad (\text{B.31}) \\ &= \frac{1}{2\alpha} (\alpha \|v\| - \|l\|)^2 - \frac{\|l\|^2}{2\alpha} \geq -\frac{\|l\|^2}{2\alpha}. \end{aligned}$$

Let $c_1 := \inf\{J(v); v \in V\}$ and let (v_n) be the minimizing sequence. Then

$$\alpha \|v_n - v_m\|^2 \leq a(v_n - v_m, v_n - v_m) \quad (\text{B.32})$$

$$= 2a(v_n, v_n) + 2a(v_m, v_m) - a(v_n + v_m, v_n + v_m) \quad (\text{B.33})$$

$$= 4J(v_n) + 4J(v_m) - 8J\left(\frac{v_n + v_m}{2}\right) \quad (\text{B.34})$$

$$\leq 4J(v_n) + 4J(v_m) - 8c_1, \quad (\text{B.35})$$

since V is convex and thus $\frac{1}{2}(v_n + v_m) \in V$. Now $J(v_n), J(v_m) \rightarrow c_1$ implies $\|v_n - v_m\| \rightarrow 0$ for $n, m \rightarrow \infty$. Thus (v_n) is a Cauchy sequence in H and $u = \lim_{n \rightarrow \infty} v_n$ exists. Since V is closed we also have $u \in V$. The continuity of J implies $J(u) = \lim_{n \rightarrow \infty} J(v_n) = \inf_{v \in V} J(v)$.

We now show that the solution is unique. Suppose u_1 and u_2 are both solutions. Clearly $u_1, u_2, u_1, u_2, \dots$ is a minimizing sequence. As we saw above, every minimizing sequence is a Cauchy sequence. This is only possible if $u_1 = u_2$.

Finally,

Existence Theorem: Let L be a second order uniformly elliptic partial differential operator. Then the Dirichlet problem always has a weak solution in $H^1(\Omega)$. It is the minimum of the variational problem

$$\frac{1}{2}a(v, v) - (f, v)_0 \rightarrow \min! \quad (\text{B.36})$$

over $H_0^1(\Omega)$.

Proof: Let $c := \sup\{|a_{ik}(x)|; x \in \Omega, 1 \leq i, k \leq n\}$. Then the Cauchy-Schwarz inequality implies

$$\left| \sum_{i,k} \int a_{ik} \partial_i u \partial_k v dx \right| \leq c \sum_{i,k} \int |\partial_i u \partial_k v| dx \quad (\text{B.37})$$

$$\leq c \sum_{i,k} \left[\int (\partial_i u)^2 dx \int (\partial_k v)^2 dx \right]^{\frac{1}{2}} \quad (\text{B.38})$$

$$\leq C \|u\|_1 \|v\|_1, \quad (\text{B.39})$$

where $C = cn^2$. If we also assume that $C \geq \sup\{|a_0(x)|; x \in \Omega\}$, then we get

$$\left| \int a_0 uv dx \right| \leq C \int |uv| dx \leq C \cdot \|u\|_0 \cdot \|v\|_0 \quad (\text{B.40})$$

in an analogous way. Combining these we have

$$a(u, v) \leq C \|u\|_1 \|v\|_1. \quad (\text{B.41})$$

Next the uniform ellipticity implies the pointwise estimate

$$\sum_{i,k} a_{ik} \partial_i v \partial_k v \geq \alpha \sum_i (\partial_i v)^2 \quad (\text{B.42})$$

for C^1 functions. Integrating both sides and using $a_0 \geq 0$ leads to

$$a(v, v) \geq \alpha \sum_i \int_{\Omega} (\partial_i v)^2 dx = \alpha \|v\|_1^2 \quad \text{for all } v \in H^1(\Omega) \quad (\text{B.43})$$

By Freidrich's inequality, $\|\cdot\|_1$ and $\|\cdot\|_0$ are equivalent norms on H_0^1 . Thus a is an H^1 -elliptic bilinear form on $H_0^1(\Omega)$. By the Lax-Milgram Theorem there exists a unique weak solution which is also a solution of the variational problem.

B.1.3 Finite elements

The solution of the variational problem in a subspace S_h

$$J(v) := \frac{1}{2}a(v, v) - \langle l, v \rangle \rightarrow \min_{S_h} \quad (\text{B.44})$$

can be computed using the Characterisation Theorem. In particular u_h is a solution provided

$$a(u_h, v) = \langle l, v \rangle \quad \text{for all } v \in S_h. \quad (\text{B.45})$$

$$a(u_h, v) = \langle l, v \rangle \quad \text{for all } v \in S_h.$$

Suppose $\{\psi_1, \psi_2, \dots, \psi_N\}$ is a basis for S_h . Then (B.45) is equivalent to

$$a(u_h, \psi_i) = \langle l, \psi_i \rangle, \quad i = 1, 2, \dots, N.$$

Assuming that u_h has the form

$$u_h = \sum_{k=1}^N z_k \psi_k, \quad (\text{B.47})$$

we are led to the system of equations

$$\sum_{k=1}^N a(\psi_k, \psi_i) z_k = \langle l, \psi_i \rangle, \quad i = 1, 2, \dots, N, \quad (\text{B.48})$$

which we can write in matrix-vector form as

$$Az = b, \quad (\text{B.49})$$

where $A_{ik} := a(\psi_i, \psi_k)$ and $b_i := \langle l, \psi_i \rangle$.

There are several related methods including:

- **Rayleigh-Ritz:** Here the minimum of J is sought in the space S_h . Instead of the basis-free derivation usually one finds u_h by solving the equation $(\frac{\partial}{\partial z_i} J(\sum_k z_k \psi_k) = 0$.
- **Galerkin:** The weak equation is solved for problems where the bilinear form is not necessarily symmetric. If the weak equations arise from a variational problem with a positive quadratic form then often the term Ritz-Galerkin Method is used.

Cea's Lemma: Suppose the bilinear form a is V -elliptic with $H_0^m(\Omega) \subset V \subset H^m(\Omega)$. In addition suppose u and u_h are the solutions of the variational problem V and $S_h \subset V$ respectively. Then

$$\|u - u_h\|_m \leq \frac{C}{\alpha} \inf_{v_h \in S_h} \|u - v_h\|_m. \quad (\text{B.50})$$

Proof: By definition of u and u_h ,

$$a(u, v) = \langle l, v \rangle \text{ for all } v \in V, \quad (\text{B.51})$$

$$a(u_h, v) = \langle l, v \rangle \text{ for all } v \in S_h. \quad (\text{B.52})$$

Since $S_h \subset V$ it follows by subtraction that

$$a(u - u_h, v) = 0 \text{ for all } v \in S_h. \quad (\text{B.53})$$

Let $v_h \in S_h$. With $v = v_h - u_h \in S_h$ it now follows immediately from Eq. (B.53) that $a(u - u_h, v_h - u_h) = 0$ and

$$\alpha \|u - u_h\|_m^2 \leq a(u - u_h, u - u_h) \quad (\text{B.54})$$

$$= a(u - u_h, u - v_h) + a(u - u_h, v_h - u_h) \quad (\text{B.55})$$

$$\leq C \|u - u_h\|_m \|u - v_h\|_m. \quad (\text{B.56})$$

After dividing by $\|u - u_h\|_m$ we get

$$\alpha \|u - u_h\|_m \leq C \|u - v_h\|_m \quad (\text{B.57})$$

as required.

B.2 Application to Field theory

We now look at the work of Bender et al [51, 52] where they apply finite element methods to Operator field equations by taking operators as their coefficients for their polynomials such that the equal-time commutation relations are captured. We will look at the implementation of this idea from their original paper and then comment on what this has lead to.

For example we look at the Heisenberg equations of motion for a one-dimensional quantum system. If the Hamiltonian is

$$H = \frac{p^2}{2} + V(q), \quad (\text{B.58})$$

the Heisenberg equations are

$$\frac{dq(t)}{dt} = p(t) \quad (\text{B.59})$$

$$\frac{dp(t)}{dt} = f(q(t)), \quad (\text{B.60})$$

where $f(q) = -V'(q)$. The quantum mechanical problem consists of solving these for the operators $p(t)$ and $q(t)$ given the equal-time commutation relations (ETCR)

$$[q(t), p(t)] = i. \quad (\text{B.61})$$

We solve this problem first on a single finite element. We approximate $q(t)$ and $p(t)$ by linear functions of t :

$$q(t) = (1 - \frac{t}{h})q_0 + \frac{t}{h}q_1, \quad (\text{B.62})$$

$$p(t) = (1 - \frac{t}{h})p_0 + \frac{t}{h}p_1, \quad (\text{B.63})$$

$0 \leq t \leq h$. Substituting these expressions into our equations of motion and evaluating the result at the center of the time interval, $t_0 = \frac{h}{2}$ gives

$$\frac{(q_1 - q_0)}{h} = \frac{1}{2}(p_0 + p_1) \quad (\text{B.64})$$

$$\frac{(p_1 - p_0)}{h} = f(\frac{1}{2}(q_0 + q_1)). \quad (\text{B.65})$$

Are these consistent with the commutation relations? At $t = 0$ we have $[q_0, p_0] = i$. If we solve the equations of motion we can compute p_1 and q_1 . Are these consistent with the ETCR too? Commuting Eq. (B.64) on the right with $p_0 + p_1$ we get

$$[q_1 - q_0, p_0 + p_1] = 0 \quad (\text{B.66})$$

and commuting Eq. (B.65) on the left with $q_0 + q_1$ we get

$$[q_0 + q_1, p_1 - p_0] = 0. \quad (\text{B.67})$$

Adding these we see that

$$[q_1, p_1] = [q_0, p_0] = i. \quad (\text{B.68})$$

Thus we prove that finite element is consistent with the ETCR's.

Note that the ETCR's hold at the end points of the finite elements and not in the interior. Also the result depends on imposing the Heisenberg equations at the centre of the element at $t = \frac{h}{2}$.

We now solve these equations. Using (B.64) we can say

$$p_1 = \frac{2}{h}(q_1 - q_0) - p_0 \quad (\text{B.69})$$

and substitute this into (B.65). We express this in terms of $g(x) = f(x) - \frac{4x}{h^2}$ in order to only have expressions with $t = t_0$ on the LHS.

$$\frac{1}{h} \left[\frac{2}{h} (q_1 - q_0) - p_0 - p_0 \right] = f\left(\frac{1}{2}(q_0 + q_1)\right) \quad (\text{B.70})$$

$$\frac{2}{h^2} (q_1 - q_0) - \frac{2p_0}{h} = g\left(\frac{1}{2}(q_0 + q_1)\right) + \frac{4\frac{1}{2}(q_0 + q_1)}{h^2} \quad (\text{B.71})$$

$$\frac{2}{h^2} (q_1 - q_0) - \frac{2(q_0 + q_1)}{h^2} - \frac{2p_0}{h} = g\left(\frac{1}{2}(q_0 + q_1)\right) \quad (\text{B.72})$$

$$\frac{-4}{h^2} (q_0) - \frac{2p_0}{h} = g\left(\frac{1}{2}(q_0 + q_1)\right). \quad (\text{B.73})$$

Using this we can say

$$q_1 = -q_0 + 2g^{-1}\left(-\left(\frac{2}{h}\right)p_0 - \left(\frac{4}{h^2}\right)q_0\right) \quad (\text{B.74})$$

and

$$p_1 = -p_0 - \frac{4}{h}q_0 + \frac{4}{h}g^{-1}\left(-\left(\frac{2}{h}\right)p_0 - \left(\frac{4}{h^2}\right)q_0\right). \quad (\text{B.75})$$

We can then simply iterate this N times in order to determine p_N and q_N .

This can be extended to scalar field theory by taking a bilinear approximation for the field which satisfies the ETCR at $t = t_0$ and also for $t = t_1$; as well as in general by induction as above. Not only that but using the same approach we can work with the Dirac equation without doubling.

The Dirac equation is notoriously difficult to deal with. If we simply take a lattice approximation for the continuum action with a forward difference scheme used for space derivatives, the result is not Hermitian. In fact the Hermitian conjugate involves a backward difference scheme for the derivative. This suggests using symmetric difference but this, as we know from [5], leads to fermion doubling.

It is possible to construct an action which is Hermitian and has no fermion doubling, as was shown by Banks, Kogut and Susskind [28], however this explicitly violates chiral symmetry.

If we proceed using ETCR with fermions we again use a forward difference scheme but here Hermiticity is maintained since undifferentiated fields appear as averages. These finite element formulations of lattice fermions escapes the no-go theorems [63, 61] because the Hamiltonian is non-local.

This formulation has been developed further by incorporating at first Abelian [53] and then Non-Abelian [54] gauge theories. It appears though that unitarity must be sacrificed in order to obtain locality or vice versa. It is worth mentioning that there is no fermion doubling using this approach and because it is based on the operator equations of motion it is not constrained by the statistical limitations of traditional lattice field theory.

As discussed in Sec.6.6, FDS is related though quite different to FE^2 and the commutation relations are not central in our work. The work of Bender et al though does demonstrate that FE like methods can be used to good effect³ in field theory and provides a good guide to the path ahead in our own work.

²FDS uses an analogue method as opposed to the variational approach of FE.

³Work using smeared lattice fermions [102] seems to get round some of the traditional problems, as in the no-go theorems, and has connections to FE methods.

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Apr 19, 02 7:40

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Page 1/2

(Message inbox:11068)

Date: Thu, 18 Apr 2002 17:28:17 BST
 To: siddhartha.sen@tcd.ie
 From: stefan hutzler <shutzler@tcd.ie>
 Subject: polygons

Return-Path: shutzler@tcd.ie
 X-Mmdf-To: sen
 MIME-Version: 1.0

Dear Siddhartha,

Simon Cox and myself were having this discussion about the "ideal" structure of foam and we came to a point where I thought that maybe you could give us some advice.

If one (wrongly) assumes the average cell in a foam as a regular polyhedron with planar faces then one can obtain an approximation for the average number of faces, vertices and edges of such a polyhedron foam cell.

One finds that the average number of faces is $f=13.39$
 the average number of vertices is $v = 22.79$
 and the average number of sides to each face is $s=5.10$

These values are not unreasonable as one sees by comparing them with the Kelvin cell and the Weaire-Phelan structure:

Note that the Kelvin cell has
 $f=14$
 $v=24$
 $s=5.14$

while Weaire Phelan has
 $f= 13.5$
 $v=$ (can't remember)
 $s=$ (can't remember)

similar to the numbers computed above.

We have the following QUESTION:

What would be the area of a 5.1 sided regular polygon, what would be the volume of the above ideal foam cell? That is, is there some subbranch of mathematics on non-integer sided polygons and bodies composed of them? Or maybe I am just totally naive in assuming that mathematics generalises ALL possible topics?

Looking forward to your reply,
 Many thanks,

Stefan

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Friday April 19, 2002

Apr 19, 02 7:40

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Page 2/2

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