M345A47 Finite Elements: Analysis and Implementation

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CONTENTS

1	Numerical analysis	1
1	Introduction 1.1 Poisson's equation in the unit square 1.2 Triangulations 1.3 Our first finite element space 1.4 Integral formulations and L_2 1.5 Finite element derivative 1.6 Towards the finite element discretisation 1.7 Practical implementation	3 3 4 4 5 5 7
2	2.4 Some more exotic elements	9 10 11 13 14
3	3.2 Measuring interpolation errors	17 17 17 18 20
4	 4.1 Finite element spaces and other Hilbert spaces 4.2 Linear forms on Hilbert spaces 4.3 Variational problems on Hilbert spaces 	23 23 25 27 28
5	5.1 Weak derivatives	33 34 35 37 37 39 40
II	Implementation Exercise	43
0	0.2 Extension (mastery) exercise	45 45 45

	0.4	Skeleton code documentation	7					
	0.5	How to do the implementation exercises	7					
	0.6	Pull requests for feedback						
	0.7	Testing your work						
	0.8	Coding style and commenting						
	0.9	Tips and tricks for the implementation exercise	8					
1	Num	erical quadrature 4						
	1.1	Exact and incomplete quadrature						
	1.2	Examples in one dimension						
	1.3	Reference elements						
	1.4	Python implementations of reference elements						
	1.5	Quadrature rules on reference elements						
	1.6	Legendre-Gauß quadrature in one dimension						
	1.7	Extending Legendre-Gauß quadrature to two dimensions						
	1.8	Implementing quadrature rules in Python	2					
2	Cons	tructing finite elements 5	3					
	2.1	A worked example	3					
	2.2	Types of node	4					
	2.3	The Lagrange element nodes	4					
	2.4	Solving for basis functions	5					
	2.5	Implementing finite elements in Python	5					
	2.6	Implementing the Lagrange Elements	6					
	2.7	Tabulating basis functions	6					
	2.8	Gradients of basis functions	6					
	2.9	Interpolating functions to the finite element nodes	8					
3	Mesh	ies 5	;9					
	3.1	Mesh entities	jç					
	3.2	Reference cell entities	0					
	3.3	Adjacency	j(
	3.4	Mesh geometry	1					
	3.5	A mesh implementation in Python	1					
4	Func	unction spaces: associating data with meshes						
	4.1	Local numbering and continuity	3					
	4.2	Implementing local numbering	<u>.</u>					
	4.3	Global numbering	<u>.</u> 4					
	4.4	The cell-node map	5					
	4.5	Implementing function spaces in Python	5					
5	Func	tions in finite element spaces	7					
	5.1	A python implementation of functions in finite element spaces						
	5.2	Interpolating values into finite element spaces	7					
	5.3	Integration						
6	Assei	mbling and solving finite element problems 7	13					
	6.1	Assembling the right hand side						
	6.2	Assembling the left hand side matrix						
	6.3	The method of manufactured solutions						
	6.4	Errors and convergence						
	6.5	Implementing finite element problems						
7	Diric	hlet boundary conditions 7	/O					
•	7.1	An algorithm for homogeneous Dirichlet conditions						
	7.1	Implementing boundary conditions						
	7.3	Inhomogeneous Dirichlet conditions						

8	Nonli	Nonlinear problems				
	8.1	A model problem	8			
	8.2	Residual form	8			
	8.3	Linearisation and Gâteaux Derivatives	82			
	8.4	A Taylor expansion and Newton's method	83			
	8.5	Implementing a nonlinear problem	84			
Bi	bliogra	aphy	87			

Part I Numerical analysis

INTRODUCTION

In this section we provide an introduction that establishes some initial ideas about how the finite element method works and what it is about.

The finite element method is an approach to solving partial differential equations (PDEs) on complicated domains. It has the flexibility to build discretisations that can increase the order of accuracy, and match the numerical discretisation to the physical problem being modelled. It has an elegant mathematical formulation that lends itself both to mathematical analysis and to flexible code implementation. In this course we blend these two directions together.

1.1 Poisson's equation in the unit square

In this introduction we concentrate on the specific model problem of Poisson's equation in the unit square.

Definition 1 (Poisson's equation in the unit square) Let $\Omega = [0,1] \times [0,1]$. For a given function f, we seek u such that

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)u := -\nabla^2 u = f, \quad u(0,y) = u(1,y) = 0, \quad \frac{\partial u}{\partial y}(x,0) = \frac{\partial u}{\partial y}(x,1) = 0. \tag{1.1}$$

In this problem, the idea is that we are given a specific known function f (for example, $f = sin(2\pi x)sin(2\pi y)$), and we have to find the corresponding unknown function u that satisfies the equation (including the boundary conditions). Here we have combined a mixture of Dirichlet boundary conditions specifying the value of the function u, and Neumann boundary conditions specifying the value of the normal derivative $\partial u/\partial n$. This is because these two types of boundary conditions are treated differently in the finite element method, and we would like to expose both treatments in the same example. The treatment of boundary conditions is one of the strengths of the finite element method.

1.2 Triangulations

The description of our finite element method starts by considering a triangulation.

Definition 2 (Triangulation) Let Ω be a polygonal subdomain of \mathbb{R}^2 . A triangulation \mathcal{T} of Ω is a set of triangles $\{K_i\}_{i=1}^N$, such that:

- 1. int $K_i \cap K_j = \emptyset$, $i \neq j$, where int denotes the interior of a set (no overlaps).
- 2. $\bigcup K_i = \bar{\Omega}$, the closure of Ω (triangulation covers Ω).
- 3. No vertex of the interior of any triangle is located in the interior of any other triangle in \mathcal{T} (triangle vertices only meet other triangle vertices).

1.3 Our first finite element space

The idea is that we will approximate functions which are polynomial (at some chosen degree) when restricted to each triangle, with some chosen continuity conditions between triangles. We shall call the space of possible functions under these choices a finite element space. In this introduction, we will just consider the following space.

Definition 3 (The P1 **finite element space)** Let T be a triangulation of Ω . Then the P1 finite element space is a space V_h containing all functions v such that

1.
$$v \in C^0(\Omega)$$
,

2. $v|_{K_i}$ is a linear function for each $K_i \in \mathcal{T}$.

We also define the following subspace,

$$\mathring{V}_h = \{ v \in V_h : v(0, y) = v(1, y) = 0 \}.$$
(1.2)

This is the subspace of the P1 finite element space V_h of functions that satisfy the Dirichlet boundary conditions. We will search only amongst \mathring{V}_h for our approximate solution to the Poisson equation. This is referred to as strong boundary conditions. Note that we do not consider any subspaces related to the Neumann conditions. These will emerge later.

1.4 Integral formulations and L_2

The finite element method is based upon integral formulations of partial differential equations. Rather than checking if two functions are equal by checking their value at every point, we will just check that they are equal in an integral sense. We do this by introducing the L^2 norm, which is a way of measuring the "magnitude" of a function.

Definition 4 For a real-valued function f on a domain Ω , with Lebesgue integral

$$\int_{\Omega} f(x) dx,$$

we define the L^2 norm of f,

$$||f||_{L^2}(\Omega) = \left(\int_{\Omega} |f(x)|^2 dx\right)^{1/2}.$$

This motivates us to say that two functions are equal if the L^2 norm of their difference is zero. It only makes sense to do that if the functions individually have finite L^2 norm, which then also motivates the L^2 function space.

Definition 5 We define $L^2(\Omega)$ as the set of functions

$$L^{2}(\Omega) = \{ f : ||f||_{L^{2}}(\Omega) < \infty \},\,$$

and identify two functions f and g if $||f - g||_{L^2(\Omega)} = 0$, in which case we write $f \equiv g$ in L^2 .

Example 6 Consider the two functions f and g defined on $\Omega = [0,1] \times [0,1]$ with

$$f(x,y) = \left\{ \begin{array}{ll} 1 & x \geq 0.5, \\ 0 & x < 0.5, \end{array} \right. g(x,y) = \left\{ \begin{array}{ll} 1 & x > 0.5, \\ 0 & x \leq 0.5. \end{array} \right.$$

Since f and g only differ on the line x = 0.5 which has zero area, then $||f - g||_{L^2(\Omega)} = 0$, and so $f \equiv g$ in L^2 .

1.5 Finite element derivative

Functions in V_h do not have derivatives everywhere. This means that we have to work with a more general definition (and later we shall learn when it does and does not work).

Definition 7 (Finite element partial derivative) The finite element partial derivative $\frac{\partial^{FE}}{\partial x_i}u$ of u is defined in $L^2(\Omega)$ such that restricted to K_i , we have

$$\frac{\partial^{FE} u}{\partial x_i}|_{K_i} = \frac{\partial u}{\partial x_i}.$$

Here we see why we needed to introduce L^2 : we have a definition that does not have a unique value on the edge between two adjacent triangles. This is verified in the following exercises.

Exercise 8 Let V_h be a P1 finite element space for a triangulation \mathcal{T} of Ω . For all $u \in V_h$, show that the definition above uniquely defines $\frac{\partial^F E_u}{\partial x_i}$ in $L^2(\Omega)$.

Exercise 9 Let $u \in C^1(\Omega)$ (the space of functions with finite-valued partial derivatives at every point in Ω). Show that the finite element partial derivative and the usual derivative are equal in $L^2(\Omega)$.

In view of this second exercise, in this section we will consider all derivatives to be finite element derivatives. In later sections we shall consider an even more general definition of the derivative which contains both of these definitions.

1.6 Towards the finite element discretisation

We will now use the finite element derivative to develop the finite element discretisation. We assume that we have a solution u to Equation (1.1) that is smooth (i.e. $u \in C^1$). (Later, we will consider more general types of solutions to this equation, but this assumption just motivates things for the time being.)

We take $v \in \mathring{V}_h$, multiply by Equation (1.1), and integrate over the domain. Integration by parts in each triangle then gives

$$\sum_i \left(\int_{K_i} \nabla v \cdot \nabla u \, dx - \int_{\partial K_i} v n \cdot \nabla u \, dS \right) = \int_{\Omega} v f \, dx,$$

where n is the unit outward pointing normal to K_i .

Next, we consider each interior edge f in the triangulation, formed as the intersection between two neighbouring triangles $K_i \cap K_j$. If i > j, then we label the K_i side of f with a +, and the K_j side with a -. Then, denoting Γ as the union of all such interior edges, we can rewrite our equation as

$$\int_{\Omega} \nabla v \cdot \nabla u \, dx - \int_{\Gamma} v n^{+} \cdot \nabla u + v n^{-} \cdot \nabla u \, dS - \int_{\partial \Omega} v n \cdot \nabla u \, dS = \int_{\Omega} v f \, dx,$$

where n^{\pm} is the unit normal to f pointing from the \pm side into the \mp side. Since $n^{-}=-n^{+}$, the interior edge integrals vanish.

Further, on the boundary, either v vanishes (at x=0 and x=1) or $n\cdot \nabla u$ vanishes (at y=0 and y=1), and we obtain

$$\int_{\Omega} \nabla v \cdot \nabla u \, dx = \int_{\Omega} v f \, dx.$$

The finite element approximation is then defined by requiring that this equation holds for all $v \in \mathring{V}_h$ and when we restrict $u \in \mathring{V}_h$.

Definition 10 The finite element approximation $u_h \in \mathring{V}_h$ to the solution u_h of Poisson's equation is defined by

$$\int_{\Omega} \nabla v \cdot \nabla u_h \, dx = \int_{\Omega} v f \, dx, \quad \forall v \in \mathring{V}_h. \tag{1.3}$$

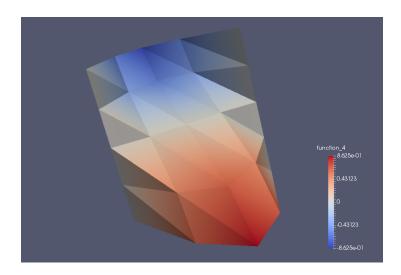


Fig. 1.1: Numerical solution on a 4×4 mesh.

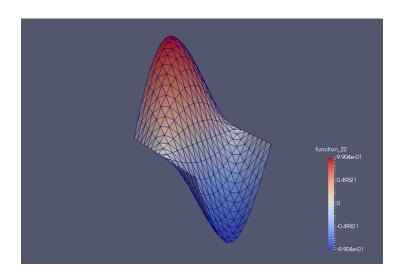


Fig. 1.2: Numerical solution on a 16×16 mesh.

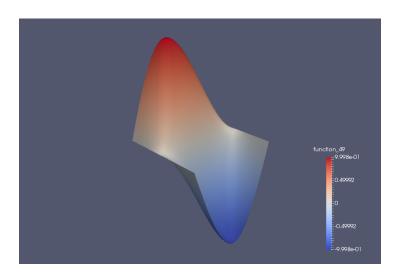


Fig. 1.3: Numerical solution on a 128×128 mesh.

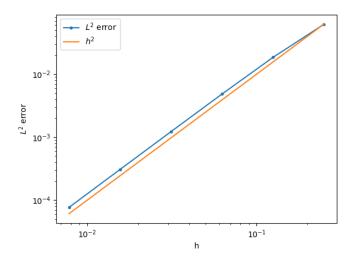


Fig. 1.4: Plot showing error versus mesh resolution. We observe the error decreases proportionally to h^2 , where h is the maximum triangle edge size in the triangulation.

We now present some numerical results for the case $f = 2\pi^2 \sin(\pi x) \sin(\pi y)$.

We see that for this example, the error is decreasing as we increase the number of triangles, for the meshes considered.

In general, our formulation raises a number of questions.

- 1. Is u_h unique?
- 2. What is the size of the error $u u_h$?
- 3. Does this error go to zero as the mesh is refined?
- 4. For what types of functions f can these questions be answered?
- 5. What other kinds of finite element spaces are there?
- 6. How do we extend this approach to other PDEs?
- 7. How can we calculate u_h using a computer?

We shall aim to address these questions, at least partially, through the rest of this course. For now, we concentrate on the final question, in general terms.

In this course we shall mostly concentrate on finite element methods for elliptic PDEs, of which Poisson's equation is an example, using continuous finite element spaces, of which P1 is an example. The design, analysis and implementation of finite methods for PDEs is a huge field of current research, and includes parabolic and elliptic PDEs and other PDEs from elasticity, fluid dynamics, electromagnetism, mathematical biology, mathematical finance, astrophysics and cosmology, etc. This course is intended as a starting point to introduce the general concepts that can be applied in all of these areas.

1.7 Practical implementation

The finite element approximation above is only useful if we can actually compute it. To do this, we need to construct an efficient basis for P1, which we call the nodal basis.

Definition 11 (P1 nodal basis) Let $\{z_i\}_{i=1}^M$ indicate the vertices in the triangulation \mathcal{T} . For each vertex z_i , we define a basis function $\phi_i \in V_h$ by

$$\phi_i(z_j) = \delta_{ij} := \begin{cases} 1 & i = j, \\ 0 & i \neq j. \end{cases}$$

We can define a similar basis for V_h by removing the basis functions ϕ_i corresponding to vertices z_i on the Dirichlet boundaries x=0 and x=1; the dimension of the resulting basis is \bar{M} .

If we expand u_h and v in the basis for \mathring{V}_h ,

$$u_h(x) = \sum_{i=1}^{\bar{M}} u_i \phi_i(x), \quad v(x) = \sum_{i=1}^{\bar{M}} v_i \phi_i(x),$$

into Equation (1.3), then we obtain

$$\sum_{i=1}^{\bar{M}} v_i \left(\sum_{j=1}^{\bar{M}} \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, dx v_j - \int_{\Omega} \phi_i f \, dx \right) = 0.$$

Since this equation must hold for all $v \in \mathring{V}_h$, then it must hold for all basis coefficients v_i , and we obtain the matrix-vector system

$$K\mathbf{u} = \mathbf{f}$$

where

$$K_{ij} = \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, dx,$$
$$\mathbf{u} = (u_1, u_2, \dots, u_{\bar{M}})^T,$$
$$\mathbf{f} = (f_1, f_2, \dots, f_{\bar{M}})^T, \quad f_i = \int_{\Omega} \phi_i f \, dx.$$

Once we have solved for u, we can use these basis coefficients to reconstruct the solution u_h . The system is square, but we do not currently know that K is invertible. This is equivalent to the finite element approximation having a unique solution u_h , which we shall establish in later sections. This motivates why we care that u_h exists and is unique.

Putting solvability aside for the moment, the goal of the implementation sections of this course is to explain how to efficiently form K and f, and solve this system. For now we note a few following aspects that suggest that this might be possible. First, the matrix K and vector f can be written as sums over elements,

$$K_{ij} = \sum_{K \in \mathcal{T}} \int_{K} \nabla \phi_{i} \cdot \nabla \phi_{j} \, dx,$$
where $f_{i} = \sum_{K \in \mathcal{T}} \int_{K} \phi_{i} f \, dx.$

For each entry in the sum for K_{ij} , the integrand is composed entirely of polynomials (actually constants in this particular case, but we shall shortly consider finite element spaces using polynomials of higher degree). This motivates our starting point in exposing the computer implementation, namely the integration of polynomials over triangles using quadrature rules. This will also motivate an efficient way to construct derivatives of polynomials evaluated at quadrature points. Further, we shall shortly develop an interpolation operator $\mathcal I$ such that $\mathcal I_f \in V_h$. If we replace f by $\mathcal I_f$ in the approximations above, then the evaluation of f_i can also be performed via quadrature rules.

Even further, the matrix K is very sparse, since in most triangles, both ϕ_i and ϕ_j are zero. Any efficient implementation must make use of this and avoid computing integrals that return zero. This motivates the concept of global assembly, the process of looping over elements, computing only the contributions to K that are non-zero from that element. Finally, the sparsity of K means that the system should be solved using numerical linear algebra algorithms that can exploit this sparsity.

Having set out the main challenges of the computational implementation, we now move on to define and discuss a broader range of possible finite element spaces.

FINITE ELEMENT SPACES: LOCAL TO GLOBAL

In this section, we discuss the construction of general finite element spaces. Given a triangulation \mathcal{T} of a domain Ω , finite element spaces are defined according to

- 1. the form the functions take (usually polynomial) when restricted to each cell (a triangle, in the case considered so far),
- 2. the continuity of the functions between cells.

We also need a mechanism to explicitly build a basis for the finite element space. We first do this by looking at a single cell, which we call the local perspective. Later we will take the global perspective, seeing how function continuity is enforced between cells.

2.1 Ciarlet's finite element

The first part of the definition is formalised by Ciarlet's definition of a finite element.

Definition 12 (Ciarlet's finite element) Let

- 1. the element domain $K \subset \mathbb{R}^n$ be some bounded closed set with piecewise smooth boundary,
- 2. the space of shape functions P be a finite dimensional space of functions on K, and
- 3. the set of nodal variables $\mathcal{N} = (N_0, \dots, N_k)$ be a basis for the dual space P'.

Then $(K, \mathcal{P}, \mathcal{N})$ is called a finite element.

For the cases considered in this course, K will be a polygon such as a triangle, square, tetrahedron or cube, and P will be a space of polynomials. Here, P' is the dual space to P, defined as the space of linear functions from P to \mathbb{R} . Examples of dual functions to P include:

- 1. The evaluation of $p \in P$ at a point $x \in K$.
- 2. The integral of $p \in P$ over a line $l \in K$.
- 3. The integral of $p \in P$ over K.
- 4. The evaluation of a component of the derivative of $p \in P$ at a point $x \in K$.

Exercise 13 Show that the four examples above are all linear functions from P to \mathbb{R} .

Ciarlet's finite element provides us with a standard way to define a basis for the P, called the nodal basis.

Definition 14 ((local) nodal basis) Let $(K, \mathcal{P}, \mathcal{N})$ be a finite element. The nodal basis is the basis $\{\phi_0, \phi_2, \dots, \phi_k\}$ of \mathcal{P} that is dual to \mathcal{N} , i.e.

$$N_i(\phi_i) = \delta_{ij}, \quad 0 \le i, j \le k.$$

We now introduce our first example of a Ciarlet element.

Definition 15 (The 1-dimensional Lagrange element) The 1-dimensional Lagrange element $(K, \mathcal{P}, \mathcal{N})$ of degree k is defined by

- 1. K is the interval [a, b] for $-\infty < a < b < \infty$.
- 2. P is the (k + 1)-dimensional space of degree k polynomials on K,
- 3. $\mathcal{N} = \{N_0, \dots, N_k\}$ with

$$N_i(v) = v(x_i), x_i = a + (b-a)i/k, \quad \forall v \in \mathcal{P}, i = 0, \dots, k.$$

Exercise 16 Show that the nodal basis for P is given by

$$\phi_i(x) = \frac{\prod_{j=0, j \neq i}^k (x - x_j)}{\prod_{j=0, j \neq i}^k (x_i - x_j)}, \quad i = 0, \dots, k.$$

2.2 Vandermonde matrix and unisolvence

More generally, It is useful computationally to write the nodal basis in terms of another arbitrary basis $\{\psi_i\}_{i=0}^k$. This transformation is represented by the Vandermonde matrix.

Definition 17 (Vandermonde matrix) Given a dual basis \mathcal{N} and a basis $\{\psi_j\}_{i=0}^k$,

the Vandermonde matrix is the matrix V with coefficients

$$V_{ij} = N_j(\psi_i).$$

This relationship is made clear by the following lemma.

Lemma 18 The expansion of the nodal basis $\{\phi_i\}_{i=0}^k$ in terms of another basis $\{\psi_i\}_{i=0}^k$ for \mathcal{P} ,

$$\phi_i(x) = \sum_{j=0}^k \mu_{ij} \psi_j(x),$$

has coefficients μ_{ij} , $0 \le i, j \le k$ given by

$$\mu = V^{-1}$$
,

where μ is the corresponding matrix.

Proof 19 The nodal basis definition becomes

$$\delta_{ij} = N_j(\phi_i) = \sum_{l=0}^k \mu_{il} N_j(\psi_l) = \sum_{l=0}^k \mu_{il} V_{lj} = (\mu V)_{ij},$$

where μ is the matrix with coefficients μ_{ij} , and V is the matrix with coefficients $N_j(\psi_i)$.

Given a triple $(K, \mathcal{P}, \mathcal{N})$, it is necessary to verify that \mathcal{N} is indeed a basis for \mathcal{P}' , i.e. that the Ciarlet element is well-defined. Then the nodal basis is indeed a basis for \mathcal{P} by construction. The following lemma provides a useful tool for checking this.

Lemma 20 (dual condition) Let K, \mathcal{P} be as defined above, and let $\{N_0, N_1, \ldots, N_k\} \in \mathcal{P}'$. Let $\{\psi_0, \psi_1, \ldots, \psi_k\}$ be a basis for \mathcal{P} .

Then the following three statements are equivalent.

- 1. $\{N_0, N_1, \ldots, N_k\}$ is a basis for \mathcal{P}' .
- 2. The Vandermonde matrix with coefficients

$$V_{ij} = N_j(\psi_i), 0 \le i, j \le k,$$

is invertible.

3. If $v \in \mathcal{P}$ satisfies $N_i(v) = 0$ for i = 0, ..., k, then $v \equiv 0$.

Proof 21 Let $\{N_0, N_1, \ldots, N_k\}$ be a basis for \mathcal{P}' . This is equivalent to saying that given element E of \mathcal{P}' , we can find basis coefficients $\{e_i\}_{i=0}^k \in \mathbb{R}$ such that

$$E = \sum_{i=0}^{k} e_i N_i.$$

This in turn is equivalent to being able to find a vector $e = (e_0, e_1, \dots, e_k)^T$ such that

$$b_i = E(\psi_i) = \sum_{j=0}^k e_j N_j(\psi_i) = \sum_{j=0}^k e_j V_{ij},$$

i.e. the equation Ve = b is solvable. This means that (1) is equivalent to (2).

On the other hand, we may expand any $v \in \mathcal{P}$ according to

$$v(x) = \sum_{i=0}^{k} f_i \psi_i(x).$$

Then

$$N_i(v) = 0 \iff \sum_{j=0}^k f_j N_i(\psi_j) = 0, \quad i = 0, 1, \dots, k,$$

by linearity of N_i . So (2) is equivalent to

$$\sum_{j=0}^{k} f_j N_i(\psi_j) = 0, \quad i = 0, 1, \dots, k \implies f_j = 0, j = 0, 1, \dots, k,$$

which is equivalent to V^T being invertible, which is equivalent to V being invertible, and so (3) is equivalent to (2).

This result leads us to introducing the following terminology.

Definition 22 (Unisolvence.) We say that \mathcal{N} determines \mathcal{P} if it satisfies condition 3 of Lemma 20. If this is the case, we say that $(K, \mathcal{P}, \mathcal{N})$ is unisolvent.

We can now go and directly apply this lemma to the 1D Lagrange elements.

Corollary 23 The 1D degree k Lagrange element is a finite element.

Proof 24 Let $(K, \mathcal{P}, \mathcal{N})$ be the degree k Lagrange element. We need to check that \mathcal{N} determines \mathcal{P} . Let $v \in \mathcal{P}$ with $N_i(v) = 0$ for all $N_i \in \mathcal{N}$. This means that

$$v(a + (b - a)i/k) = 0, i = 0, 1, \dots, k,$$

which means that v vanishes at k+1 points in K. Since v is a degree k polynomial, it must be zero by the fundamental theorem of algebra.

2.3 2D and 3D finite elements

We would like to construct some finite elements with 2D and 3D domains K. The fundamental theorem of algebra does not directly help us there, but the following lemma is useful when checking that \mathcal{N} determines \mathcal{P} in those cases.

Lemma 25 Let $p(x): \mathbb{R}^d \to \mathbb{R}$ be a polynomial of degree $k \geq 1$ that vanishes on a hyperplane Π_L defined by

$$\Pi_L = \{x : L(x) = 0\},\,$$

for a non-degenerate affine function $L(x): \mathbb{R}^d \to \mathbb{R}$. Then p(x) = L(x)q(x) where q(x) is a polynomial of degree k-1.

Proof 26 Choose coordinates (by shifting the origin and applying a linear transformation) such that $x = (x_1, ..., x_d)$ with $L(x) = x_d$, so Π_L is defined by $x_d = 0$. Then the general form for a polynomial is

$$P(x_1, \dots, x_d) = \sum_{i_d=0}^k \left(\sum_{|i_1+\dots+i_{d-1}| \le k-i_d} c_{i_1,\dots,i_{d-1},i_d} x_d^{i_d} \prod_{l=1}^{d-1} x_l^{i_l} \right),$$

Then, $p(x_1, ..., x_{d-1}, 0) = 0$ for all $(x_1, ..., x_{d-1})$, so

$$0 = \left(\sum_{|i_1 + \dots + i_{d-1}| \le k} c_{i_1, \dots, i_{d-1}, 0} \prod_{l=1}^{d-1} x_l^{i_l}\right)$$

which means that

$$c_{i_1,\dots,i_{d-1},0} = 0, \quad \forall |i_1 + \dots + i_{d-1}| \le k.$$

This means we may rewrite

$$P(x) = L(x) \underbrace{\left(\sum_{i_d=1}^k \sum_{|i_1+\ldots+i_{d-1}| \le k-i_d} c_{i_1,\ldots,i_{d-1},i_d} x_d^{i_d-1} \prod_{l=1}^{d-1} x_l^{i_l} \right)}_{P(x) = \underbrace{x_d}_{L(x)} \underbrace{\left(\sum_{i_d=0}^{k-1} \sum_{|i_1+\ldots+i_{d-1}| \le k-i_d} c_{i_1,\ldots,i_{d-1},i_d} x_d^{i_d-1} \prod_{l=1}^{d-1} x_l^{i_l} \right)}_{Q(x)},$$

with deg(Q) = k - 1.

Equipped with this tool we can consider some finite elements in two dimensions.

Definition 27 (Lagrange elements on triangles) The triangular Lagrange element of degree k $(K, \mathcal{P}, \mathcal{N})$, denoted Pk, is defined as follows.

- 1. K is a (non-degenerate) triangle with vertices z_1 , z_2 , z_3 .
- 2. \mathcal{P} is the space of degree k polynomials on K.
- 3. $\mathcal{N} = \{N_{i,j} : 0 \le i \le k, \ 0 \le j \le i\}$ defined by $N_{i,j}(v) = v(x_{i,j})$ where

$$x_{i,j} = z_1 + (z_2 - z_1)\frac{i}{k} + (z_3 - z_1)\frac{j}{k}.$$

We illustrate this for the cases k = 1, 2.

Example 28 (P1 elements on triangles) The nodal basis for P1 elements is point evaluation at the three vertices.

Example 29 (P2 elements on triangles) The nodal basis for P2 elements is point evaluation at the three vertices, plus point evaluation at the three edge centres.

We now need to check that that the degree k Lagrange element is a finite element, i.e. that \mathcal{N} determines \mathcal{P} . We will first do this for P1.

Lemma 30 The degree 1 Lagrange element is a finite element.

Proof 31 Let Π_1 , Π_2 , Π_3 be the three lines containing the vertices z_2 and z_3 , z_1 and z_3 , and z_1 and z_3 respectively, and defined by $L_1=0$, $L_2=0$, and $L_3=0$ respectively. Consider a linear polynomial p vanishing at z_1 , z_2 , and z_3 . The restriction $p|_{\Pi_1}$ of p to Π_1 is a linear function vanishing at two points, and therefore p=0 on Π_1 , and so $p=L_1(x)Q(x)$, where Q(x) is a degree 0 polynomial, i.e. a constant c. We also have

$$0 = p(z_1) = cL_1(z_1) \implies c = 0,$$

since $L_1(z_1) \neq 0$, and hence $p(x) \equiv 0$. This means that \mathcal{N} determines \mathcal{P} .

This technique can then be extended to degree 2.

Lemma 32 The degree 2 Lagrange element is a finite element.

Proof 33 Let p be a degree 2 polynomial with $N_i(p)$ for all of the degree 2 dual basis elements. Let Π_1 , Π_2 , Π_3 , L_1 , L_2 and L_3 be defined as for the proof of Lemma . $p|_{\Pi_1}$ is a degree 2 scalar polynomial vanishing at 3 points, and therefore p=0 on Π_1 , and so $p(x)=L_1(x)Q_1(x)$ with $\deg(Q_1)=1$. We also have $0=p|_{\Pi_2}=L_1Q_1|_{\Pi_2}$, so $Q_1|_{\Pi_2}=0$ and we conclude that $p(x)=cL_1(x)L_2(x)$. Finally, p also vanishes at the midpoint of L_3 , so we conclude that c=0 as required.

The technique extends further to degree 3.

Exercise 34 Show that the degree 3 Lagrange element is a finite element.

Going beyond degree 3, we have more than 1 nodal variable taking point evaluation inside the triangle. To deal with this, we use the nested triangular structure of the Lagrange triangle.

Lemma 35 The degree k Lagrange element is a finite element for k > 3.

Proof 36 We prove by induction. Assume that the degree k-3 Lagrange element is a finite element. Let p be a degree k polynomial with $N_i(p)$ for all of the degree k dual basis elements. Let Π_1 , Π_2 , Π_3 , L_1 , L_2 and L_3 be defined as for the proof of lemma 30. The restriction $p|_{\Pi_1}$ is a degree k polynomial in one variable that vanishes at k+1 points, and therefore $p(x)=L_1(x)Q_1(x)$, with $\deg(Q_1)=k-1$. p and therefore Q also vanishes on Π_2 , so $Q_1(x)=L_2(x)Q_2(x)$.

Repeating the argument again means that $p(x) = L_1(x)L_2(x)L_3(x)Q_3(x)$, with $\deg(Q_3) = k-3$. Q_3 must vanish on the remaining points in the interior of K, which are arranged in a smaller triangle K' and correspond to the evaluation points for a degree k-3 Lagrange finite element on K'. From the inductive hypothesis, and using the results for k=1,2,3, we conclude that $Q_3 \equiv 0$, and therefore $p\equiv 0$ as required.

2.4 Some more exotic elements

We now consider some finite elements that involve derivative evaluation. The Hermite elements involve evaluation of first derivatives as well as point evaluations.

Definition 37 (Cubic Hermite elements on triangles) The cubic Hermite element is defined as follows:

- 1. K is a (nondegenerate) triangle,
- 2. \mathcal{P} is the space of cubic polynomials on K,
- 3. $\mathcal{N} = \{N_1, N_2, \dots, N_{10}\}$ defined as follows:
 - (N_1, \ldots, N_3) : evaluation of p at vertices,
 - (N_4, \ldots, N_9) : evaluation of the gradient of p at the 3 triangle vertices.
 - N_{10} : evaluation of p at the centre of the triangle.

It turns out that the Hermite element is insufficient to guarantee functions with continuous derivatives between triangles. This problem is solved by the Argyris element.

Definition 38 (Quintic Argyris elements on triangles) The quintic Argyris element is defined as follows:

- 1. K is a (nondegenerate) triangle,
- 2. P is the space of quintic polynomials on K,
- 3. N defined as follows:
 - evaluation of p at 3 vertices,
 - evaluation of gradient of p at 3 vertices,
 - evaluation of Hessian of p at 3 vertices,
 - evaluation of the gradient normal to 3 triangle edges.

2.5 Global continuity

Next we need to know how to glue finite elements together to form spaces defined over a triangulation (mesh). To do this we need to develop a language for specifying connections between finite element functions between element domains.

Definition 39 (Finite element space) Let \mathcal{T} be a triangulation made of triangles K_i , with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$. A space V of functions on \mathcal{T} is called a finite element space if for each $u \in V$, and for each $K_i \in \mathcal{T}$, $u|_{K_i} \in \mathcal{P}_i$.

Note that the set of finite elements do not uniquely determine a finite element space, since we also need to specify continuity requirements between triangles, which we will do in this chapter.

Definition 40 (Finite element space) A finite element space V is a C^m finite element space if $u \in C^m$ for all $u \in V$.

The following lemma guides use in how to inspect the continuity of finite element functions.

Lemma 41 (Continuity lemma) *Let* T *be a triangulation on* Ω *, and let* V *be a finite element space defined on* T. *The following two statements are equivalent.*

- 1. V is a C^m finite element space.
- 2. The following two conditions hold.
- For each vertex z in \mathcal{T} , let $\{K_i\}_{i=1}^m$ be the set of triangles that contain z. Then $u|_{K_1}(z) = u|_{K_2}(z) = \ldots = u|_{K_m}(z)$, for all functions $u \in V$, and similarly for all of the partial derivatives of degrees up to m.
- For each edge e in \mathcal{T} , let K_1 , K_2 be the two triangles containing e. Then $u|_{K_1}(z) = u|_{K_2}(z)$, for all points z on the interior of e, and similarly for all of the partial derivatives of degrees up to m.

Proof 42 V is polynomial on each triangle K, so continuity at points on the interior of each triangle K is immediate. We just need to check continuity at points on vertices, and points on the interior of edges, which is equivalent to the two parts of the second condition.

This means that we just need to guarantee that the polynomial functions and their derivatives agree at vertices and edges (similar ideas extend to higher dimensions). We achieve this by assigning nodal variables (and their associated nodal basis functions) appropriately to vertices, edges etc. of each triangle K. First we need to introduce this terminology.

Definition 43 (local and global mesh entities) Let K be a triangle. The local mesh entities of K are the vertices, the edges, and K itself. The global mesh entities of a triangulation T are the vertices, edges and triangles comprising T.

Having made this definition, we can now talk about how nodal variables can be assigned to local mesh entities in a geometric decomposition.

Definition 44 (local geometric decomposition) Let $(K, \mathcal{P}, \mathcal{N})$ be a finite element. We say that the finite element has a (local) geometric decomposition if each dual basis function N_i can be associated with a single mesh entity $w \in W$ such that for any $f \in \mathcal{P}$, $N_i(f)$ can be calculated from f and derivatives of f evaluated on w.

To discuss C^m continuity, we need to introduce some further vocabulary about the topology of K.

Definition 45 (closure of a local mesh entity) Let w be a local mesh entity for a triangle. The closure of w is the set of local mesh entities contained in w (including w itself).

This allows us to define the degree of continuity of the local geometric decomposition.

Definition 46 (C^m geometric decomposition) Let $(K, \mathcal{P}, \mathcal{N})$ be a finite element with geometric decomposition W. We say that W is a C^m geometric decomposition, if for each local mesh entity w, for any $f \in \mathcal{P}$, the restriction $f|_w$ of f (and the restriction $D^k f|_w$ of the k-th derivative of f to w for $k \leq m$) can be obtained from the set of dual basis functions associated with entities in the closure of w, applied to f.

The idea behind this definition is that if two triangles K_1 and K_2 are joined at a vertex, with finite elements $(K_1, \mathcal{P}_1, \mathcal{N}_1)$ and $(K_2, \mathcal{P}_2, \mathcal{N}_2)$, then if the \mathcal{N}_1 variables associated with the vertex applied to a function u agree with the corresponding \mathcal{N}_2 variables also associated with that vertex also applied to u, then the function u will be C^m continuous through the vertex. Similarly, if K_1 and K_2 are joined at an edge, then if the corresponding \mathcal{N}_1

and \mathcal{N}_2 nodal variables associated with that edge agree when applied to u, then u will be C^m continuous through that edge. We just need to define these correspondences.

We explore this definition through a couple of exercises.

Exercise 47 (Show that the Lagrange elements of degree k have C^0 geometric decompositions.)

Exercise 48 (Show that the Argyris element has a C^1 geometric decomposition.)

We now use the geometric decomposition to construct global finite element spaces over the whole triangulation (mesh). We just need to define what it means for elements of the nodal variables from the finite elements of two neighbouring triangles to "correspond".

We start by considering spaces of functions that are discontinuous between triangles, before defining C^m continuous subspaces.

Definition 49 (Discontinuous finite element space) Let \mathcal{T} be a triangulation, with finite elements $(K_i, P_i, \mathcal{N}_i)$ for each triangle K_i . The associated discontinuous finite element space V, is defined as

$$V = \{u : u|_{K_i} \in P_i, \forall K_i \in \mathcal{T}\}.$$

This defines families of discontinuous finite element spaces.

Example 50 (Discontinuous Lagrange finite element space) Let \mathcal{T} be a triangulation, with Lagrange elements of degree k, $(K_i, P_i, \mathcal{N}_i)$, for each triangle $K_i \in \mathcal{T}$. The corresponding discontinuous finite element space, denoted P'k'DG, is called the discontinuous Lagrange finite element space of degree k.

Next we need to associate each nodal variable in each element to a vertex, edge or triangle of the triangulation \mathcal{T}_h , i.e. the global mesh entitles. The following definition explains how to choose this association.

Definition 51 (Global C^m **geometric decomposition)** Let \mathcal{T} be a triangulation with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$, each with a C^m geometric decomposition. Assume that for each global mesh entity w, the n_w triangles containing w have finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$ each with M_w dual basis functions associated with w. Further, each of these basis functions can be enumerated $N_{i,j}^w \in \mathcal{N}_i$, $j=1,\ldots,M_w$, such that $N_{1,j}^w(u|_{K_1})=N_{2,j}^w(u|_{K_2})=\ldots=N_{n_w,j}^w(u|_{K_n})$, $j=1,\ldots,M_w$, for all functions $u\in C^m(\Omega)$.

This combination of finite elements on \mathcal{T} together with the above enumeration of dual basis functions on global mesh entities is called a global C^m geometric decomposition.

Now we use this global C^m geometric decomposition to build a finite element space on the triangulation.

Definition 52 (Finite element space from a global C^m **geometric decomposition)** Let \mathcal{T} be a triangulation with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$, each with a C^m geometric decomposition, and let \hat{V} be the corresponding discontinuous finite element space. Then the global C^m geometric decomposition defines a subspace V of \hat{V} consisting of all functions that u satisfy $N_{1,j}^w(u|_{K_1}) = N_{2,j}^w(u|_{K_2}) = \ldots = N_{n_w,j}^w(u|_{K_{n_w}}), \quad j=1,\ldots,M_w$ for all mesh entities $w \in \mathcal{T}$.

The following result shows that the global C^m geometric decomposition is a useful definition.

Lemma 53 Let V be a finite element space defined from a global C^m geometric decomposition. Then V is a C^m finite element space.

Proof 54 From the local C^m decomposition, functions and derivatives up to degree m on vertices and edges are uniquely determined from dual basis elements associated with those vertices and edges, and from the global C^m decomposition, the agreement of dual basis elements means that functions and derivatives up to degree m agree on vertices and edges, and hence the functions are in C^m from Lemma 41.

We now apply this to a few examples, which can be proved as exercises.

Example 55 The finite element space built from the C^0 global decomposition built from degree k Lagrange element is called the degree k continuous Lagrange finite element space, denoted P'k'.

Example 56 The finite element space built from the C^1 global decomposition built from the quintic Argyris element is called the Argyris finite element space.

In this section, we have built a theoretical toolbox for the construction of finite element spaces. In the next section, we move on to studying how well we can approximate continuous functions as finite element functions.

INTERPOLATION OPERATORS

In this section we investigate how continuous functions can be approximated by finite element functions. We start locally, looking at a single finite element, and then move globally to function spaces on a triangulation.

3.1 Local and global interpolation operators

Definition 57 (Local interpolant) Given a finite element $(K, \mathcal{P}, \mathcal{N})$, with corresponding nodal basis $\{\phi_i\}_{i=0}^k$. Let v be a function such that $N_i(v)$ is well-defined for all i. Then the local interpolant \mathcal{I}_K is an operator mapping v to \mathcal{P} such that

$$(I_K v)(x) = \sum_{i=0}^k N_i(v)\phi_i(x).$$

We now discuss some useful properties of the local interpolant.

Lemma 58 The operator I_K is linear.

Proof 59 (Exercise.)

Lemma 60

$$N_i(I_K(v)) = N_i(v), \forall 0 \le i \le k.$$

Proof 61 (Exercise.)

Lemma 62 I_K is the identity when restricted to \mathcal{P} .

Proof 63 (Exercise.)

By combining together the local interpolants in each triangle of the triangulation, we obtain the global interpolant into the finite element space.

Definition 64 (Global interpolant) Let V_h be a finite element space constructed from a triangulation \mathcal{T}_h with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$, each with a C^m geometric decomposition. The global interpolant \mathcal{I}_h is defined by $\mathcal{I}_h u \in V_h$ such that

$$\mathcal{I}_h u|_K = I_K u$$

for each $K \in \mathcal{T}_h$.

3.2 Measuring interpolation errors

Next we look at how well we can approximate continuous functions using the interpolation operator, i.e. we want to measure the approximation error $\mathcal{I}_h u - u$. We are interested in integral formulations, so we want to use integral quantities to measure errors. We have already seen the L^2 norm. It is also useful to take derivatives into account when measuring the error. To discuss higher order derivatives, we introduce the multi-index.

Definition 65 (Multi-index.) For d-dimensional space, a multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ assigns the number of partial derivatives in each Cartesian direction. We write $|\alpha| = \sum_{i=1}^d \alpha_i$.

This means we can write mixed partial derivatives, for example if $\alpha = (1, 2)$ then

$$D^{\alpha}u = \frac{\partial^3 u}{\partial x \partial y^2}.$$

Now we can define some norms involving derivatives for measuring errors.

Definition 66 (H^k seminorm and norm) The H^k seminorm is defined as

$$|u|_{H^k}^2 = \sum_{|\alpha|=k} \int_{\Omega} |D^{\alpha}u|^2 dx,$$

where the sum is taken over all multi-indices of size k i.e. all the derivatives are of degree k.

The H^k norm is defined as

$$||u||_{H^k}^2 = \sum_{i=0}^k |u|_{H^i}^2.$$

where we conventionally write $|u|_{H^0} = ||u||_{L^2}$.

To help to estimate interpolation errors, we quote the following important result (which we will return to much later).

Theorem 67 (Sobolev's inequality (for continuous functions)) Let Ω be an n-dimensional domain with Lipschitz boundary, and let u be a continuous function with k continuous derivatives, i.e. $u \in C^{k,\infty}(\Omega)$. Let k be an integer with k > n/2. Then there exists a constant C (depending only on Ω) such that

$$||u||_{C^{\infty}(\Omega)} = \max_{x \in \Omega} |u(x)| \le C||u||_{H^{k}(\Omega)}.$$

Proof 68 See a functional analysis course or textbook.

This is extremely useful because it means that we can measure the H^k norm by integrating and know that it gives an upper bound on the value of u at each point. We say that u is in $C^{\infty}(\Omega)$ if $\|u\|_{C^{\infty}(\Omega)} < \infty$, and Sobolev's inequality tells us that this is the case if $\|u\|_{H^k(\Omega)} < \infty$.

This result can be easily extended to derivatives.

Corollary 69 (Sobolev's inequality for derivatives (for continuous functions)) Let Ω be a n-dimensional domain with Lipschitz boundary, and let $u \in C^{k,\infty}(\Omega)$ Let k be an integer with k-m>n/2. Then there exists a constant C (depending only on Ω) such that

$$||u||_{C^{m,\infty}(\Omega)} := \sum_{|\alpha| \le m} \max_{x \in \Omega} |D^{\alpha}u(x)| \le C||u||_{H^k(\Omega)}.$$

Proof 70 *Just apply Sobolev's inequality to the m derivatives of u.*

3.3 Approximation by averaged Taylor polynomials

The basic tool for analysing interpolation error for continuous functions is the Taylor series. Rather than taking the Taylor series about a single point, since we are interested in integral quantities, it makes sense to consider an averaged Taylor series over some region inside each cell. This will become important later when we start thinking about more general types of derivative that only exist in an integral sense.

Definition 71 (Averaged Taylor polynomial) Let $\Omega \subset \mathbb{R}^n$ be a domain with diameter d, that is star-shaped with respect to a ball B contained within Ω . For $f \in C^{k,\infty}$ the averaged Taylor polynomial $Q_{k,B}f \in \mathcal{P}_k$ is defined as

$$Q_{k,B}f(x) = \frac{1}{|B|} \int_B T^k f(y,x) \, dy,$$

where $T^k f$ is the Taylor polynomial of degree k of f,

$$T^{k}f(y,x) = \sum_{|\alpha| \le k} D^{\alpha}f(y) \frac{(x-y)^{\alpha}}{\alpha!},$$
$$\alpha! = \prod_{i=1}^{n} \alpha_{i}!,$$
$$x^{\alpha} = \prod_{i=1}^{n} x_{i}^{\alpha_{i}}.$$

Now we develop an estimate of the error $T^k f - f$.

Theorem 72 Let $\Omega \subset \mathbb{R}^n$ be a domain with diameter d, that is star-shaped with respect to a ball B contained within Ω . Then there exists a constant C(k,n) such that for $0 \le |\beta| \le k+1$ and all $f \in C^{k+1,\infty}(\Omega)$,

$$||D^{\beta}(f - Q_{k,B}f)||_{L^{2}} \le C \frac{|\Omega|^{1/2}}{|B|^{1/2}} d^{k+1-|\beta|} |f|_{H^{k+1}(\Omega)}.$$

Proof 73 The Taylor remainder theorem (see a calculus textbook) gives

$$f(x) - T_k f(y, x) = (k+1) \sum_{|\alpha| = k+1} \frac{(x-y)^{\alpha}}{\alpha!} \int_0^1 D^{\alpha} f(ty + (1-t)x) t^k dt,$$

when $f \in C^{k+1,\infty}$.

Integration over y in B and dividing by |B| gives

$$f(x) - Q_{k,B}f(x) = \frac{k+1}{|B|} \sum_{|\alpha|=k+1} \int_B \frac{(x-y)^{\alpha}}{\alpha!} \times \int_0^1 D^{\alpha} f(ty + (1-t)x) t^k dt dy.$$

Then

$$\int_{\Omega} |f(x) - Q_{k,B}f(x)|^2 dx \le C \frac{d^{2(k+1)}}{|B|^2} \sum_{|\alpha| = k+1} \int_{\Omega} \left(\int_{B} \int_{0}^{1} |D^{\alpha}f(ty + (1-t)x)| t^k dt dy \right)^2 dx,
\le C_0 \frac{d^{2(k+1)}}{|B|^2} \sum_{|\alpha| = k+1} \int_{\Omega} \int_{B} \int_{0}^{1} |D^{\alpha}f(ty + (1-t)x)|^2 dt dy \int_{B} \int_{0}^{1} t^{2k} dt dy dx.$$

Then

$$\int_{\Omega} |f(x) - Q_{k,B}f(x)|^2 dx \le C_1 \frac{d^{2(k+1)}}{|B|^2} \sum_{|\alpha| = k+1} \int_{\Omega} \int_{B} \int_{0}^{1} |D^{\alpha}f(ty + (1-t)x)|^2 dt dy dx.$$

We will get the result by changing variables and exchanging the t, y and x integrals. To avoid a singularity when t = 0 or t = 1, for each α term we can split the t integral into [0, 1/2] and [1/2, 1]. Call these terms I and II.

Denote by g_{α} the extension by zero of $D^{\alpha}f$ to \mathbb{R}^n . Then

$$I = \int_{B} \int_{0}^{1/2} \int_{\mathbb{R}^{n}} |g_{\alpha}(ty + (1-t)x)|^{2} dx dt dy,$$

$$= \int_{B} \int_{0}^{1/2} \int_{\mathbb{R}^{n}} |g_{\alpha}((1-t)x)|^{2} dx dt dy,$$

$$= \int_{B} \int_{0}^{1/2} \int_{\mathbb{R}^{n}} |g_{\alpha}(z)|^{2} (1-t)^{-n} dz dt dy,$$

$$\leq 2^{n-1} |B| \int_{\Omega} |D^{\alpha} f(z)|^{2} dz.$$

Similarly, for II,

$$II = \int_{B} \int_{1/2}^{1} \int_{\mathbb{R}^{n}} |g_{\alpha}(ty + (1 - t)x)|^{2} dx dt dy,$$

$$= \int_{B} \int_{1/2}^{1} \int_{\mathbb{R}^{n}} |g_{\alpha}(ty)|^{2} dx dt dy,$$

$$= \int_{B} \int_{1/2}^{1} \int_{\mathbb{R}^{n}} |g_{\alpha}(z)|^{2} t^{-n} dz dt dy,$$

$$\leq 2^{n-1} |B| \int_{\Omega} |D^{\alpha} f(z)|^{2} dz.$$

Hence, we obtain the required bounds for $|\beta| = 0$. For higher derivatives we use the fact that

$$D^{\beta}Q_{k,B}f(x) = Q_{k-|\beta|,B}D^{\beta}f(x),$$

which immediately leads to the estimate for $|\beta| > 0$.

Now we develop this into an estimate that depends on the diameter of the triangle we are interpolating to.

Corollary 74 Let K_1 be a triangle with diameter 1. There exists a constant C(k, n) such that

$$||f - Q_{k,B}f||_{H^k(K_1)} \le C|f|_{H^{k+1}(K_1)}.$$

Proof 75 Take the maximum over the constants for the derivative contributions of the left-hand side with d=1 and use the previous result.

3.4 Local and global interpolation errors

Now we will use the Taylor polynomial estimates to derive error estimates for the local interpolation operator. We start by looking at a triangle with diameter 1, and then use a scaling argument to obtain error estimates in terms of the diameter h. It begins by getting the following bound.

Lemma 76 Let $(K_1, \mathcal{P}, \mathcal{N})$ be a finite element such that K_1 is a triangle with diameter 1, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and $\|N_i\|_{C^{l,\infty}(K_1)'} < \infty$,

$$||N_i||_{C^{l,\infty}(K_1)'} = \sup_{\|u\|_{C^{l,\infty}(K_1)} > 0} \frac{|N_i(u)|}{\|u\|_{W_{\infty}^l(K_1)}}$$
(Dual norm of N_i)

Let k-l > n/2, and $u \in C^{k,\infty}(\Omega)$. Then

$$\|\mathcal{I}_{K_1}u\|_{H^k(K_1)} \le C\|u\|_{H^k(K_1)}.$$

Proof 77 Let $\{\phi_i\}_{i=1}^n$ be the nodal basis for \mathcal{P} . Then

$$\|\mathcal{I}_{K_{1}}u\|_{H^{k}(K_{1})} \leq \sum_{i=1}^{k} \|\phi_{i}\|_{H^{k}(K_{1})} |N_{i}(u)|$$

$$\leq \underbrace{\sum_{i=1}^{k} \|\phi_{i}\|_{H^{k}(K_{1})} \|N_{i}\|_{C^{l,\infty}(K_{1})'}}_{C_{0}} \|u\|_{C^{l,\infty}(K_{1})},$$

$$\leq C\|u\|_{H^{k}(K_{1})}$$

where the Sobolev inequality was used in the last line.

Now we can directly apply this to the interpolation operator error estimate on the triangle with diameter 1. It is the standard trick of adding and subtracting something, in this case the Taylor polynomial.

Lemma 78 Let $(K_1, \mathcal{P}, \mathcal{N})$ be a finite element such that K_1 has diameter 1, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contain all polynomials of degree k and below, with k > l + n/2. Let $u \in C^{k+1,\infty}(K_1)$. Then for $i \leq k$, the local interpolation operator satisfies

$$|\mathcal{I}_{K_1}u - u|_{H^i(K_1)} \le C_1|u|_{H^{k+1}(K_1)}.$$

Proof 79

$$\begin{aligned} |\mathcal{I}_{K_{1}}u - u|_{H^{i}(K_{1})}^{2} &\leq \|\mathcal{I}_{K_{1}}u - u\|_{H^{k}(K_{1})}^{2} \\ &= \|\mathcal{I}_{K_{1}}u - Q_{k,B}u + Q_{k,B}u - u\|_{H^{k}(K_{1})}^{2} \\ &\leq \|Q_{k,B}u - u\|_{H^{k}(K_{1})}^{2} + \|\mathcal{I}(u - Q_{k,B}u)\|_{H^{k}(K_{1})}^{2} \\ &\leq \|Q_{k,B}u - u\|_{H^{k}(K_{1})}^{2} + C^{2}\|Q_{k,B}u - u\|_{H^{k}(K_{1})}^{2}, \\ &\leq (1 + C^{2})|u|_{H^{k+1}(K_{1})}^{2}, \end{aligned}$$

where we used the fact that $I_{K_1}Q_{k,B}u=Q_{k,B}u$ in the second line and the previous lemma in the third line.

Now we apply a scaling argument to translate this to triangles with diameter h.

Lemma 80 Let $(K, \mathcal{P}, \mathcal{N})$ be a finite element such that K has diameter d, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contains all polynomials of degree k and below, with k > l + n/2. Let $u \in C^{k+1,\infty}(K_1)$. Then for $i \leq k$, the local interpolation operator satisfies

$$|\mathcal{I}_K u - u|_{H^i(K)} \le C_K d^{k+1-i} |u|_{H^{k+1}(K)}.$$

where C_K is a constant that depends on the shape of K but not the diameter.

Proof 81 Consider the change of variables $x \to \phi(x) = x/d$. This map takes K to K_1 with diameter 1. Then

$$\int_{K} |D^{\beta}(I_{K}u - u)|^{2} dx = d^{-2|\beta|+1} \int_{K_{1}} |D^{\beta}(I_{K_{1}}u \circ \phi - u \circ \phi)|^{2} dx,$$

$$\leq C_{1}^{2} d^{-2|\beta+1} \sum_{|\alpha|=k+1} \int_{K_{1}} |D^{\alpha}u \circ \phi|^{2} dx,$$

$$\leq C_{1}^{2} d^{-2|\beta+2(k+1)} \sum_{|\alpha|=k+1} \int_{K} |D^{\alpha}u|^{2} dx,$$

$$= C_{1}^{2} d^{2(-|\beta|+k+1)} |u|_{H^{k+1}(K)}^{2},$$

and taking the square root gives the result.

So far we have just developed an error estimate for the local interpolant on a single triangle. Now we extend this to finite element spaces defined on the whole triangulation.

Theorem 82 Let \mathcal{T} be a triangulation of Ω with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$, such that the minimum aspect ratio γ of the triangles K_i satisfies $\gamma > 0$, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contains all polynomials of degree k and below, with k > l + n/2. Let $k \in \mathbb{C}^{k+1,\infty}(K_1)$. Let $k \in \mathbb{C}^{k+1,\infty}(K_1)$. Let $k \in \mathbb{C}^{k+1,\infty}(K_1)$ be the maximum over all of the triangle diameters, with $k \in \mathbb{C}^{k+1,\infty}(K_1)$ and $k \in \mathbb{C}^{k+1,\infty}(K_1)$ be the maximum over all of the triangle diameters, with $k \in \mathbb{C}^{k+1,\infty}(K_1)$ and $k \in \mathbb{C}^{k+1,\infty}(K_1)$ are the formula of the triangle diameters.

$$\|\mathcal{I}_h u - u\|_{H^i(\Omega)} \le C h^{k+1-i} |u|_{H^{k+1}(\Omega)}.$$

(Recalling that we use the "broken" finite element derivative in norms for $\mathcal{I}_h u$ over Ω .

Proof 83

$$\begin{split} \|\mathcal{I}_h u - u\|_{H^i(\Omega)}^2 &= \sum_{K \in \mathcal{T}} \|\mathcal{I}_K u - u\|_{H^i(K)}^2, \\ &\leq \sum_{K \in \mathcal{T}} C_K d_K^{2(k+1-i)} |u|_{H^{k+1}(K)}^2, \\ &\leq C_{\max} h^{2(k+1-i)} \sum_{K \in \mathcal{T}} |u|_{H^{k+1}(K)}^2, \\ &= C_{\max} h^{2(k+1-i)} |u|_{H^{k+1}(\Omega)}^2, \end{split}$$

M345A47 Finite Elements: Analysis and Implementation, Edition 2020.0

where the existence of the $C_{\max} = \max_K C_K < \infty$ is due to the lower bound in the aspect ratio.

In this section, we have built a theoretical toolbox for the interpolation of functions to finite element spaces. In the next section, we move on to studying the solveability of finite element approximations.

FINITE ELEMENT PROBLEMS: SOLVABILITY AND STABILITY

In section 1, we saw the example of a finite element approximation for Poisson's equation in the unit square, which we now recall below.

Definition 84 The finite element approximation $u_h \in \mathring{V}_h$ to the solution u_h of Poisson's equation is defined by

$$\int_{\Omega} \nabla v \cdot \nabla u_h \, dx = \int_{\Omega} v f \, dx, \quad \forall v \in \mathring{V}_h. \tag{4.1}$$

A fundamental question is whether the solution u_h exists and is unique. This question is of practical interest because if these conditions are not satisfied, then the matrix-vector system for the basis coefficients of u_h will not be solvable. To answer this question for this approximation (and others for related equations), we will use some general mathematical machinery about linear problems defined on Hilbert spaces. It will turn out that this machinery will also help us show that the approximation u_h converges to the exact solution u (and in what sense).

4.1 Finite element spaces and other Hilbert spaces

In the previous sections, we introduced the concept of finite element spaces, which contain certain functions defined on a domain Ω . Finite element spaces are examples of vector spaces (hence the use of the word "space").

Definition 85 (Vector space) A vector space over the real numbers \mathbb{R} is a set V, with an addition operator $+: V \times V \to V$, plus a scalar multiplication operator $\times: \mathbb{R} \times V \to V$, such that:

- 1. There exists a unique zero element $e \in V$ such that:
- $k \times e = e$ for all $k \in \mathbb{R}$,
- $0 \times v = e \text{ for all } v \in V$,
- e + v = v for all $v \in V$.
- 1. V is closed under addition and multiplication, i.e.,

$$a \times u + v \in V$$
 for all $u, v \in V$, $a \in \mathbb{R}$.

Lemma 86 Let V be a finite element space. Then V is a vector space.

Proof 87 First, we note that the zero function u(x) := 0 is in V, and satisfies the above properties. Further, let $u, v \in V$, and $a \in \mathbb{R}$. Then, when restricted to each triangle K_i , $u + av \in P_i$. Also, for each shared mesh entity, the shared nodal variables agree, i.e. $N_{i,j}[u + av] = N_{i,j}[u + av]$, by linearity of nodal variables. Therefore, $u + av \in V$.

We now introduce bilinear forms on vector spaces. Bilinear forms are important because they will represent the left hand side of finite element approximations of linear PDEs.

Definition 88 (Bilinear form) A bilinear form $b(\cdot, \cdot)$ on a vector space V is a mapping $b: V \times V \rightarrow \mathbb{R}$, such that

- 1. $v \to b(v, w)$ is a linear map in v for all w.
- 2. $v \to b(w, v)$ is a linear map in v for all w.

It is a symmetric bilinear form if in addition, b(v, w) = b(w, v), for all $v, w \in V$.

Here are two important examples of bilinear forms on finite element spaces.

Example 89 Let V_h be a finite element space. The following are bilinear forms on V_h ,

$$b(u, v) = \int_{\Omega} uv \, dx,$$

$$b(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx.$$

To turn a vector space into a Hilbert space, we need to select an inner product.

Definition 90 (Inner product) A real inner product, denoted by (\cdot, \cdot) , is a symmetric bilinear form on a vector space V with

- 1. $(v,v) \ge 0 \ \forall v \in V$,
- 2. $(v,v) = 0 \iff v = 0$.

This enables the following definition.

Definition 91 (Inner product space) We call a vector space $(V, (\cdot, \cdot))$ equipped with an inner product an inner product space.

We now introduce two important examples of inner products for finite element spaces.

Definition 92 (L^2 inner product) Let f, g be two functions in $L^2(\Omega)$. The L^2 inner product between f and g is defined as

$$(f,g)_{L^2} = \int_{\Omega} fg \, dx.$$

The L^2 inner product satisfies condition 2 provided that we understand functions in L^2 as being equivalence classes of functions under the relation $f \equiv g \iff \int_{\Omega} (f-g)^2 dx = 0$.

Definition 93 (H^1 inner product) Let f, g be two C^0 finite element functions. The H^1 inner product between f and g is defined as

$$(f,g)_{H^1} = \int_{\Omega} fg + \nabla f \cdot \nabla g \, dx.$$

The H^1 inner product satisfies condition 2 since

$$(f, f)_{L^2} < (f, f)_{H^1}$$
.

The Schwarz inequality is a useful tool for bounding the size of inner products.

Theorem 94 (Schwarz inequality) If $(V, (\cdot, \cdot))$ is an inner product space, then

$$|(u,v)| \le (u,u)^{1/2} (v,v)^{1/2}.$$

Equality holds if and only if $u = \alpha v$ for some $\alpha \in \mathbb{R}$.

Proof 95 See a course on vector spaces.

Our solvability conditions will make use of norms that measure the size of elements of a vector space (the size of finite element functions, in our case).

Definition 96 (Norm) Given a vector space V, a norm $\|\cdot\|$ is a function from V to \mathbb{R} , with

- $1. ||v|| \ge 0, \forall v \in V,$
- 2. $||v|| = 0 \iff v = 0$,
- 3. $||cv|| = |c|||v|| \forall c \in \mathbb{R}, v \in V$,
- 4. $||v + w|| \le ||v|| + ||w||$.

For inner product spaces, there is a natural choice of norm.

Lemma 97 Let $(V, (\cdot, \cdot))$ be an inner product space. Then $||v|| = \sqrt{(v, v)}$ defines a norm on V.

Proof 98 From bilinearity we have

$$\|\alpha v\| = \sqrt{(\alpha v, \alpha v)} = \sqrt{\alpha^2(v, v)} = |\alpha| \|v\|,$$

hence property 3.

 $||v|| = (v, v)^{1/2} \ge 0$, hence property 1.

If
$$0 = ||v|| = (v, v)^{1/2} \implies (v, v) = 0 \implies v = 0$$
, hence property 2.

We finally check the triangle inequality (property 4).

$$\begin{aligned} \|u+v\|^2 &= (u+v,u+v) \\ &= (u,u) + 2(u,v) + (v,v) \\ &= \|u\|^2 + 2(u,v) + \|v\|^2 \\ &\leq \|u\|^2 + 2\|u\| \|v\| + \|v\|^2 \quad \textit{[Schwarz]}, \\ &= (\|u\| + \|v\|)^2, \end{aligned}$$

hence $||u+v|| \le ||u|| + ||v||$.

We introduce the following useful term.

Definition 99 (Normed space) A vector space V with a norm $\|\cdot\|$ is called a normed vector space, written $(V, \|\cdot\|)$.

To finish our discussion of Hilbert spaces, we need to review the concept of completeness (which you might have encountered in an analysis course). This seems not so important since finite element spaces are finite dimensional, but later we shall consider sequences of finite element spaces with smaller and smaller triangles, where completeness becomes important.

Completeness depends on the notion of a Cauchy sequence.

Definition 100 (Cauchy sequence) A Cauchy sequence on a normed vector space $(V, \|\cdot\|)$ is a sequence $\{v_i\}_{i=1}^{\infty}$ satisfying $\|v_j - v_k\| \to 0$ as $j, k \to \infty$.

This definition leads to the definition of completeness.

Definition 101 (Complete normed vector space) A normed vector space $(V, \| \cdot \|)$ is complete if all Cauchy sequences have a limit $v \in V$ such that $\|v - v_j\| \to 0$ as $j \to \infty$.

Finally, we reach the definition of a Hilbert space.

Definition 102 (Hilbert space) An inner product space $(V, (\cdot, \cdot))$ is a Hilbert space if the corresponding normed space $(V, \|\cdot\|)$ is complete.

All finite dimensional normed vector spaces are complete. Hence, C^0 finite element spaces equipped with L^2 or H^1 inner products are Hilbert spaces. Later we shall understand our finite element spaces as subspaces of infinite dimensional Hilbert spaces.

4.2 Linear forms on Hilbert spaces

We will now build some structures on Hilbert spaces that allow us to discuss variational problems on them, which includes finite element approximations such as the Poisson example discussed so far.

Linear functionals are important as they will represent the right-hand side of finite element approximations of PDEs.

Definition 103 (Continuous linear functional) *Let* H *be a Hilbert space with norm* $|\cdot|_{H}$.

1. A functional L is a map from H to \mathbb{R} .

- 2. A functional $L: H \to \mathbb{R}$ is linear if $u, v \in H$, $\alpha \in \mathbb{R} \implies L(u + \alpha v) = L(u) + \alpha L(v)$.
- 3. A functional $L: H \to \mathbb{R}$ is continuous if there exists C > 0 such that

$$|L(u) - L(v)| \le C||u - v||_H \quad \forall u, v \in H.$$

It is important that linear functionals are "nice" in the following sense.

Definition 104 (Bounded functional) A functional $L: H \to \mathbb{R}$ is bounded if there exists C > 0 such that

$$|L(u)| \le C||u||_H, \quad \forall u \in H.$$

For linear functionals we have the following relationship between boundedness and continuity.

Lemma 105 Let $L: H \to \mathbb{R}$ be a linear functional. Then L is continuous if and only if it is bounded.

Proof 106 L bounded $\implies L(u) \le C||u||_H \implies |L(u) - L(v)| = |L(u - v)| \le C||u - v||_H \ \forall u, v \in H, i.e.$ L is continuous.

On the other hand, L continuous $\Longrightarrow |L(u-v)| \le C||u-v||_H \quad \forall u,v \in H$. Pick v=0, then $|L(u)|=|L(u-0)| \le C|u-0|_H = C|u|_H$, i.e. L is bounded.

We can also interpret bounded linear functionals as elements of a vector space.

Definition 107 (Dual space) *Let* H *be a Hilbert space. The dual space* H' *is the space of continuous (or bounded) linear functionals* $L: H \to \mathbb{R}$.

This dual space can also be equipped with a norm.

Definition 108 (Dual norm) Let L be a continuous linear functional on H, then

$$||L||_{H'} = \sup_{0 \neq v \in H} \frac{L(v)}{||v||_H}.$$

There is a simple mapping from H to H'.

Lemma 109 Let $u \in H$. Then the functional $L_u : H \to \mathbb{R}$ defined by

$$L_u(v) = (u, v), \quad \forall v \in H,$$

is linear and continuous.

Proof 110 For $v, w \in H$, $\alpha \in \mathbb{R}$ we have

$$L_u(v + \alpha w) = (u, v + \alpha w) = (u, v) + \alpha(u, v) = L_u(v) + \alpha L_u(w).$$

Hence L_u is linear.

We see that L_u is bounded by Schwarz inequality,

$$|L_u(v)| = |(u, v)| \le C||v||_H \text{ with } C = ||u||_H.$$

The following famous theorem states that the converse is also true.

Theorem 111 (Riesz representation theorem) For any continuous linear functional L on H there exists $u \in H$ such that

$$L(v) = (u, v) \quad \forall v \in H.$$

Further,

$$||u||_H = ||L||_{H'}.$$

Proof 112 See a course or textbook on Hilbert spaces.

4.3 Variational problems on Hilbert spaces

We will consider finite element methods that can be formulated in the following way.

Definition 113 (Linear variational problem) Let b(u,v) be a bilinear form on a Hilbert space V, and F be a linear form on V. This defines a linear variational problem: find $u \in V$ such that

$$b(u, v) = F(v), \quad \forall v \in V.$$

We now discuss some important examples from finite element discretisations of linear PDEs.

Example 114 (Pk discretisation of (modified) Helmholtz problem with Neumann bcs) For some known function f,

$$b(u,v) = \int_{\Omega} uv + \nabla u \cdot \nabla v \, dx,$$
$$F(v) = \int_{\Omega} vf \, dx,$$

and V is the Pk continuous finite element space on a triangulation of Ω .

Example 115 (Pk discretisation of Poisson equation with partial Dirichlet bcs) For some known function f,

$$b(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx,$$
$$F(v) = \int_{\Omega} v f \, dx,$$

and V is the subspace of the Pk continuous finite element space on a triangulation of Ω such that functions vanishes on $\Gamma_0 \subseteq \partial \Omega$.

Example 116 (Pk discretisation of Poisson equation with pure Neumann bcs) For some known function f,

$$b(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx,$$
$$F(v) = \int_{\Omega} v f \, dx,$$

and V is the subspace of the Pk continuous finite element space on a triangulation of Ω such that functions satisfy

$$\int_{\Omega} u \, dx = 0.$$

We now introduce two important properties of bilinear forms that determine whether a linear variational problem is solvable or not. The first is continuity.

Definition 117 (Continuous bilinear form) A bilinear form is continuous on a Hilbert space V if there exists a constant $0 < M < \infty$ such that

$$|b(u,v)| \le M||u||_V||v||_V.$$

The second is coercivity.

Definition 118 (Coercive bilinear form) A bilinear form is coercive on a Hilbert space V if there exists a constant $0 < \gamma < \infty$ such that

$$|b(u,u)| \ge \gamma ||u||_V ||u||_V.$$

These two properties combine in the following theorem providing sufficient conditions for existence and uniqueness for solutions of linear variational problems.

Theorem 119 (Lax-Milgram theorem) Let b be a bilinear form, F be a linear form, and $(V, \| \cdot \|)$ be a Hilbert space. If b is continuous and coercive, and F is continuous, then a unique solution $u \in V$ to the linear variational problem exists, with

$$||u||_V \le \frac{1}{\gamma} ||F||_{V'}.$$

Proof 120 See a course or textbook on Hilbert spaces.

We are going to use this result to show solvability for finite element discretisations. In particular, we also want to know that our finite element discretisation continues to be solvable as the maximum triangle edge diameter h goes to zero. This motivates the following definition.

Definition 121 (Stability) Consider a sequence of triangulations \mathcal{T}_h with corresponding finite element spaces V_h labelled by a maximum triangle diameter h, applied to a variational problem with bilinear form b(u, v) and linear form L. For each V_h we have a corresponding coercivity constant γ_h .

If $\gamma_h \to \gamma > 0$, and $||F||_{V_h'} \to c < \infty$, then we say that the finite element discretisation is stable.

With this in mind it is useful to consider h-independent definitions of $\|\cdot\|_V$ (such as the L^2 and H^1 norms), which is why we introduced them.

4.4 Solvability and stability of some finite element discretisations

In this section we will introduce some tools for showing coercivity and continuity of bilinear forms, illustrated with finite element approximations of some linear PDEs where they may be applied.

We start with the simplest example, for which continuity and coercivity are immediate.

Theorem 122 (Solving the (modified) Helmholtz problem) Let b, L be the forms from the Helmholtz problem, with $||f||_{L^2} < \infty$. Let V_h be a Pk continuous finite element space defined on a triangulation \mathcal{T} . Then the finite element approximation u_h exists and the discretisation is stable in the H^1 norm.

Proof 123 First we show continuity of F. We have

$$F(v) = \int_{\Omega} fv \, dx \le ||f||_{L^2} ||v||_{L^2} \le ||f||_{L^2} ||v||_{H^1},$$

since $||v||_{L^2} \leq ||v||_{H^1}$.

Next we show continuity of b.

$$|b(u,v)| = |(u,v)_{H^1}| \le 1 \times ||u||_{H^1} ||v||_{H^1},$$

from the Schwarz inequality of the H^1 inner product. Finally we show coercivity of b.

$$b(u, u) = ||u||_{H^1}^2 \ge 1 \times ||u||_{H^1}^2,$$

The continuity and coercivity constants are both 1, independent of h, so the discretisation is stable.

For the Helmholtz problem, we have

$$b(u,v) = \int_{\Omega} uv + \nabla u \cdot \nabla v \, dx = (u,v)_{H^1},$$

i.e. b(u, v) is the H^1 inner of u and v, which makes the continuity and coercivity immediate.

For the Poisson problem, we have

$$b(u,v) = \int_{\Omega} |\nabla u|^2 dx = |u|_{H^1}^2 \neq ||u||_{H^1}^2.$$

Where we recall the H^1 seminorm from the interpolation section. Some additional results are required to show coercivity, as b(u,u) is not the H^1 norm squared any more. A seminorm has all the properties of a norm except $|u|=0 \Rightarrow u=0$, which is precisely what is needed in the Lax-Milgram theorem. For the Poisson problem, coercivity comes instead from the following mean estimate.

Lemma 124 (Mean estimate for finite element spaces) Let u be a member of a C^0 finite element space, and define

$$\bar{u} = \frac{\int_{\Omega} u \, dx}{\int_{\Omega} \, dx}.$$

Then there exists a positive constant C, independent of the triangulation but dependent on (convex) Ω , such that

$$||u - \bar{u}||_{L^2} \le C|u|_{H^1}.$$

Proof 125 (Very similar to the proof of the estimate for averaged Taylor polynomials.)

Let x and y be two points in Ω . We note that f(s) = u(y + s(x - y)) is a C^0 , piecewise polynomial function of s. Let $s_0 = 0 < s_1 < s_2 < \ldots < s_{k-1} < s_k = 1$ denote the points where y + s(x - y) intersects a triangle edge or vertex. Then f is a continuous function when restricted to each interval $[s_i, s_i + 1]$, $i = 0, \ldots, k-1$. This means that

$$f(s_{i+1}) - f(s_i) = \int_{s_i}^{s_{i+1}} f'(s) ds$$
$$= \int_{s_i}^{s_{i+1}} \nabla u(y + s(x - y)) ds,$$

where ∇u is the finite element derivative of u. Summing this up from i=0 to i=k-1, we obtain

$$u(x) = u(y) + \int_0^1 (x - y) \cdot \nabla u(y + s(x - y)) ds.$$

Then

$$\begin{split} u(x) - \bar{u} &= \frac{1}{|\Omega|} \int_{\Omega} u(x) - u(y) \, dy \\ &= \frac{1}{|\Omega|} \int_{\Omega} (x - y) \cdot \int_{s=0}^{1} \nabla u(y + s(x - y)) \, ds \, dy, \end{split}$$

Therefore

$$\begin{aligned} \|u - \bar{u}\|_{L^{2}(\Omega)}^{2} &= \frac{1}{|\Omega|^{2}} \int_{\Omega} \left(\int_{\Omega} (x - y) \cdot \int_{s=0}^{1} \nabla u (y + s(x - y)) \, ds \, dy \right)^{2} \, dx, \\ &\leq \frac{1}{|\Omega|^{2}} \int_{\Omega} \int_{\Omega} |x - y|^{2} \, dy \int_{\Omega} \int_{s=0}^{1} |\nabla u (y + s(x - y))|^{2} \, ds \, dy \, dx, \\ &\leq C \int_{\Omega} \int_{\Omega} \int_{s=0}^{1} |\nabla u (y + s(x - y))|^{2} \, ds \, dy \, dx. \end{aligned}$$

We split this final quantity into two parts (to avoid singularities),

$$||u - \bar{u}||_{L^2(\Omega)}^2 \le C(I + II),$$

where

$$I = \int_{\Omega} \int_{s=0}^{1/2} \int_{\Omega} |\nabla u(y + s(x - y))|^2 \, dy \, ds \, dx,$$

$$II = \int_{\Omega} \int_{s=1/2}^{2} \int_{\Omega} |\nabla u(y + s(x - y))|^2 \, dx \, ds \, dy,$$

which we will now estimate separately.

To evaluate I, change variables $y \to y' = y + s(x-y)$, defining $\Omega_s' \subset \Omega$ as the image of Ω under this transformation. Then,

$$\begin{split} I &= \int_{\Omega} \int_{s=0}^{1/2} \frac{1}{(1-s)^2} \int_{\Omega_s'} |\nabla u(y')|^2 \, dy' \, ds \, dx, \\ &\leq \int_{\Omega} \int_{s=0}^{1/2} \frac{1}{(1-s)^2} \int_{\Omega} |\nabla u(y')|^2 \, dy' \, ds \, dx, \\ &= \frac{|\Omega|}{2} |\nabla u|_{H^1(\Omega)}^2. \end{split}$$

To evaluate II, change variables $x \to x' = y + s(x - y)$, defining $\Omega'_s \subset \Omega$ as the image of Ω under this transformation. Then,

$$II = \int_{\Omega} \int_{s=1/2}^{2} \frac{1}{s^{2}} \int_{\Omega'_{s}} |\nabla u(x')|^{2} dx' ds dy,$$

$$\leq \int_{\Omega} \int_{s=0}^{1/2} \frac{1}{s^{2}} \int_{\Omega} |\nabla u(x')|^{2} dx' ds dy,$$

$$= |\Omega| |\nabla u|_{H^{1}(\Omega)}^{2}.$$

Combining,

$$||u - \bar{u}||_{L^2(\Omega)}^2 \le C(I + II) = \frac{3C|\Omega|}{2}|u|_{H^1(\Omega)}^2,$$

which has the required form.

The mean estimate can now be used to show solvability for the Poisson problem with pure Neumann conditions.

Theorem 126 (Solving the Poisson problem with pure Neumann conditions) Let b, L, V, be the forms for the pure Neumann Poisson problem, with $||f||_{L^2} < \infty$. Let V_h be a Pk continuous finite element space defined on a triangulation \mathcal{T} , and define

$$\bar{V}_h = \{ u \in V_h : \bar{u} = 0 \}.$$

Then for \bar{V}_h , the finite element approximation u_h exists and the discretisation is stable in the H^1 norm.

Proof 127 Using the mean estimate, for $u \in \bar{V}_h$, we have

$$||u||_{L^2}^2 = ||u - \underbrace{\bar{u}}_{=0}||_{L^2}^2 \le C^2 |u|_{H^1}^2.$$

Hence we obtain the coercivity result,

$$||u||_{H^1}^2 = ||u||_{L^2}^2 + |u|_{H^1}^2 \le (1 + C^2)|u|_{H^1}^2 = (1 + C^2)b(u, u).$$

Continuity follows from Schwarz inequality,

$$|b(u,v)| \le |u|_{H^1} |v|_{H^1} \le ||u||_{H^1} ||v||_{H^1}.$$

The coercivity constant is independent of h, so the approximation is stable.

Proving the coercivity for the Poisson problem with Dirichlet or partial Dirichlet boundary conditions requires some additional results. We start by showing that the divergence theorem also applies to finite element derivatives of C^0 finite element functions.

Lemma 128 (Finite element divergence theorem) Let ϕ be a C^1 vector-valued function. and $u \in V$ be a member of a C^0 finite element space. Then

$$\int_{\Omega} \nabla \cdot (\phi u) \, dx = \int_{\partial \Omega} \phi \cdot nu \, dS,$$

where n is the outward pointing normal to $\partial\Omega$.

Proof 129

$$\int_{\Omega} \nabla \cdot (\phi u) \, dx = \sum_{K \in \mathcal{T}} \int_{K} \nabla \cdot (\phi u) \, dx,$$

$$= \sum_{K \in \mathcal{T}} \int_{\partial K} \phi \cdot n_{K} u \, dS,$$

$$= \int_{\partial \Omega} \phi \cdot nu \, dS + \underbrace{\int_{\Gamma} \phi \cdot (n^{+} + n^{-}) u \, dS}_{=0}.$$

This allows us to prove the finite element trace theorem, which relates the H^1 norm of a C^0 finite element function to the L^2 norm of the function restricted to the boundary.

Theorem 130 (Trace theorem for continuous finite elements) Let V_h be a continuous finite element space, defined on a triangulation \mathcal{T} , on a polygonal domain Ω . Then

$$||u||_{L^2(\partial\Omega)} \le C||u||_{H^1(\Omega)},$$

where C is a constant that depends only on the geometry of Ω .

Proof 131 The first step is to construct a C^1 function ξ satisfying $\xi \cdot n = 1$ on Ω . We do this by finding a triangulation \mathcal{T}_0 (unrelated to \mathcal{T}), and defining an C^1 Argyris finite element space V_0 on it. We then choose ξ so that both Cartesian components are in V_0 , satisfying the boundary condition.

Then,

$$\begin{aligned} \|u\|_{L^{2}(\partial\Omega)}^{2} &= \int_{\partial\Omega} u^{2} dS = \int_{\partial\Omega} \xi \cdot nu^{2} dS, \\ &= \int_{\Omega} \nabla \cdot (\xi u^{2}) dx, \\ &= \int_{\Omega} u^{2} \nabla \cdot \xi + 2u \xi \cdot \nabla u dx, \\ &\leq \|u\|_{L^{2}}^{2} \|\nabla \cdot \xi\|_{\infty} + 2|\xi|_{\infty} \|u\|_{L^{2}} |u|_{H^{1}}, \end{aligned}$$

So,

$$||u||_{L^{2}(\partial\Omega)}^{2} \leq ||u||_{L^{2}}^{2} ||\nabla \cdot \xi||_{\infty} + |\xi|_{\infty} \left(||u||_{L^{2}}^{2} + |u|_{H^{1}}^{2} \right),$$

$$\leq C||u||_{H^{1}}^{2},$$

where we have used the geometric-arithmetic mean inequality $2ab \le a^2 + b^2$.

We can now use the trace inequality to estabilish solvability for the Poisson problem with (full or partial) Dirichlet conditions.

Theorem 132 (Solving the Poisson problem with partial Dirichlet conditions) Let b, L, V, be the forms for the (partial) Dirichlet Poisson problem, with $||f||_{L^2} < \infty$. Let V_h be a Pk continuous finite element space defined on a triangulation \mathcal{T} , and define

$$\mathring{V}_h = \{u \in V_h : u|_{\Gamma_0}\}.$$

Then for V_h , the finite element approximation u_h exists and the discretisation is stable in the H^1 norm.

Proof 133 [Proof taken from Brenner and Scott]. We have

$$\begin{aligned} \|v\|_{L^{2}(\Omega)} &\leq \|v - \bar{v}\|_{L^{2}(\Omega)} + \|\bar{v}\|_{L^{2}(\Omega)}, \\ &\leq C|v|_{H^{1}(\Omega)} + \frac{|\Omega|^{1/2}}{|\Gamma_{0}|} \left| \int_{\Gamma_{0}} \bar{v} \, dS \right|, \\ &\leq C|v|_{H^{1}(\Omega)} + \frac{|\Omega|^{1/2}}{|\Gamma_{0}|} \left(\left| \int_{\Gamma_{0}} v \, dS + \int_{\Gamma_{0}} \bar{v} - v \, dS \right| \right). \end{aligned}$$

We have

$$\left| \int_{\Gamma_0} (v - \bar{v}) \, ds \right| \le |\Gamma_0|^{1/2} ||v - \bar{v}||_{L^2(\partial\Omega)},$$
$$\le |\Gamma_0|^{1/2} C |v|_{H^1(\Omega)}.$$

Combining, we get

$$||v||_{L^2(\Omega)} \le C_1 |v|_{H^1(\Omega)},$$

and hence coercivity,

$$||v||_{H^1(\Omega)}^2 \le (1 + C_1^2)b(v, v).$$

M345A47 Finite Elements: Analysis and Implementation, Edition 2020.0

The coercivity constant is independent of h, so the approximation is stable.

In this section, We have developed some techniques for showing that variational problems arising from finite element discretisations for Helmholtz and Poisson problems have unique solutions, that are stable in the H^1 -norm. This means that we can be confident that we can solve the problems on a computer and the solution won't become singular as the mesh is refined. Now we would like to go further and ask what is happening to the numerical solutions as the mesh is refined. What are they converging to?

We will address these questions in the next section.

CONVERGENCE OF FINITE ELEMENT APPROXIMATIONS

In this section we develop tools to prove convergence of finite element approximations to the exact solutions of PDEs.

5.1 Weak derivatives

Consider a triangulation \mathcal{T} with recursively refined triangulations \mathcal{T}_h and corresponding finite element spaces V_h . Given stable finite element variational problems, we have a sequence of solutions u_h as $h \to 0$, satisfying the h-independent bound

$$||u_h||_{H^1(\Omega)} \leq C.$$

What are these solutions converging to? We need to find a Hilbert space that contains all V_h as $h \to 0$, that extends the H^1 norm to the $h \to 0$ limit of finite element functions.

Our first task is to define a derivative that works for all finite element functions, without reference to a mesh. This requires some preliminary definitions, starting by considering some very smooth functions that vanish on the boundaries together with their derivatives (so that we can integrate by parts as much as we like).

Definition 134 (Compact support on Ω) A function u has compact support on Ω if there exists $\epsilon > 0$ such that u(x) = 0 when $\min_{y \in \partial \Omega} |x - y| < \epsilon$.

Definition 135 $(C_0^{\infty}(\Omega))$ We denote by $C_0^{\infty}(\Omega)$ the subset of $C^{\infty}(\Omega)$ corresponding to functions that have compact support on Ω .

Next we will define a space containing the generalised derivative.

Definition 136 (L_{loc}^1) For triangles $K \subset \text{int}(\Omega)$, we define

$$||u||_{L^1(K)} = \int_K |u| \, dx,$$

and

$$L_K^1 = \left\{ u : \|u\|_{L^1(K)} < \infty \right\}.$$

Then

$$L^1_{loc} = \left\{ f : f \in L^1(K) \quad \forall K \subset \operatorname{int}\left(\Omega\right) \right\}.$$

Finally we are in a position to introduce the generalisation of the derivative itself.

Definition 137 (Weak derivative) The weak derivative $D_w^{\alpha} f \in L_{loc}^1(\Omega)$ of a function $f \in L_{loc}^1(\Omega)$ is defined by

$$\int_{\Omega} \phi D_w^{\alpha} f \, dx = (-1)^{|\alpha|} \int_{\Omega} D^{\alpha} \phi f \, dx, \quad \forall \phi \in C_0^{\infty}(\Omega).$$

Not that we do not see any boundary terms since ϕ vanishes at the boundary along with all derivatives.

Now we check that the derivative agrees with our finite element derivative definition.

Lemma 138 Let V be a C^0 finite element space. Then, for $u \in V$, the finite element derivative of u is equal to the weak derivative of u.

Proof 139 Taking any $\phi \in C_0^{\infty}(\Omega)$, we have

$$\begin{split} \int_{\Omega} \phi \frac{\partial}{\partial x_{i}}|_{FE} u \, dx &= \sum_{K} \int_{K} \phi \frac{\partial u}{\partial x_{i}} \, dx, \\ &= \sum_{K} \left(-\int_{K} \frac{\partial \phi}{\partial x_{i}} u \, dx + \int_{\partial K} \phi n_{i} u \, dS \right), \\ &= -\sum_{K} \int_{K} \frac{\partial \phi}{\partial x_{i}} u \, dx = -\int_{\Omega} \frac{\partial \phi}{\partial x_{i}} u \, dx, \end{split}$$

as required.

Exercise 140 Let V be a C^1 finite element space. For $u \in V$, show that the finite second derivatives of u is equal to the weak second derivative of u.

Exercise 141 Let V be a discontinuous finite element space. For $u \in V$, show that the weak derivative does not coincide with the finite element derivative in general (find a counter-example).

Lemma 142 For $u \in C^{|\alpha|}(\Omega)$, the usual "strong" derivative D^{α} of u is equal to the weak derivative D^{α}_w of u.

Proof 143 Exercise. [very similar to previous proof]

Due to these equivalences, we do not need to distinguish between strong, weak and finite element first derivatives for C^0 finite element functions. All derivatives are assumed to be weak from now on.

5.2 Sobolev spaces

We are now in a position to define a space that contains all C^0 finite element spaces. This means that we can consider the limit of finite element approximations as $h \to 0$.

Definition 144 (The Sobolev space H^1) $H^1(\Omega)$ is the function space defined by

$$H^1(\Omega) = \{ u \in L^1_{loc} : ||u||_{H^1(\Omega)} < \infty \}.$$

Going further, the Sobolev space H^k is the space of all functions with finite H^k norm.

Definition 145 (The Sobolev space H^k) $H^k(\Omega)$ is the function space defined by

$$H^k(\Omega) = \left\{u \in L^1_{loc} : \|u\|_{H^k(\Omega)} < \infty\right\}$$

Since $||u||_{H^k(\Omega)} \le ||u||_{H^l(\Omega)}$ for k < l, we have $H^k \subset H^l$ for k < l.

If we are to consider limits of finite element functions in these Sobolev spaces, then it is important that they are closed, i.e. limits remain in the spaces.

Lemma 146 (H^k spaces are Hilbert spaces) The space $H^k(\Omega)$ is closed.

Let $\{u_i\}$ be a Cauchy sequence in H^k . Then $\{D^{\alpha}u_i\}$ is a Cauchy sequence in $L^2(\Omega)$ (which is closed), so $\exists v^{\alpha} \in L^2(\Omega)$ such that $D^{\alpha}u_i \to v^{\alpha}$ for $|\alpha| \leq k$. If $w_j \to w$ in $L^2(\Omega)$, then for $\phi \in C_0^{\infty}(\Omega)$,

$$\int_{\Omega} (w_j - w) \phi \, dx \le \|w_j - w\|_{L^2(\Omega)} \|\phi\|_{L^{\infty}} \to 0.$$

We use this equation to get

$$\int_{\Omega} v^{\alpha} \phi \, dx = \lim_{i \to \infty} \int_{\Omega} \phi D^{\alpha} u_i \, dx,$$

$$= \lim_{i \to \infty} (-1)^{|\alpha|} \int_{\Omega} u_i D^{\alpha} \phi \, dx,$$

$$= (-1)^{|\alpha|} \int_{\Omega} v D^{\alpha} \phi \, dx,$$

i.e. v^{α} is the weak derivative of u as required.

We quote the following much deeper results without proof.

Theorem 147 (H = W) Let Ω be any open set. Then $H^k(\Omega) \cap C^{\infty}(\Omega)$ is dense in $H^k(\Omega)$.

The interpretation is that for any function $u \in H^k(\Omega)$, we can find a sequence of C^{∞} functions u_i converging to u. This is very useful as we can compute many things using C^{∞} functions and take the limit.

Theorem 148 (Sobolev's inequality) Let Ω be an n-dimensional domain with Lipschitz boundary, let k be an integer with k > n/2. Then there exists a constant C such that

$$||u||_{L^{\infty}(\Omega)} = \operatorname{ess\,sup}_{x \in \Omega} |u(x)| \le C||u||_{H^{k}(\Omega)}.$$

Further, there is a C^0 continuous function in the $L^{\infty}(\Omega)$ equivalence class of u.

Previously we saw this result for continuous functions. Here it is presented for H^k functions, with an extra statement about the existence of a C^0 function in the equivalence class. The interpretation is that if $u \in H^k$ then there is a continuous function u_0 such that the set of points where $u \neq u_0$ has zero area/volume.

Corollary 149 (Sobolev's inequality for derivatives) Let Ω be a n-dimensional domain with Lipschitz boundary, let k be an integer with k-m > n/2. Then there exists a constant C such that

$$||u||_{W^m_{\infty}(\Omega)} := \sum_{|\alpha| \le m} ||D^{\alpha}u||_{L^{\infty}(\Omega)} \le C||u||_{H^k(\Omega)}.$$

Further, there is a C^m continuous function in the $L^{\infty}(\Omega)$ equivalence class of u.

Proof 150 Just apply Sobolev's inequality to the m derivatives of u.

5.3 Variational formulations of PDEs

We can now consider linear variational problems defined on H^k spaces, by taking a bilinear form b(u, v) and linear form F(v), seeking $u \in H^k$ (for chosen H^k) such that

$$b(u, v) = F(v), \quad \forall v \in H^k.$$

Since H^k is a Hilbert space, the Lax-Milgram theorem can be used to analyse, the existence of a unique solution to an H^k linear variational problem.

For example, the Helmholtz problem solvability is immediate.

Theorem 151 (Well-posedness for (modified) Helmholtz)) The Helmholtz variational problem on H^1 satisfies the conditions of the Lax-Milgram theorem.

Proof 152 The proof for C^0 finite element spaces extends immediately to H^1 .

Next, we develop the relationship between solutions of the Helmholtz variational problem and the strong-form Helmholtz equation,

$$u - \nabla^2 u = f$$
, $\frac{\partial u}{\partial n} = 0$, on $\partial \Omega$.

The basic idea is to check that when you take a solution of the Helmholtz variational problem and integrate by parts (provided that this makes sense) then you reveal that the solution solves the strong form equation. Functions in H^k make boundary values hard to interpret since they are not guaranteed to have defined values on the boundary. We make the following definition.

Definition 153 (Trace of H^1 **functions)** Let $u \in H^1(\Omega)$ and choose $u_i \in C^{\infty}(\Omega)$ such that $u_i \to u$. We define the trace $u|_{\partial\Omega}$ on $\partial\Omega$ as the limit of the restriction of u_i to $\partial\Omega$. This definition is unique from the uniqueness of limits.

We can extend our trace inequality for finite element functions directly to H^1 functions.

Lemma 154 (Trace theorem for H^1 **functions)** *Let* $u \in H^1(\Omega)$ *for a polygonal domain* Ω . *Then the trace* $u|_{\partial\Omega}$ *satisfies*

$$||u||_{L^2(\partial\Omega)} \le C||u||_{H^1(\Omega)}.$$

The interpretation of this result is that if $u \in H^1(\Omega)$ then $u|_{\partial\Omega} \in L^2(\partial\Omega)$.

Proof 155 Adapt the proof for C^0 finite element functions, choosing $u \in C^{\infty}(\Omega)$, and pass to the limit in $H^1(\Omega)$.

This tells us when the integration by parts formula makes sense.

Lemma 156 Let $u \in H^2(\Omega)$, $v \in H^1(\Omega)$. Then

$$\int_{\Omega} (-\nabla^2 u) v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial \Omega} \frac{\partial u}{\partial n} v \, dS.$$

Proof 157 First note that $u \in H^2(\Omega) \implies \nabla u \in (H^1(\Omega))^d$. Then

Then, take $v_i \in C^{\infty}(\Omega)$ and $u_i \in C^{\infty}(\Omega)$ converging to v and u, respectively, and $v_i \nabla u_i \in C^{\infty}(\Omega)$ converges to $v \nabla u$. These satisfy the equation; we obtain the result by passing to the limit.

Now we have everything we need to show that solutions of the strong form equation also solve the variational problem. It is just a matter of substituting into the formula and applying integration by parts.

Lemma 158 For $f \in L^2$, let $u \in H^2(\Omega)$ solve

$$u - \nabla^2 u = f$$
, $\frac{\partial u}{\partial n} = 0$ on $\partial \Omega$,

in the L^2 sense, i.e. $||u - \nabla^2 u - f||_{L^2} = 0$. Then u solves the variational form of the Helmholtz equation.

Proof 159 $u \in H^2 \implies ||u||_{H^2} < \infty \implies ||u||_{H^1} < \infty \implies u \in H^1$. Multiplying by test function $v \in H^1$, and using the previous proposition gives

$$\int_{\Omega} uv + \nabla u \cdot \nabla v \, dx = \int_{\Omega} fv \, dx, \quad \forall v \in H^{1}(\Omega),$$

as required.

Now we go the other way, showing that solutions of the variational problem also solve the strong form equation. To do this, we need to assume a bit more smoothness of the solution, that it is in H^2 instead of just H^1 .

Theorem 160 Let $f \in L^2(\Omega)$ and suppose that $u \in H^2(\Omega)$ solves the variational Helmholtz equation on a polygonal domain Ω . Then u solves the strong form Helmholtz equation with zero Neumann boundary conditions.

Proof 161 Using integration by parts for $u \in H^2$, $v \in C_0^{\infty}(\Omega) \in H^1$, we have

$$\int_{\Omega} (u - \nabla^2 u - f) v \, dx = \int_{\Omega} uv + \nabla u \cdot \nabla v - vf \, dx = 0.$$

It is a standard result that $C_0^\infty(\Omega)$ is dense in $L^2(\Omega)$ (i.e., every L^2 function can be approximated arbitrarily closely by a C_0^∞ function), and therefore we can choose a sequence of v converging to $u - \nabla^2 u - f$ and we obtain $\|u - \nabla^2 u - f\|_{L^2(\Omega)} = 0$.

Now we focus on showing the boundary condition is satisfied. We have

$$0 = \int_{\Omega} uv + \nabla u \cdot \nabla v - fv \, dx$$
$$= \int_{\Omega} uv + \nabla u \cdot \nabla v - (u - \nabla^2 u)v \, dx$$
$$= \int_{\partial \Omega} \frac{\partial u}{\partial n} v \, dS.$$

We can find arbitrary $v \in L_2(\partial\Omega)$, hence $\|\frac{\partial u}{\partial n}\|_{L^2(\partial\Omega)} = 0$.

5.4 Galerkin approximations of linear variational problems

Going a bit more general again, assume that we have a well-posed linear variational problem on H^k , connected to a strong form PDE. Now we would like to approximate it. This is done in general using the Galerkin approximation.

Definition 162 (Galerkin approximation) Consider a linear variational problem of the form:

find $u \in H^k$ such that

$$b(u, v) = F(v), \quad \forall v \in H^k.$$

For a finite element space $V_h \subset V = H^k(\Omega)$, the Galerkin approximation of this H^k variational problem seeks to find $u_h \in V_h$ such that

$$b(u_h, v) = F(v), \quad \forall v \in V_h.$$

We just restrict the trial function u and the test function v to the finite element space. C^0 finite element spaces are subspaces of H^1 , C^1 finite element spaces are subspaces of H^2 and so on.

If b(u, v) is continuous and coercive on H^k , then it is also continuous and coercive on V_h by the subspace property. Hence, we know that the Galerkin approximation exists, is unique and is stable. This means that it will be possible to solve the matrix-vector equation.

Moving on, if we can solve the equation, we would like to know if it is useful. What is the size of the error $u - u_h$? For Galerkin approximations this question is addressed by Céa's lemma.

Theorem 163 (Céa's lemma.) Let $V_h \subset V$, and let u solve a linear variational problem on V, whilst u_h solves the equivalent Galerkin approximation on V_h . Then

$$||u - u_h||_V \le \frac{M}{\gamma} \min_{v \in V_h} ||u - v||_V,$$

where M and γ are the continuity and coercivity constants of b(u, v), respectively.

Proof 164 We have

$$b(u, v) = F(v) \quad \forall v \in V, b(u_h, v) = F(v) \quad \forall v \in V_h.$$

Choosing $v \in V_h \subset V$ means we can use it in both equations, and subtraction and linearity lead to the "Galerkin orthogonality" condition

$$b(u - u_h, v) = 0, \quad \forall v \in V_h.$$

Then, for all $v \in V_h$,

$$\gamma \|u - u_h\|_V^2 \le b(u - u_h, u - u_h),$$

$$= b(u - u_h, u - v) + \underbrace{b(u - u_h, v - u_h)}_{=0},$$

$$\le M \|u - u_h\|_V \|u - v\|_V.$$

So,

$$\gamma \|u - u_h\|_V \le M|u - v\|_V.$$

Minimising over all v completes the proof.

5.5 Interpolation error in H^k spaces

The interpretation of Céa's lemma is that the error is proportional to the minimal error in approximating u in V_h . To do this, we can simply choose $v = I_h u$ in Céa's lemma, to get

$$||u - u_h||_V \le \frac{M}{\gamma} \min_{v \in V_h} ||u - v||_V \le \frac{M}{\gamma} ||u - I_h u||_V.$$

Hence, Céa's lemma reduces the problem of estimating the error in the numerical solution to estimating error in the interpolation of the exact solution. We have already examined this in the section on interpolation operators, but in the context of continuous functions. The problem is that we do not know that the solution u is continuous, only that it is in H^k for some k.

We now quickly revisit the results of the interpolation section to extend them to H^k spaces. The proofs are mostly identical, so we just give the updated result statements and state how to modify the proofs.

Firstly we recall the averaged Taylor polynomial. Since it involves only integrals of the derivatives, we can immediately use weak derivatives here.

Definition 165 (Averaged Taylor polynomial with weak derivatives) Let $\Omega \subset \mathbb{R}^n$ be a domain with diameter d, that is star-shaped with respect to a ball B with radius ϵ , contained within Ω . For $f \in H^{k+1}(\Omega)$ the averaged Taylor polynomial $Q_{k,B}f \in \mathcal{P}_k$ is defined as

$$Q_{k,B}f(x) = \frac{1}{|B|} \int_B T^k f(y,x) \, dy,$$

where $T^k f$ is the Taylor polynomial of degree k of f,

$$T^k f(y,x) = \sum_{|\alpha| \le k} D^{\alpha} f(y) \frac{(x-y)^{\alpha}}{\alpha!},$$

evaluated using weak derivatives.

This definition makes sense since the Taylor polynomial coefficients are in $L^1_{loc}(\Omega)$ and thus their integrals over B are defined.

The next step was to examine the error in the Taylor polynomial.

Theorem 166 Let $\Omega \subset \mathbb{R}^n$ be a domain with diameter d, that is star-shaped with respect to a ball B with radius ϵ , contained within Ω . There exists a constant C(k,n) such that for $0 \le |\beta| \le k+1$ and all $f \in H^{k+1}(\Omega)$,

$$||D^{\beta}(f - Q_{k,B}f)||_{L^{2}} \le C \frac{|\Omega|^{1/2}}{|B|^{1/2}} d^{k+1-|\beta|} ||\nabla^{k+1}f||_{L^{2}(\Omega)}.$$

Proof 167 To show this, we assume that $f \in C^{\infty}(\Omega)$, in which case the result of Theorem 72 applies. Then we obtain the present result by approximating f by a sequence of $C^{\infty}(\Omega)$ functions and passing to the limit.

We then repeat the following corollary.

Corollary 168 Let K_1 be a triangle with diameter 1. There exists a constant C(k, n) such that

$$||f - Q_{k,B}f||_{H^k(K_1)} \le C|\nabla^{k+1}f|_{H^{k+1}(K_1)}.$$

Proof 169 Same as Lemma 74.

The next step was the bound on the interpolation operator. Now we just have to replace $C^{l,\infty}$ with W^l_{∞} as derivatives may not exist at every point.

Lemma 170 Let $(K_1, \mathcal{P}, \mathcal{N})$ be a finite element such that K_1 is a triangle with diameter 1, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and $\|N_i\|_{W^l_{\infty}(K_1)'} < \infty$,

$$||N_i||_{W^l_{\infty}(K_1)'} = \sup_{||u||_{W^l_{\infty}(K_1)} > 0} \frac{|N_i(u)|}{||u||_{W^l_{\infty}(K_1)}}.$$

Let $u \in H^k(K_1)$ with k > l + n/2. Then

$$\|\mathcal{I}_{K_1}u\|_{H^k(K_1)} \le C\|u\|_{H^k(K_1)}.$$

Proof 171 Same as Lemma 76. replacing $C^{l,\infty}$ with W^l_{∞} , and using the full version of the Sobolev inequality in Lemma 148.

The next steps then just follow through.

Lemma 172 Let $(K_1, \mathcal{P}, \mathcal{N})$ be a finite element such that K_1 has diameter 1, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contain all polynomials of degree k and below, with k > l + n/2. Let $u \in H^{k+1}(K_1)$. Then for $i \leq k$, the local interpolation operator satisfies

$$|\mathcal{I}_{K_1}u - u|_{H^i(K_1)} \le C_1|u|_{H^{k+1}(K_1)}.$$

Proof 173 Same as Lemma 78.

Lemma 174 Let $(K, \mathcal{P}, \mathcal{N})$ be a finite element such that K has diameter d, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contains all polynomials of degree k and below, with k > l + n/2. Let $u \in H^{k+1}(K)$. Then for $i \leq k$, the local interpolation operator satisfies

$$|\mathcal{I}_K u - u|_{H^i(K)} \le C_K d^{k+1-i} |u|_{H^{k+1}(K)}.$$

where C_K is a constant that depends on the shape of K but not the diameter.

Proof 175 Repeat the scaling argument of Lemma 80.

Theorem 176 Let \mathcal{T} be a triangulation with finite elements $(K_i, \mathcal{P}_i, \mathcal{N}_i)$, such that the minimum aspect ratio r of the triangles K_i satisfies r > 0, and such that the nodal variables in \mathcal{N} involve only evaluations of functions or evaluations of derivatives of degree $\leq l$, and \mathcal{P} contains all polynomials of degree k and below, with k > l + n/2. Let $u \in H^{k+1}(\Omega)$. Let k be the maximum over all of the triangle diameters, with $k \leq l \leq l$. Let k be the corresponding k finite element space. Then for k and k a

$$\|\mathcal{I}_h u - u\|_{H^i(\Omega)} \le Ch^{k+1-i} |u|_{H^{k+1}(\Omega)}.$$

Proof 177 Identical to Theorem 82.

5.6 Convergence of the finite element approximation to the Helmholtz problem

Now that we have the required interpolation operator results, we can return to applying Céa's lemma to the convergence of the finite element approximation to the Helmholtz problem.

Corollary 178 The degree k Lagrange finite element approximation u_h to the solution u of the variational Helmholtz problem satisfies

$$||u_h - u||_{H^1(\Omega)} \le Ch^k ||u||_{H^2(\Omega)}.$$

Proof 179 We combine Céa's lemma with the previous estimate, since

$$\min_{v \in V_h} \|u - v\|_{H^1(\Omega)} \le \|u - I_h u\|_{H^1(\Omega)} \le Ch^k \|u\|_{H^2(\Omega)},$$

having chosen i = 1.

Céa's lemma gives us error estimates in the norm of the space where the variational problem is defined, where the continuity and coercivity results hold. In the case of the Helmholtz problem, this is H^1 . We would also like estimates of the error in the L^2 norm, and it will turn out that these will have a more rapid convergence rate as $h \to 0$.

To do this we quote the following without proof.

Theorem 180 (Elliptic regularity) Let w solve the equation

$$w - \nabla^2 w = f, \quad \frac{\partial w}{\partial n} = 0 \text{ on } \partial \Omega,$$

on a convex (results also hold for other types of "nice" domains) domain Ω , with $f \in L^2$. Then there exists constant C > 0 such that

$$|w|_{H^2(\Omega)} \le C||f||_{L^2(\Omega)}.$$

Similar results hold for general elliptic operators, such as Poisson's equation with the types of boundary conditions discussed above. Elliptic regularity is great to have, because it says that the solution of the H^1 variational problem is actually in H^2 , provided that $f \in L^2$.

We now use this to obtain the following result, using the Aubin-Nitsche trick.

Theorem 181 The degree m Lagrange finite element approximation u_h to the solution u of the variational Helmholtz problem satisfies

$$||u_h - u||_{L^2(\Omega)} \le Cd^{m+1}||u||_{H^2(\Omega)}.$$

Proof 182 We use the Aubin-Nitsche duality argument. Let w be the solution of

$$w - \nabla^2 w = u - u_h$$

with the same Neumann boundary conditions as for u.

Since $u - u_h \in H^1(\Omega) \subset L^2(\Omega)$, we have $w \in H^2(\Omega)$ by elliptic regularity.

Then we have (by multiplying by a test function an integrating by parts),

$$b(w,v) = (u - u_h, v)_{L^2(\Omega)}, \quad \forall v \in H^1(\Omega),$$

and so

$$||u - u_h||_{L^2(\Omega)}^2 = (u - u_h, u - u_h) = b(w, u - u_h), = b(w - \mathcal{I}_h w, u - u_h) \text{ (orthogonality)},$$

$$\leq C||u - u_h||_{H^1(\Omega)}||w - \mathcal{I}_h w||_{H^1(\Omega)},$$

$$\leq Ch||u - u_h||_{H^1(\Omega)}|w|_{H^2(\Omega)}$$

$$\leq C_1 h^{m+1}||u - u_h||_{L^2(\Omega)}|u|_{H^2(\Omega)}$$

and dividing both sides by $||u-u_h||_{L^2(\Omega)}$ gives the result.

Thus we gain one order of convergence rate with h by using the L^2 norm instead of the H^1 norm.

5.7 Epilogue

This completes our analysis of the convergence of the Galerkin finite element approximation to the Helmholtz problem. Similar approaches can be applied to analysis of other elliptic PDEs, using the following programme.

- 1. Find a variational formulation of the PDE with a bilinear form that is continuous and coercive (and hence well-posed by Lax-Milgram) on H^k for some k.
- 2. Find a finite element space $V_h \subset H^k$. For H^1 , this requires a C^0 finite element space, and for H^2 , a C^1 finite element space is required.
- 3. The Galerkin approximation to the variational formulation is obtained by restricting the solution and test functions to V_h .
- 4. Continuity and coercivity (and hence well-posedness) for the Galerkin approximation is assured since $V_h \subset H^k$. This means that the Galerkin approximation is solvable and stable.
- 5. The estimate of the error estimate in terms of *h* comes from Céa's lemma plus the error estimate for the nodal interpolation operator.

This course only describes the beginning of the subject of finite element methods, for which research continues to grow in both theory and application. There are many methods and approaches that go beyond the basic Galerkin approach described above. These include

• Discontinuous Galerkin methods, which use discontinuous finite element spaces with jump conditions between cells to compensate for not having the required continuity. These problems do not fit into the standard Galerkin framework and new techniques have been developed to derive and analyse them.

Mixed finite element methods, which consider systems of partial differential equations such as the Poisson
equation in first-order form,

$$u - \nabla p = 0, \quad \nabla \cdot u = f.$$

The variational forms corresponding to these systems are not coercive, but they are well-posed anyway, and additional techniques have been developed.

- Non-conforming methods, which work even though $V_h \not\subset H^k$. For example, the Crouzeix-Raviart element uses linear functions that are only continuous at edge centres, so the functions are not in C^0 and the functions do not have a weak derivative. However, using the finite element derivative in the weak form for H^1 elliptic problems still gives a solvable system that converges at the optimal rate. Additional techniques have been developed to analyse this.
- Interior penalty methods, which work even though $V_h \not\subset H^k$. These methods are used to solve H^k elliptic problems using H^l finite element spaces with l < k, using jump conditions to obtain a stable discretisation. Additional techniques have been developed to analyse this.
- Stabilised and multiscale methods for finite element approximation of PDEs whose solutions have a wide range of scales, for example they might have boundary layers, turbulent structures or other phenomena. Resolving this features is often too expensive, so the goal is to find robust methods that behave well when the solution is not well resolved. Additional techniques have been developed to analyse this.
- Hybridisable methods that involve flux functions that are supported only on cell facets.
- Currently there is a lot of activity around discontinuous Petrov-Galerkin methods, which select optimal test functions to maximise the stability of the discrete operator. This means that they can be applied to problems such as wave propagation which are otherwise very challenging to find stable methods for. Also, these methods come with a bespoke error estimator that can allow for adaptive meshing starting from very coarse meshes. Another new and active area is virtual element methods, where the basis functions are not explicitly defined everywhere (perhaps just on the boundary of cells). This facilitates the use of arbitrary polyhedra as cells, leading to very flexible mesh choices.

All of these methods are driven by the requirements of different physical applications.

Other rich areas of finite element research include

- the development of bespoke, efficient iterative solver algorithms on parallel computers for finite element discretisations of PDEs. Here, knowledge of the analysis of the discretisation can lead to solvers that converge in a number of iterations that is independent of the mesh parameter h.
- adaptive mesh algorithms that use analytical techniques to estimate or bound the numerical error after the numerical solution has been computed, in order to guide iterative mesh refinement in particular areas of the domain.

5.7. Epilogue 41

M345A47 Finite Elements: Analysis and Implementation, Edition 2020.0					

Part II Implementation Exercise

THE IMPLEMENTATION EXERCISE

The object of the implementation exercise is to gain an understanding of the finite element method by producing a working one and two dimensional finite element solver library. Along the way you will have the opportunity to pick up valuable scientific computing skills in coding, software engineering and rigorous testing.

There will be no conventional lectures for this part of the module. Instead, there will be twice weekly 1 hour computer lab sessions during the term. Some of this time will involve explanations at the board, but much of the time will be an opportunity to develop your finite element implementation and receive help on how to do so.

0.1 Formalities and marking scheme

The implementation exercise is due at the end of term. That is, by 1600 on Friday 22 March. You must submit your work uploading the git commit code on Blackboard. You can convenently find this code on the commits page for your repository on github. For the avoidance of doubt, the commit you submit must date from before the deadline!

The marking scheme will be as follows:

- **First/distinction (70-100)** All parts of the implementation are correct and all tests pass. The code style is always very clear and the implementation of every exercise is transparent and elegant.
- **Upper second/merit (60-70)** The implementation is correct but let down somewhat by poor coding style. Alternatively, submissions which are correct and well written up to and including solving the Helmholtz problem but which do not include a correct solution to boundary conditions will earn an upper second.
- **Lower second/pass (50-60)** There are significant failings in the implementation resulting in many test failures, and/or the coding style is sufficiently poor that the code is hard to understand.
- **Fail** (0-50) The implementation is substantially incomplete. Correct implementations may have been provided for some of the earlier exercises but the more advanced parts of the implementation exercise have not been attempted or do not work.

0.2 Extension (mastery) exercise

Fourth year and masters students must also complete the mastery exercise, which will be issued half way through the term. This will be worth 20% of the implementation exercise marks and will be marked on the same scheme as above.

0.3 Obtaining the skeleton code

This section assumes you've already done the *Git tutorial*.

0.3.1 Setting up your repository

We're using a tool called GitHub classroom to automate the creation of your copies of the repository. To create your repository, click here.

0.3.2 Cloning a local copy

At the command line on your working machine type:

```
git clone <url> finite-element-course
```

Substituting your git repository url for <url>. Your git repository url can be found by clicking on *clone or down-load* at the top right of your repository page on GitHub.

0.3.3 Setting up your venv

We're going to use a Python venv. This is a private Python environment in which we'll install the packages we need, including our own implementation exercise. This minimises interference between this project and anything else which might be using Python on the system. We can run a script from the git repository to make the venv:

```
./finite-element-course/scripts/fe_install_venv venv
```

This has to install several packages in the veny, so it might take a few minutes to run.

On Windows, the set of commands is somewhat different. In this case you would run:

```
./finite-element-course/scripts/fe_install_venv_win venv
```

0.3.4 Activating your venv

Every time you want to work on the implementation exercise, you need to activate the venv. On Linux or Mac do this with:

```
source venv/bin/activate
```

while on Windows the command is:

```
source venv/Scripts/activate
```

Obviously if you are typing this in a directory other than the one containing the veny, you need to modify the path accordingly.

0.3.5 Setting up an implementation branch

We'll keep the master branch of your repository in the original condition so we can compare to it later, and collect any updates which occur during the term. Instead, we'll create an implementation branch to actually work on:

```
cd finite-element-course git checkout -b implementation
```

Your working directory is now a current checkout of your implementation branch. You'll also want to push this branch to GitHub:

```
git push --set-upstream origin implementation
```

0.3.6 Watching for updates and issues

You should make sure you are notified of all updates on the main repository and all issues anyone raises. For this, you should navigate to the main repository. On the top right there is an eye icon. Select the drop-down box and switch to watching.

0.3.7 Updating your fork

When you see that the main repository has been updated, you'll need to update your repository to incorporate those changes. *Just this once*, you need to tell your local git repo about the main repository:

```
\verb|git| \verb|remote| add upstream| \verb| https://github.com/finite-element/finite-element-course.git| \\
```

Now, every time you want to update you do the following:

- 1. Make sure you have committed all your local changes and pushed them to GitHub.
- 2. Execute the following commands:

```
git checkout master  # Switch to the master branch.

git pull upstream master  # Update from the main repository.

git push  # Push the updated master branch to GitHub.

git checkout implementation  # Switch back to the implementation branch.

git merge master  # Merge the new changes from master into_

implementation.

git push  # Push the updated implementation branch to_

GitHub.
```

0.4 Skeleton code documentation

There is web documentation for the complete fe utils. There is also an alphabetical index and a search page.

0.5 How to do the implementation exercises

The implementation exercises build up a finite element library from its component parts. Quite a lot of the coding infrastructure you will need is provided already. Your task is to write the crucial mathematical operations at key points. The mathematical operations required are described on this website, interspersed with exercises which require you to implement and test parts of the mathematics.

The code on which you will build is in the fe_utils directory of your repository. The code has embedded documentation which is used to build the fe_utils web documentation.

As you do the exercises, **commit your code** to your repository. This will build up your finite element library. You should commit code early and often - small commits are easier to understand and debug than large ones. **Never** commit back to the master branch of your fork, that should always remain a clean copy of the main repository.

0.6 Pull requests for feedback

Hint: A video about creating pull requests is available here

There will be a formal opportunity to recieve feedback on your code progress twice during the term. To take part, you should set up a pull request from your implementation branch to the master branch of your repository. This will enable the lecturer to write line by line comments on your code.

0.6.1 Creating your pull request

- 1. Click on the New pull request button at the top of your repository page on GitHub.
- 2. Make sure **left** dropdown box ("base") is set to master.
- 3. Make sure right dropdown box ("compare") is set to implementation.
- 4. Type a suitable title in the title box. For example Request for feedback 30/1/19.
- 5. If you have any comments you would like to pass on to the lecturer (for example questions about how you should have done a particular exercise) then type these in the Description box.
- 6. Click Create pull request.

0.7 Testing your work

As you complete the exercises, there will often be test scripts which exercise the code you have just written. These are located in the test directory and employ the pytest testing framework. You run the tests with:

```
py.test test_script.py
```

from the bash command line, replacing test_script.py with the appropriate test file name. The -x option to py.test will cause the test to stop at the first failure it finds, which is often the best place to start fixing a problem. For those familiar with debuggers, the --pdb option will drop you into the Python debugger at the first error.

You can also run all the tests by running py.test on the tests directory. This works particularly well with the -x option, resulting in the tests being run in course order and stopping at the first failing test:

```
py.test -x tests/
```

0.8 Coding style and commenting

Computer code is not just functional, it also conveys information to the reader. It is important to write clear, intelligible code. The readability and clarity of your code will count for marks.

The Python community has agreed standards for coding, which are documented in PEP8. There are programs and editor modes which can help you with this. The skeleton implementation follows PEP8 quite closely. You are encouraged, especially if you are a more experienced programmer, to follow PEP8 in your implementation. However nobody is going to lose marks for PEP8 failures.

0.9 Tips and tricks for the implementation exercise

Work from the documentation. The notes, and particularly the exercise specifications, contain important information about how and what to implement. If you just read the source code then you will miss out on important information.

Read the hints The pink sections in the notes starting with a lightbulb are hints. Usually they contain suggestions about how to go about writing your answer, or suggest Python functions which you might find useful.

Don't forget the 1D case Your finite element library needs to work in one and two dimensions.

Return a numpy.array() Many of the functions you have to write return arrays. Make sure you actually return an array and not a list (it's usually fine to build the answer as a list, but convert it to an array before you return it).

NUMERICAL QUADRATURE

Hint: A video recording of this tutorial is available here

The core computational operation with which we are concerned in the finite element method is the integration of a function over a known reference element. It's no big surprise, therefore, that this operation will be at the heart of our finite element implementation.

The usual way to efficiently evaluate arbitrary integrals numerically is numerical quadrature. This basic idea will already be familiar to you from undergraduate maths (or maybe even high school calculus) as it's the generalisation of the trapezoidal rule and Simpson's rule for integration.

The core idea of quadrature is that the integral of a function f(X) over an element e can be approximated as a weighted sum of function values evaluated at particular points:

$$\int_{e} f(X) = \sum_{q} f(X_q) w_q + O(h^n)$$

$$\tag{1.1}$$

we term the set $\{X_q\}$ the set of *quadrature points* and the corresponding set $\{w_q\}$ the set of *quadrature weights*. A set of quadrature points and their corresponding quadrature weights together comprise a *quadrature rule* for e. For an arbitrary function f, quadrature is only an approximation to the integral. The global truncation error in this approximation is invariably of the form $O(h^n)$ where h is the diameter of the element.

If f is a polynomial in X with degree p such that $p \le n-2$ then it is easy to show that integration using a quadrature rule of degree n results in exactly zero error.

Definition 183 The degree of precision of a quadrature rule is the largest p such that the quadrature rule integrates all polynomials of degree p without error.

1.1 Exact and incomplete quadrature

In the finite element method, integrands are very frequently polynomial. If the quadrature rule employed for a particular interval has a sufficiently high degree of precision such that there is no quadrature error in the integration, we refer to the quadrature as *exact* or *complete*. In any other case we refer to the quadrature as *incomplete*.

Typically, higher degree quadrature rules have more quadrature points than lower degree rules. This results in a trade-off between the accuracy of the quadrature rule and the number of function evaluations, and hence the computational cost, of an integration using that rule. Complete quadrature results in lower errors, but if the error due to incomplete quadrature is small compared with other errors in the simulation, particularly compared with the discretisation error, then incomplete quadrature may be advantageous.

1.2 Examples in one dimension

We noted above that a few one dimensional quadrature rules are commonly taught in introductory integration courses. The first of these is the midpoint rule:

$$\int_{0}^{h} f(X)dX = hf(0.5h) + O(h^{3})$$
(1.2)

In other words, an approximation to the integral of f over an interval can be calculated by multiplying the value of f at the mid-point of the interval by the length of the interval. This amounts to approximating the function over the integral by a constant value.

If we improve our approximation of f to a straight line over the interval, then we arrive at the trapezoidal (or trapezium) rule:

$$\int_{0}^{h} f(X)dX = \frac{h}{2}f(0) + \frac{h}{2}f(h) + O(h^{4})$$
(1.3)

while if we employ a quadratic function then we arrive at Simpson's rule:

$$\int_0^h f(X)dX = \frac{h}{6}f(0) + \frac{2h}{3}f\left(\frac{h}{2}\right) + \frac{h}{6}f(h) + O(h^5)$$
(1.4)

1.3 Reference elements

As a practical matter, we wish to write down quadrature rules as arrays of numbers, independent of h. In order to achieve this, we will write the quadrature rules for a single, reference element. When we wish to actually integrate a function over cell, we will change coordinates to the reference cell. We will return to the mechanics of this process later, but for now it means that we need only consider quadrature rules on the reference cells we choose.

A commonly employed one dimensional reference cell is the unit interval [0, 1], and that is the one we shall adopt here (the other popular alternative is the interval [-1, 1], which some prefer due to its symmetry about the origin).

In two dimensions, the cells employed most commonly are triangles and quadrilaterals. For simplicity, in this course we will only consider implementing the finite element method on triangles. The choice of a reference interval implies a natural choice of reference triangle. For the unit interval the natural correspondence is with the triangle with vertices [(0,0),(1,0),(0,1)], though different choices of vertex numbering are possible.

1.4 Python implementations of reference elements

The ReferenceCell class provides Python objects encoding the geometry and topology of the reference cell. At this stage, the relevant information is the dimension of the reference cell and the list of vertices. The topology will become important when we consider *meshes*. The reference cells we will require for this course are the ReferenceInterval and ReferenceTriangle.

1.5 Quadrature rules on reference elements

Having adopted a convention for the reference element, we can simply express quadrature rules as lists of quadrature points with corresponding quadrature weights. For example Simpson's rule becomes:

$$w = \left[\frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right]$$

$$X = [(0), (0.5), (1)].$$
(1.5)

We choose to write the quadrature points as 1-tuples for consistency with the n-dimensional case, in which the points will be n-tuples.

The lowest order quadrature rule on the reference triangle is a single point quadrature:

$$w = \begin{bmatrix} \frac{1}{2} \end{bmatrix}$$

$$X = \left[\left(\frac{1}{3}, \frac{1}{3} \right) \right]$$
(1.6)

This rule has a degree of precision of 1.

Hint: The weights of a quadrature rule always sum to the volume of the reference element. Why is this?

1.6 Legendre-Gauß quadrature in one dimension

The finite element method will result in integrands of different polynomial degrees, so it is convenient if we have access to quadrature rules of arbitrary degree on demand. In one dimension the Legendre-Gauß quadrature rules are a family of rules of arbitrary precision which we can employ for this purpose. Helpfully, numpy provides an implementation which we are able to adopt. The Legendre-Gauß quadrature rules are usually defined for the interval [-1, 1] so we need to change coordinates in order to arrive at a quadrature rule for our reference interval:

$$X_{q} = \frac{X'_{q} + 1}{2}$$

$$w_{q} = \frac{w'_{q}}{2}$$
(1.7)

where $(\{X_q'\}, \{w_q'\})$ is the quadrature rule on the interval [-1, 1] and $(\{X_q\}, \{w_q\})$ is the rule on the unit interval. Legendre-Gauß quadrature on the interval is optimal in the sense that it uses the minimum possible number of points for each degree of precision.

1.7 Extending Legendre-Gauß quadrature to two dimensions

We can form a unit square by taking the Cartesian product of two unit intervals: $(0,1) \otimes (0,1)$. Similarly, we can form a quadrature rule on a unit square by taking the product of two interval quadrature rules:

$$X_{sq} = \{(x_p, x_q) \mid x_p, x_q \in X\}$$

$$w_{sq} = \{w_p w_q \mid w_p, w_q \in w\}$$
(1.8)

where (X, w) is an interval quadrature rule. Furthermore, the degree of accuracy of (X_{sq}, w_{sq}) will be the same as that of the one-dimensional rule.

However, we need a quadrature rule for the unit triangle. We can achieve this by treating the triangle as a square with a zero length edge. The Duffy transform maps the unit square to the unit triangle:

$$(x_{\text{tri}}, y_{\text{tri}}) = (x_{\text{sq}}, y_{\text{sq}}(1 - x_{\text{sq}}))$$
 (1.9)

By composing the Duffy transform with (1.8) we can arrive at a quadrature rule for the triangle:

$$X_{\text{tri}} = \{ (x_p, x_q(1 - x_p)) \mid x_p \in X_h, x_q \in X_v \}$$

$$w_{\text{tri}} = \{ w_p w_q(1 - x_p) \mid w_p \in w_h, w_q \in w_v \}$$
(1.10)

where (X_v, w_v) is a reference interval quadrature rule with degree of precision n and (X_h, w_h) is a reference interval quadrature rule with degree of precision n+1. The combined quadrature rule $(X_{\rm tri}, w_{\rm tri})$ will then be n. The additional degree of precision required for (X_h, w_h) is because the Duffy transform effectively increases the polynomial degree of the integrand by one.

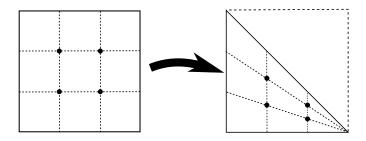


Fig. 1.1: The Duffy transform maps a square to a triangle by collapsing one side.

1.8 Implementing quadrature rules in Python

The fe_utils.quadrature module provides the QuadratureRule class which records quadrature points and weights for a given ReferenceCell. The gauss_quadrature() function creates quadrature rules for a prescribed degree of precision and reference cell.

Exercise 184 The integrate () method is left unimplemented. Using (1.1), implement this method.

A test script for your method is provided in the test directory as test_01_integrate.py. Run this script to test your code:

py.test test/test_01_integrate.py

from the Bash command line. Make sure you commit your modifications and push them to your fork of the course repository.

Hint: You can implement integrate () in one line using a list comprehension and numpy.dot().

Hint: Don't forget to activate your Python venv!

CONSTRUCTING FINITE ELEMENTS

Hint: A video recording of the introduction to this chapter is available here

At the core of the finite element method is the representation of finite-dimensional function spaces over elements. This concept was formalised by [Cia02]:

Definition 185 A finite element is a triple (K, P, N) in which K is a cell, P is a space of functions $K \to \mathbb{R}^n$ and N, the set of nodes, is a basis for P^* , the dual space to P.

Note that this definition includes a basis for P^* , but not a basis for P. It turns out to be most convenient to specify the set of nodes for an element, and then derive an appropriate basis for P from that. In particular:

Definition 186 Let $N = \{\phi_j^*\}$ be a basis for P^* . A nodal basis, $\{\phi_i\}$ for P is a basis for P with the property that $\phi_i^*(\phi_i) = \delta_{ij}$.

2.1 A worked example

Hint: A video recording of this section is available here

To illustrate the construction of a nodal basis, let's consider the linear polynomials on a triangle. We first need to define our reference cell. The obvious choice is the triangle with vertices $\{(0,0),(1,0),(0,1)\}$

Functions in this space have the form a + bx + cy. So the function space has three unknown parameters, and its basis (and dual basis) will therefore have three members. In order to ensure the correct continuity between elements, the dual basis we need to use is the evaluation of the function at each of the cell vertices. That is:

$$\phi_0^*(f) = f((0,0))$$

$$\phi_1^*(f) = f((1,0))$$

$$\phi_2^*(f) = f((0,1))$$
(2.1)

We know that ϕ_i has the form a + bx + cy so now we can use the definition of the nodal basis to determine the unknown coefficients:

$$\begin{pmatrix} \phi_0^*(\phi_i) \\ \phi_1^*(\phi_i) \\ \phi_2^*(\phi_i) \end{pmatrix} = \begin{pmatrix} \delta_{i,0} \\ \delta_{i,1} \\ \delta_{i,2} \end{pmatrix}$$
 (2.2)

So for ϕ_0 we have:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ b_0 \\ c_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$
 (2.3)

Which has solution $\phi_0 = 1 - x - y$. We can write the equations for all the basis functions at once as a single matrix equation:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_0 & a_1 & a_2 \\ b_0 & b_1 & b_2 \\ c_0 & c_1 & c_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
(2.4)

By which we establish that the full basis is given by:

$$\phi_0 = 1 - x - y$$

$$\phi_1 = x$$

$$\phi_2 = y$$
(2.5)

2.2 Types of node

We have just encountered nodes given by the evaluation of the function at a given point. Other forms of functional are also suitable for use as finite element nodes. Examples include the integral of the function over the cell or some sub-entity and the evaluation of the gradient of the function at some point. For some vector-valued function spaces, the nodes may be given by the evaluation of the components of the function normal or tangent to the boundary of the cell at some point.

In this course we will only consider point evaluation nodes. The implementation of several other forms of node are covered in [Kir04].

2.3 The Lagrange element nodes

Hint: A video recording of this section is available here

The number of coefficients of a degree p polynomial in d dimensions is given by $\binom{p+d}{d}$. The simplest set of nodes which we can employ is simply to place these nodes in a regular grid over the reference cell. Given the classical relationship between binomial coefficients and Pascal's triangle (and between trinomial coefficients and Pascal's pyramid), it is unsurprising that this produces the correct number of nodes.

The set of equally spaced points of degree p on the triangle is:

$$\left\{ \left(\frac{i}{p}, \frac{j}{p}\right) \middle| 0 \le i + j \le p \right\} \tag{2.6}$$

The finite elements with this set of nodes are called the *equispaced Lagrange* elements and are the most commonly used elements for relatively low order computations.

Note: At higher order the equispaced Lagrange basis is poorly conditioned and creates unwanted oscillations in the solutions. However for this course Lagrange elements will be sufficient.

Exercise 187 Use (2.6) to implement lagrange_points(). Make sure your algorithm also works for one-dimensional elements. Some basic tests for your code are to be found in test/test_02_lagrange_points.py. You can also test your lagrange points on the triangle by running:

plot_lagrange_points degree

Where degree is the degree of the points to plot.

2.4 Solving for basis functions

Hint: A video recording of this section is available here

The matrix in (2.4) is a generalised Vandermonde¹ matrix. Given a list of points $(x_i, y_i) \in \mathbb{R}^2, 0 \le i < m$ the corresponding degree n generalised Vandermonde matrix is given by:

$$V = \begin{bmatrix} 1 & x_0 & y_0 & x_0^2 & x_0 y_0 & y_0^2 & \dots & x_0^n & x_0^{n-1} y_0 & \dots & x_0 y_0^{n-1} & y_0^n \\ 1 & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 & \dots & x_1^n & x_1^{n-1} y_1 & \dots & x_1 y_1^{n-1} & y_1^n \\ \vdots & & & & & & & & & & \\ 1 & x_m & y_m & x_m^2 & x_m y_m & y_m^2 & \dots & x_m^n & x_m^{n-1} y_m & \dots & x_m y_m^{n-1} & y_m^n \end{bmatrix}$$
(2.7)

If we construct the Vandermonde matrix for the nodes of a finite element, then the equation for the complete set of basis function polynomial coefficients is:

$$VC = I (2.8)$$

where the j-th column of C contains the polynomial coefficients of the basis function corresponding to the j-th node. For (2.8) to be well-posed, there must be a number of nodes equal to the number of coefficients of a degree n polynomial. If this is the case, then it follows immediately that:

$$C = V^{-1} \tag{2.9}$$

The same process applies to the construction of basis functions for elements in one or three dimensions, except that the Vandermonde matrix must be modified to exclude powers of y (in one dimension) or to include powers of z.

Note: The monomial basis for polynomial spaces employed here becomes increasingly ill-conditioned at higher order, so it may be advantageous to employ a different basis in the construction of the Vandermonde matrix. See [Kir04] for an example.

Exercise 188 Use (2.7) to implement vandermonde_matrix(). Think carefully about how to loop over each row to construct the correct powers of x and y. For the purposes of this exercise you should ignore the grad argument.

Tests for this function are in test/test_03_vandermonde_matrix.py

Hint: You can use numpy array operations to construct whole columns of the matrix at once.

2.5 Implementing finite elements in Python

Hint: A video recording of this section is available here

The Ciarlet triple (K,P,N) also provides a good abstraction for the implementation of software objects corresponding to finite elements. In our case K will be a ReferenceCell. In this course we will only implement finite element spaces consisting of complete polynomial spaces so we will specify P by providing the maximum degree of the polynomials in the space. Since we will only deal with point evaluation nodes, we can represent N by a series of points at which the evaluation should occur.

¹ A Vandermonde matrix is the one-dimensional case of the generalised Vandermonde matrix.

Exercise 189 Implement the rest of the FiniteElement __init__() method. You should construct a Vandermonde matrix for the nodes and invert it to create the basis function coefs. Store these as self. basis_coefs.

Some basic tests of your implementation are in test/test_04_init_finite_element.py.

Hint: The numpy.linalg.inv() function may be used to invert the matrix.

2.6 Implementing the Lagrange Elements

Hint: A video recording of this section is available here

The FiniteElement class implements a general finite element object assuming we have provided the cell, polynomial, degree and nodes. The LagrangeElement class is a subclass of FiniteElement which will implement the particular case of the equispaced Lagrange elements.

Exercise 190 Implement the __init__() method of LagrangeElement. Use lagrange_points() to obtain the nodes. For the purpose of this exercise, you may ignore the entity_nodes argument.

After you have implemented tabulate() in the next exercise, you can use plot_lagrange_basis_functions to visualise your Lagrange basis functions.

2.7 Tabulating basis functions

Hint: A video recording of this section is available here

A core operation in the finite element method is integrating expressions involving functions in finite element spaces. This is usually accomplished using *numerical quadrature*. This means that we need to be able to evaluate the basis functions at a set of quadrature points. The operation of evaluating a set of basis functions at a set of points is called *tabulation*.

Recall that the coefficients of the basis functions are defined with respect to the monomial basis in (2.9). To tabulate the basis functions at a particular set of points therefore requires that the monomial basis be evaluated at that set of points. In other words, the Vandermonde matrix needs to be evaluated at the quadrature points. Suppose we have a set of points $\{X_i\}$ and a set of basis functions $\{\phi_j\}$ with coefficients with respect to the monomial basis given by the matrix C. Then the tabulation matrix is given by:

$$T_{ij} = \phi_j(X_i) = \sum_b V(X_i)_b C_{bj} = (V(X_i) \cdot C)_{ij}$$
(2.10)

Exercise 191 Implement tabulate(). You can use a Vandermonde matrix to evaluate the polynomial terms and take the matrix product of this with the basis function coefficients. The method should have at most two executable lines. For the purposes of this exercise, ignore the grad argument.

The test file test/test_05_tabulate.py checks that tabulating the nodes of a finite element produces the identity matrix.

2.8 Gradients of basis functions

Hint: A video recording of this section is available here

A function f defined over a single finite element with basis $\{\phi_i\}$ is represented by a weighted sum of that basis:

$$f = \sum_{i} f_i \phi_i \tag{2.11}$$

In order to be able to represent and solve PDEs, we will naturally also have terms incorporating derivatives. Since the coefficients f_i are spatially constant, derivative operators pass through to apply to the basis functions:

$$\nabla f = \sum_{i} f_i \nabla \phi_i \tag{2.12}$$

This means that we will need to be able to evaluate the gradient of the basis functions at quadrature points. Recall once again that the basis functions are evaluated by multiplying the Vandermonde matrix evaluated at the relevant points by the matrix of basis function coefficients. Hence:

$$\nabla \phi(X) = \nabla \left(V(X) \cdot C \right) = \left(\nabla V(X) \right) \cdot C \tag{2.13}$$

The last step follows because C is not a function of X, so it passes through ∇ . The effect of this is that evaluating the gradient of a function in a finite element field just requires the evaluation of the gradient of the Vandermonde matrix.

Exercise 192 Extend vandermonde_matrix() so that setting grad to True produces a rank 3 generalised Vandermonde tensor whose indices represent points, monomial basis function, and gradient component respectively. That is:

$$\nabla V_{ijk} = \frac{\partial V_j(X_i)}{\partial x_k} \tag{2.14}$$

In other words, each entry of V is replaced by a vector of the gradient of that polynomial term. For example, the entry x^2y^3 would be replaced by the vector $[2xy^3, 3x^2y^2]$.

The test/test_06_vandermonde_matrix_grad.py file has tests of this extension. You should also ensure that you still pass test/test_03_vandermonde_matrix.py.

Hint: The transpose () method of numpy arrays enables generalised transposes swapping any dimensions.

Hint: At least one of the natural ways of implementing this function results in a whole load of nan values in the generalised Vandermonde matrix. In this case, you might find numpy.nan_to_num() useful.

Exercise 193 Extend tabulate() to pass the grad argument through to vandermonde_matrix(). Then generalise the matrix product in tabulate() so that the result of this function (when grad is true) is a rank 3 tensor:

$$T_{ijk} = \nabla(\phi_i(X_i)) \cdot \mathbf{e}_k \tag{2.15}$$

where $e_0 \dots e_{\dim -1}$ is the coordinate basis on the reference cell.

The test/test_07_tabulate_grad.py script tests this extension. Once again, make sure you still pass test/test_05_tabulate.py

Hint: A video recording of this exercise is available here

Hint: The numpy.einsum() function implements generalised tensor contractions using Einstein summation notation. For example:

A = numpy.einsum("ijk,jl->ilk", T, C)

is equivalent to $A_{ilk} = \sum_{j} T_{ijk} C_{jl}$.

2.9 Interpolating functions to the finite element nodes

Hint: A video recording of this section is available here

Recall once again that a function can be represented on a single finite element as:

$$f = \sum_{i} f_i \phi_i \tag{2.16}$$

Since $\{\phi_i\}$ is a nodal basis, it follows immediately that:

$$f_i = \phi_i^*(f) \tag{2.17}$$

where ϕ_i^* is the node associated with the basis function ϕ_i . Since we are only interested in nodes which are the point evaluation of their function input, we know that:

$$f_i = f(X_i) (2.18)$$

where X_i is the point associated with the *i*-th node.

Exercise 194 Implement interpolate().

Once you have done this, you can use the script provided to plot functions of your choice interpolated onto any of the finite elements you can make:

plot_interpolate_lagrange "sin(2*pi*x[0])" 2 5

Hint: You can find help on the arguments to this function with:

plot_interpolate_lagrange -h

THREE

MESHES

Hint: A video recording of this chapter is available here

When employing the finite element method, we represent the domain on which we wish to solve our PDE as a mesh. In order to work with meshes, we need to have a somewhat more formal mathematical notion of a mesh. The mesh concepts we will employ here are loosely based on those in [Log09], and are typical of mesh representations for the finite element method.

3.1 Mesh entities

A mesh is composed of topological entities, such as vertices, edges, polygons and polyhedra.

Definition 195 The (topological) dimension of a mesh is the largest dimension among all of the topological entities in a mesh.

In this course we will not consider meshes of manifolds immersed in higher dimensional spaces (for example the surface of a sphere immersed in \mathbb{R}^3) so the topological dimension of the mesh will always match the geometric dimension of space in which we are working, so we will simply refer to the *dimension* of the mesh.

Definition 196 A topological entity of codimension n is a topological entity of dimension d-n where d is the dimension of the mesh.

Armed with these definitions we are able to define names for topological entities of various dimension and codimension:

entity name	dimension	codimension
vertex	0	
edge	1	
face	2	
facet		1
cell		0

The cells of a mesh can be polygons or polyhedra of any shape, however in this course we will restrict ourselves to meshes whose cells are intervals or triangles. The only other two-dimensional cells frequently employed are quadrilaterals.

The topological entities of each dimension will be given unique numbers in order that degrees of freedom can later be associated with them. We will identify topological entities by an index pair (d,i) where i is the index of the entity within the set of d-dimensional entities. For example, entity (0,10) is vertex number 10, and entity (1,10) is edge 10. Fig. 3.1 shows an example mesh with the topological entities labelled.

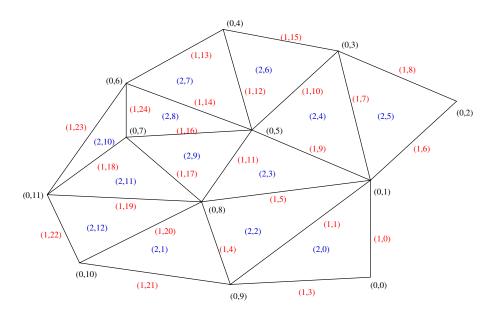


Fig. 3.1: A triangular mesh showing labelled topological entities: vertices (black), edges (red), and cells (blue).

3.2 Reference cell entities

The reference cells similarly have locally numbered topological entities, these are shown in Fig. 3.2. The numbering is a matter of convention: that adopted here is that edges share the number of the opposite vertex. The orientation of the edges is also shown, this is always from the lower numbered vertex to the higher numbered one.

The ReferenceCell class stores the local topology of the reference cell. Read the source and ensure that you understand the way in which this information is encoded.

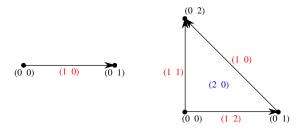


Fig. 3.2: Local numbering and orientation of the reference entities.

3.3 Adjacency

In order to implement the finite element method, we need to integrate functions over cells, which means knowing which basis functions are nonzero in a given cell. For the function spaces used in the finite element method, these basis functions will be the ones whose nodes lie on the topological entities adjacent to the cell. That is, the vertices, edges and (in 3D) the faces making up the cell, as well as the cell itself. One of the roles of the mesh is therefore to provide a lookup facility for the lower-dimensional mesh entities adjacent to a given cell.

Definition 197 Given a mesh M, then for each $\dim(M) \ge d_1 > d_2 \ge 0$ the adjacency function $\operatorname{Adj}_{d_1,d_2} : \mathbb{N} \to \mathbb{N}^k$ is the function such that:

$$Adj_{d_1,d_2}(i) = (i_0, \dots i_k)$$

where (d_1, i) is a topological entity and $(d_2, i_0), \ldots, (d_2, i_k)$ are the adjacent d_2 -dimensional topological entities numbered in the corresponding reference cell order. If every cell in the mesh has the same topology then k will be

60 Chapter 3. Meshes

fixed for each (d_1, d_2) pair. The correspondence between the orientation of the entity (d_1, i) and the reference cell of dimension d_1 is established by specifying that the vertices are numbered in ascending order¹. That is, for any entity (d_1, i) :

$$(i_0, \dots i_k) = \operatorname{Adj}_{d_1, 0}(i) \implies i_0 < \dots < i_k$$

A consequence of this convention is that the global orientation of all the entities making up a cell also matches their local orientation.

Example 198 *In the mesh shown in Fig. 3.1 we have:*

$$Adj_{2,0}(3) = (1,5,8).$$

In other words, vertices 1, 5 and 8 are adjacent to cell 3. Similarly:

$$Adi_{2,1}(3) = (11, 5, 9).$$

Edges 11, 5, and 9 are local edges 0, 1, and 2 of cell 3.

3.4 Mesh geometry

The features of meshes we have so far considered are purely topological: they deal with the adjacency relationships between topological entities, but do not describe the locations of those entities in space. Provided we restrict our attention to meshes in which the element edges are straight (ie not curved), we can represent the geometry of the mesh by simply recording the coordinates of the vertices. The positions of the higher dimensional entities then just interpolate the vertices of which they are composed. We will later observe that this is equivalent to representing the geometry in a vector-valued piecewise linear finite element space.

3.5 A mesh implementation in Python

The Mesh class provides an implementation of mesh objects in 1 and 2 dimensions. Given the list of vertices making up each cell, it constructs the rest of the adjacency function. It also records the coordinates of the vertices.

The UnitSquareMesh class creates a Mesh object corresponding to a regular triangular mesh of a unit square. Similarly, the UnitIntervalMesh class performs the corresponding (rather trivial) function for a unit one dimensional mesh.

You can observe the numbering of mesh entities in these meshes using the plot_mesh script. Run:

plot_mesh -h

for usage instructions.

¹ The numbering convention adopted here is very convenient, but only works for meshes composed of simplices (vertices, intervals, triangles and tetrahedra). A more complex convention would be required to support quadrilateral meshes.

62 Chapter 3. Meshes

FUNCTION SPACES: ASSOCIATING DATA WITH MESHES

A finite element space over a mesh is constructed by associating a finite element with each cell of the mesh. We will refer to the basis functions of this finite element space as *global* basis functions, while those of the finite element itself we will refer to as *local* basis functions. We can establish the relationship between the finite element and each cell of the mesh by associating the nodes (and therefore the local basis functions) of the finite element with the topological entities of the mesh. This is a two stage process. First, we associate the nodes of the finite element with the local topological entities of the reference cell. This is often referred to as *local numbering*. Then we associate the correct number of degrees of freedom with each global mesh entity. This is the *global numbering*.

4.1 Local numbering and continuity

Hint: A video recording of this section is available here

Which nodes should be associated with which topological entities? The answer to this question depends on the degree of continuity required between adjacent cells. The nodes associated with topological entites on the boundaries of cells (the vertices in one dimension, the vertices and edges in two dimensions, and the vertices, edges and faces in three dimensions) are shared between cells. The basis functions associated with nodes on the cell boundary will therefore be continuous between the cells which share that boundary.

For the Lagrange element family, we require global C_0 continuity. This implies that the basis functions are continuous everywhere. This has the following implications for the association of basis functions with local topological entites:

vertices At the function vertices we can achieve continuity by requiring that there be a node associated with each mesh vertex. The basis function associated with that node will therefore be continuous. Since we have a nodal basis, all the other basis functions will vanish at the vertex so the global space will be continuous at this point.

edges Where the finite element space has at least 2 dimensions we need to ensure continuity along edges. The restriction of a degree p polynomial over a d-dimensional cell to an edge of that cell will be a one dimensional degree p polynomial. To fully specify this polynomial along an edge requires p+1 nodes. However there will already be two nodes associated with the vertices of the edge, so p-1 additional nodes will be associated with the edge.

faces For three-dimensional (tetrahedral) elements, the basis functions must also be continuous across faces. This requires that sufficient nodes lie on the face to fully specify a two dimensional degree p polynomial. However the vertices and edges of the face already have nodes associated with them, so the number of nodes required to be associated with the face itself is actually the number required to represent a degree p-2 polynomial in two dimensions: $\binom{p-1}{2}$.

This pattern holds more generally: for a C_0 function space, the number of nodes which must be associated with a local topological entity of degree d is $\binom{p-1}{d}$.

Fig. 4.1 illustrates the association of nodes with reference entities for Lagrange elements on triangles. The numbering of nodes will depend on how lagrange_points() is implemented. The numbering used here is just one of the obvious choices.

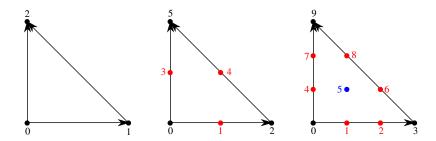


Fig. 4.1: Association of nodes with reference entities for the degree 1, 2, and 3 equispaced Lagrange elements on triangles. Black nodes are associated with vertices, red nodes with edges and blue nodes with the cell (face). The numbering of the nodes is arbitrary.

4.2 Implementing local numbering

Hint: A video recording of this section is available here

Local numbering can be implemented by adding an additional data structure to the FiniteElement class. For each local entity this must record the local nodes associated with that entity. This can be achieved using a dictionary of dictionaries structure. For example employing the local numbering of nodes employed in Fig. 4.1, the entity_node dictionary for the degree three equispaced Lagrange element on a triangle is given by:

Note that the order of the nodes in each list is important: it must always consistently reflect the orientation of the relevant entity in order that all the cells which share that entity consistently interpret the nodes. In this case this has been achieved by listing the nodes in order given by the direction of the orientation of each edge.

Exercise 199 Extend the __init__() method of LagrangeElement so that it passes the correct entity_node dictionary to the FiniteElement it creates.

The test/test_08_entity_nodes.py script tests this functionality.

Hint: You can either work out the right algorithm to generate entity_nodes with the right node indices, or you can modify lagrange_points() so that it produces the nodes in entity order, thus making the construction of entity_nodes straightforward.

You may find the point_in_entity() method of the ReferenceCell class useful.

4.3 Global numbering

Hint: A video recording of this section is available here

Given a mesh and a finite element, the global numbering task is to uniquely associate the appropriate number of global node numbers with each global entity. One such numbering is to allocate global numbers in ascending entity dimension order, and within each dimension in order of the index of each global topological entity. The formula for the first global node associated with entity (d, i) is then:

$$G(d,i) = \left(\sum_{\delta < d} N_{\delta} E_{\delta}\right) + i N_d$$

where N_d is the number of nodes which this finite element associates with each entity of dimension d, and E_d is the number of dimension d entities in the mesh. The full list of nodes associated with entity (d, i) is therefore:

$$[G(d,i),\ldots,G(d,i)+N_d-1]$$
 (4.1)

4.4 The cell-node map

Hint: A video recording of this section is available here

The primary use to which we wish to put the finite element spaces we are constructing is, naturally, the solution of finite element problems. The principle operation we will therefore need to support is integration over the mesh of mathematical expressions involving functions in finite element spaces. This will be accomplished by integrating over each cell in turn, and then summing over all cells. This means that a key operation we will need is to find the nodes associated with a given cell.

It is usual in finite element software to explicitly store the map from cells to adjacent nodes as a two-dimensional array with one row corresponding to each cell, and with columns corresponding to the local node numbers. The entries in this map will have the following values:

$$M[c, e(\delta, \epsilon)] = [G(\delta, i), \dots, G(\delta, i) + N_{\delta} - 1] \qquad \forall 0 \le \delta \le \dim(c), \forall 0 \le \epsilon < \hat{E}_{\delta}$$

$$(4.2)$$

where:

$$i = \mathrm{Adj}_{\dim(c),\delta}[c,\epsilon],$$
 (4.3)

 $e(\delta, \epsilon)$ is the local entity-node list for this finite element for the (δ, ϵ) local entity, Adj has the meaning given under *Adjacency*, \hat{E}_{δ} is the number of dimension δ entities in each cell, and G and N have the meanings given above. This algorithm requires a trivial extension to adjacency:

$$Adj_{\dim(c),\dim(c)}[c,0] = c \tag{4.4}$$

Hint: In (4.2), notice that for each value of δ and ϵ , $e(\delta, \epsilon)$ is a vector of indices, so the equation sets the value of zero, one, or more defined entries in row c of M for each δ and ϵ .

4.5 Implementing function spaces in Python

Hint: A video recording of this section is available here

¹ Many correct global numberings are possible, that presented here is simple and correct, but not optimal from the perspective of the memory layout of the resulting data.

M345A47 Finite Elements: Analysis and Implementation, Edition 2020.0

As noted above, a finite element space associates a mesh and a finite element, and contains (in some form) a global numbering of the nodes.

Exercise 200 Implement the __init__ () method of fe_utils.function_spaces.FunctionSpace. The key operation is to set cell_nodes using (4.2).

You can plot the numbering you have created with the plot_function_space_nodes script. As usual, run the script passing the -h option to discover the required arguments.

Hint: Many of the terms in (4.2) are implemented in the objects in fe_utils. For example:

- $\mathrm{Adj}_{\dim(c),\delta}$ is implemented by the adjacency () method of the Mesh.
- You have $e(\delta,\epsilon)$ as entity_nodes. Note that in this case you need separate square brackets for each index:

element.entity_nodes[delta][epsilon]

Hint: cell_nodes needs to be integer-valued. If you choose to use numpy.zeros() to create a matrix which you then populate with values, you need to explicitly specify that you want a matrix of integers. This can be achieved by passing the dtype argument to numpy.zeros(). For example numpy.zeros((nrows, ncols), dtype=int).

FUNCTIONS IN FINITE ELEMENT SPACES

Recall that the general form of a function in a finite element space is:

$$f(x) = \sum_{i} f_i \phi_i(x) \tag{5.1}$$

Where the $\phi_i(x)$ are now the global basis functions achieved by stitching together the local basis functions defined by the *finite element*.

5.1 A python implementation of functions in finite element spaces

Hint: A video recording of this section is available here

The Function class provides a simple implementation of function storage. The input is a FunctionSpace which defines the mesh and finite element to be employed, to which the Function adds an array of degree of freedom values, one for each node in the FunctionSpace.

5.2 Interpolating values into finite element spaces

Hint: A video recording of this section is available here

Suppose we have a function $g(x): \mathbb{R}^n \to \mathbb{R}$ which we wish to approximate as a function f(x) in some finite element space V. In other words, we want to find the f_i such that:

$$\sum_{i} f_i \phi_i(x) \approx g(x) \tag{5.2}$$

The simplest way to do this is to *interpolate* g(x) onto V. In other words, we evaluate:

$$f_i = n_i(g(x)) (5.3)$$

where n_i is the node associated with ϕ_i . Since we are only concerned with point evaluation nodes, this is equivalent to:

$$f_i = g(x_i) (5.4)$$

where x_i is the coordinate vector of the point defining the node n_i . This looks straightforward, however the x_i are the *global* node points, and so far we have only defined the node points in *local* coordinates on the reference element.

5.2.1 Changing coordinates between reference and physical space

We'll refer to coordinates on the global mesh as being in *physical space* while those on the reference element are in *local space*. We'll use case to distinguish local and global objects, so local coordinates will be written as X and global coordinates as x. The key observation is that within each cell, the global coordinates are the linear interpolation of the global coordinate values at the cell vertices. In other words, if $\{\Psi_j\}$ is the local basis for the **linear** lagrange elements on the reference cell and \hat{x}_j are the corresponding global vertex locations on a cell c then:

$$x = \sum_{j} \hat{x}_{j} \Psi_{j}(X) \quad \forall x \in c.$$
 (5.5)

Remember that we know the location of the nodes in local coordinates, and we have the tabulate() method to evaluate all the basis functions of an element at a known set of points. So if we write:

$$A_{i,j} = \Psi_j(X_i) \tag{5.6}$$

where {X_i} are the node points of our finite element, then:

$$x = A \cdot \hat{x} \tag{5.7}$$

Where \hat{x} is the $(\dim +1, \dim)$ array whose rows are the current element vertex coordinates, and x is the (nodes, \dim) array whose rows are the global coordinates of the nodes in the current element. We can then apply g() to each row of x in turn and record the result as the Function value for that node.

Hint: The observant reader will notice that this algorithm is inefficient because the function values at nodes on the boundaries of elements are evaluated more than once. This can be avoided with a little tedious bookkeeping but we will not concern ourselves with that here.

5.2.2 Looking up cell coordinates and values

Hint: A video recording of this section is available here

In the previous section we used the vertex coordinates of a cell to find the node coordinates, and then we calculated Function values at those points. The coordinates are stored in a single long list associated with the Mesh, and the Function contains a single long list of values. We need to use *indirect addressing* to access these values. This is best illustrated using some Python code.

Suppose f is a Function. For brevity, we write fs = f.function_space, the FunctionSpace associated with f. Now, we first need a linear element and a corresponding FunctionSpace:

```
cg1 = fe_utils.LagrangeElement(fs.mesh.cell, 1)
cg1fs = fe_utils.FunctionSpace(fs.mesh, cg1)
```

Then the vertex indices of cell number c in the correct order for the linear Lagrange element are:

```
cglfs.cell_nodes[c, :]
```

and therefore the set of coordinate vectors for the vertices of element c are:

```
fs.mesh.vertex_coords[cg1fs.cell_nodes[c, :], :]
```

That is, the cglfs.cell_nodes array is used to look up the right vertex coordinates. By a similar process we can access the values associated with the nodes of element c:

f.values[fs.cell_nodes[c, :]]

5.2.3 A Python implementation of interpolation

Hint: A video recording of this section is available here

Putting together the change of coordinates with the right indirect addressing, we can provide the Function class with a interpolate () method which interpolates a user-provided function onto the Function.

Exercise 201 Read and understand the interpolate() method. Use plot_sin_function to investigate interpolating different functions onto finite element spaces at different gresolutions and polynomial degrees.

Hint: There is no implementation work associated with this exercise, but the programming constructs used in interpolate() will be needed when you implement integration.

5.3 Integration

Hint: A video recording of this section is available here

We now come to one of the fundamental operations in the finite element method: integrating a Function over the domain. The full finite element method actually requires the integration of expressions of unknown test and trial functions, but we will start with the more straightforward case of integrating a single, known, Function over a domain Ω :

$$\int_{\Omega} f dx \quad f \in V \tag{5.8}$$

where dx should be understood as being the volume measure with the correct dimension for the domain and V is some finite element space over Ω . We can express this integral as a sum of integrals over individual cells:

$$\int_{\Omega} f dx = \sum_{c \in \Omega} \int_{c} f dx. \tag{5.9}$$

So we have in fact reduced the integration problem to the problem of integrating f over each cell. In *a previous* part of the module we implemented quadrature rules which enable us to integrate over specified reference cells. If we can express the integral over some arbitrary cell c as an integral over a reference cell c_0 then we are done. In fact this simply requires us to employ the change of variables formula for integration:

$$\int_{C} f(x) dx = \int_{C_0} f(X) |J| dX$$
(5.10)

where |J| is the absolute value of the determinant of the Jacobian matrix. J is given by:

$$J_{\alpha\beta} = \frac{\partial x_{\alpha}}{\partial X_{\beta}}. (5.11)$$

Hint: We will generally adopt the convention of using Greek letters to indicate indices in spatial dimensions, while we will use Roman letters in the sequence i, j, \ldots for basis function indices. We will continue to use q for the index over the quadrature points.

5.3. Integration 69

Evaluating (5.11) depends on having an expression for x in terms of X. Fortunately, (5.5) is exactly this expression, and applying the usual rule for differentiating functions in finite element spaces produces:

$$J_{\alpha\beta} = \sum_{j} (\tilde{x}_{j})_{\alpha} \nabla_{\beta} \Psi_{j}(X)$$
(5.12)

where $\{\Psi_j\}$ is once again the degree 1 Lagrange basis and $\{\tilde{x}_j\}$ are the coordinates of the corresponding vertices of cell c. The presence of X in (5.12) implies that the Jacobian varies spatially across the reference cell. However since $\{\Psi_j\}$ is the degree 1 Lagrange basis, the gradients of the basis functions are constant over the cell and so it does not matter at which point in the cell the Jacobian is evaluated. For example we might choose to evaluate the Jacobian at the cell origin X=0.

Hint: When using simplices with curved sides, and on all but the simplest quadrilateral or hexahedral meshes, the change of coordinates will not be affine. In that case, to preserve full accuracy it will be necessary to compute the Jacobian at every quadrature point. However, non-affine coordinate transforms are beyond the scope of this course.

5.3.1 Expressing the function in the finite element basis

Hint: A video recording of this section is available here

Let $\{\Phi_i(X)\}\$ be a **local** basis for V on the reference element c_0 . Then our integral becomes:

$$\int_{c} f(x) dx = \int_{c_0} \sum_{i} F(M(c, i)) \Phi_i(X) |J| dX$$
(5.13)

where F is the vector of global coefficient values of f, and M is the cell node map.

5.3.2 Numerical quadrature

Hint: A video recording of this section is available here

The actual evaluation of the integral will employ the quadrature rules we discussed in *a previous section*. Let $\{X_q\}, \{w_q\}$ be a quadrature rule of sufficient degree of precision that the quadrature is exact. Then:

$$\int_{c} f(x) dx = \sum_{q} \sum_{i} F(M(c, i)) \Phi_{i}(X_{q}) |J| w_{q}$$
(5.14)

5.3.3 Implementing integration

Hint: A video recording of this section is available here

Exercise 202 Use (5.12) to implement the jacobian () method of Mesh. test/test_09_jacobian.py is available for you to test your results.

Hint: The $\nabla_{\beta}\Psi_{j}(X)$ factor in (5.12) is the same for every cell in the mesh. You could make your implementation more efficient by precalculating this term in the __init__() method of Mesh.

Exercise 203 Use (5.9) and (5.14) to implement integrate(). test_10_integrate_function.py may be used to test your implementation.

Hint: Your method will need to:

- 1. Construct a suitable QuadratureRule.
- 2. tabulate() the basis functions at each quadrature point.
- 3. Visit each cell in turn.
- 4. Construct the jacobian() for that cell and take the absolute value of its determinant (numpy. absolute and numpy.linalg.det() will be useful here).
- 5. Sum all of the arrays you have constructed over the correct indices to a contribution to the integral (numpy.einsum() may be useful for this).

Hint: You might choose to read ahead before implementing integrate(), since the errornorm() function is very similar and may provide a useful template for your work.

5.3. Integration 71

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ASSEMBLING AND SOLVING FINITE ELEMENT PROBLEMS

Hint: A video recording of this section is available here

Having constructed functions in finite element spaces and integrated them over the domain, we now have the tools in place to actually assemble and solve a simple finite element problem. To avoid having to explicitly deal with boundary conditions, we choose in the first instance to solve a Helmholtz problem 1 , find u in some finite element space V such that:

$$-\nabla^2 u + u = f$$

$$\nabla u \cdot \mathbf{n} = 0 \text{ on } \Gamma$$
 (6.1)

where Γ is the domain boundary and n is the outward pointing normal to that boundary. f is a known function which, for simplicity, we will assume lies in V. Next, we form the weak form of this equation by multiplying by a test function in V and integrating over the domain. We integrate the Laplacian term by parts. The problem becomes, find $u \in V$ such that:

$$\int_{\Omega} \nabla v \cdot \nabla u + vu \, dx - \underbrace{\int_{\Gamma} v \nabla u \cdot \mathbf{n} \, ds}_{=0} = \int_{\Omega} v f \, dx \qquad \forall v \in V$$
(6.2)

If we write $\{\phi_i\}_{i=0}^{n-1}$ for our basis for V, and recall that it is sufficient to ensure that (6.2) is satisfied for each function in the basis then the problem is now, find coefficients u_i such that:

$$\int_{\Omega} \sum_{j} (\nabla \phi_i \cdot \nabla (u_j \phi_j) + \phi_i u_j \phi_j) \, dx = \int_{\Omega} \phi_i \sum_{k} f_k \phi_k \, dx \qquad \forall \, 0 \le i < n$$
(6.3)

Since the left hand side is linear in the scalar coefficients u_j , we can move them out of the integral:

$$\sum_{j} \left(\int_{\Omega} \nabla \phi_{i} \cdot \nabla \phi_{j} + \phi_{i} \phi_{j} \, \mathrm{d}x \, u_{j} \right) = \int_{\Omega} \phi_{i} \, \sum_{k} f_{k} \phi_{k} \, \mathrm{d}x \qquad \forall \, 0 \leq i < n$$
 (6.4)

We can write this as a matrix equation:

$$A\mathbf{u} = \mathbf{f} \tag{6.5}$$

where:

$$A_{ij} = \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j + \phi_i \phi_j \, dx$$
 (6.6)

$$\mathbf{u}_j = u_j \tag{6.7}$$

$$\mathbf{f}_i = \int_{\Omega} \phi_i \sum_k f_k \phi_k \, \mathrm{d}x \tag{6.8}$$

 $^{^{1}}$ Strictly speaking this is the positive definite Helmholtz problem. Changing the sign on u produces the indefinite Helmholtz problem, which is significantly harder to solve.

6.1 Assembling the right hand side

Hint: A video recording of this section is available here

The assembly of these integrals exploits the same decomposition property we exploited previously to integrate functions in finite element spaces. For example, (6.8) can be rewritten as:

$$\mathbf{f}_i = \sum_c \int_c \phi_i \sum_k f_k \phi_k \, \mathrm{d}x \tag{6.9}$$

This has a practical impact once we realise that only a few basis functions are non-zero in each element. This enables us to write an efficient algorithm for right hand side assembly. Assume that at the start of our algorithm:

$$\mathbf{f}_i = 0. \tag{6.10}$$

Now for each cell c, we execute:

$$\mathbf{f}_{M(c,\hat{i})} \stackrel{+}{=} \int_{c} \Phi_{\hat{i}} \left(\sum_{\hat{k}} f_{M(c,\hat{k})} \Phi_{\hat{k}} \right) |J| \, \mathrm{d}X \qquad \forall 0 \le \hat{i} < N$$

$$(6.11)$$

Where M is the cell-node map for the finite element space V, N is the number of nodes per element in V, and $\{\Phi_{\hat{i}}\}_{\hat{i}=0}^{N-1}$ are the local basis functions. In other words, we visit each cell and conduct the integral for each local basis function, and add that integral to the total for the corresponding global basis function.

By choosing a suitable quadrature rule, $\{X_a\}, \{w_a\}$, we can write this as:

$$\mathbf{f}_{M(c,\hat{i})} \stackrel{+}{=} \left(\sum_{q} \Phi(X_q)_{\hat{i}} \left(\sum_{\hat{k}} f_{M(c,\hat{k})} \Phi(X_q)_{\hat{k}} \right) w_q \right) |J| \qquad \forall 0 \le \hat{i} < N, \, \forall c$$
 (6.12)

6.2 Assembling the left hand side matrix

Hint: A video recording of this section is available here

The left hand side matrix follows a similar pattern, however there are two new complications. First, we have two unbound indices (i and j), and second, the integral involves derivatives. We will address the question of derivatives first.

6.2.1 Pulling gradients back to the reference element

On element c, there is a straightforward relationship between the local and global bases:

$$\phi_{M(c,i)}(x) = \Phi_i(X) \tag{6.13}$$

We can also, as we showed in *Changing coordinates between reference and physical space*, express the global coordinate x in terms of the local coordinate X.

What about $\nabla \phi$? We can write the gradient operator in component form and apply (6.13):

$$\frac{\partial \phi_{M(c,i)}(x)}{\partial x_{\alpha}} = \frac{\partial \Phi_{i}(X)}{\partial x_{\alpha}} \quad \forall \, 0 \le \alpha < \dim$$
 (6.14)

However, the expression on the right involves the gradient of a local basis function with respect to the global coordinate variable x. We employ the chain rule to express this gradient with respect to the local coordinates, X:

$$\frac{\partial \phi_{M(c,i)}(x)}{\partial x_{\alpha}} = \sum_{\beta=0}^{\dim -1} \frac{\partial X_{\beta}}{\partial x_{\alpha}} \frac{\partial \Phi_{i}(X)}{\partial X_{\beta}} \quad \forall \, 0 \le \alpha < \dim$$
 (6.15)

Using the *definition of the Jacobian*, and using ∇_x and ∇_X to indicate the global and local gradient operators respectively, we can equivalently write this expression as:

$$\nabla_x \phi_{M(c,i)}(x) = J^{-T} \nabla_X \Phi_i(X) \tag{6.16}$$

where $J^{-T} = (J^{-1})^T$ is the transpose of the inverse of the cell Jacobian matrix.

6.2.2 The assembly algorithm

Hint: A video recording of this section is available here

We can start by pulling back (6.6) to local coordinates:

$$\mathbf{A}_{ij} = 0.$$

$$\mathbf{A}_{M(c,\hat{i}),M(c,\hat{j})} \stackrel{\pm}{=} \int_{c} \left(\left(J^{-T} \nabla_{X} \Phi_{\hat{i}} \right) \cdot \left(J^{-T} \nabla_{X} \Phi_{\hat{j}} \right) + \Phi_{\hat{i}} \Phi_{\hat{j}} \right) |J| \, \mathrm{d}X \quad \forall 0 \leq \hat{i}, \hat{j} < N, \, \forall c$$

$$(6.17)$$

We now employ a suitable quadrature rule, $\{X_q\}, \{w_q\}$, to calculate the integral:

$$\mathbf{A}_{M(c,\hat{i}),M(c,\hat{j})} \stackrel{+}{=} \sum_{q} \left(\left(J^{-T} \nabla_{X} \Phi_{\hat{i}}(X_{q}) \right) \cdot \left(J^{-T} \nabla_{X} \Phi_{\hat{j}}(X_{q}) \right) + \Phi_{\hat{i}}(X_{q}) \Phi_{\hat{j}}(X_{q}) \right) |J| w_{q} \quad \forall 0 \leq \hat{i}, \hat{j} < N, \forall c$$

$$(6.18)$$

Some readers may find this easier to read using index notation over the geometric dimensions:

$$\mathbf{A}_{M(c,\hat{i}),M(c,\hat{j})} \stackrel{+}{=} \sum_{q} \left(\sum_{\alpha\beta\gamma} J_{\beta\alpha}^{-1} \left(\nabla_{X} \Phi_{\hat{i}}(X_{q}) \right)_{\beta} J_{\gamma\alpha}^{-1} \left(\nabla_{X} \Phi_{\hat{j}}(X_{q}) \right)_{\gamma} + \Phi_{\hat{i}}(X_{q}) \Phi_{\hat{j}}(X_{q}) \right) |J| w_{q} \quad \forall 0 \leq \hat{i}, \hat{j} < N, \forall c$$

$$(6.19)$$

6.2.3 A note on matrix insertion

For each cell c, the right hand sides of equations (6.18) and (6.19) have two free indices, \hat{i} and \hat{j} . The equation therefore assembles a local $N \times N$ matrix corresponding to one integral for each test function, trial function pair on the current element. This is then added to the global matrix at the row and column pairs given by the cell node map $M(c,\hat{i})$ and $M(c,\hat{j})$.

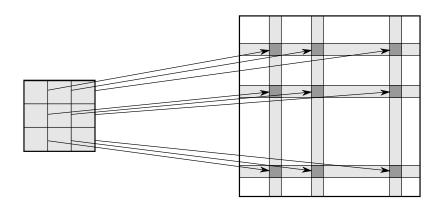


Fig. 6.1: Computing integrals for each local test and trial function produces a local dense (in this case, 3×3) matrix. The entries in this matrix are added to the corresponding global row and column positions in the global matrix.

Hint: One might naïvely expect that if nodes is the vector of global node numbers for the current cell, m is the matrix of local integral values and A is the global matrix, then the Python code might look like:

```
A[nodes, nodes] += m # DON'T DO THIS!
```

Unfortunately, numpy interprets this as an instruction to insert a vector into the diagonal of A, and will complain that the two-dimensional right hand side does not match the one-dimensional left hand side. Instead, one has to employ the numpy.ix_() function:

```
A[np.ix_(nodes, nodes)] += m # DO THIS!
```

No such problem exists for adding values into the global right hand side vector. If 1 is the global right hand side vector and v is the vector of local right hand integrals, then the following will work just fine:

```
l[nodes] += v
```

6.2.4 Sparse matrices

Hint: A video recording of this section is available here

Each row of the global matrix corresponds to a single global basis function. The number of non-zeros in this row is equal to the number of other basis functions which are non-zero in the elements where the original basis function is non-zero. The maximum number of non-zeros on a row may vary from a handful for a low degree finite element to a few hundred for a fairly high degree element. The important point is that it is essentially independent of the size of the mesh. This means that as the number of cells in the mesh increases, the proportion of the matrix entries on each row which have the value zero increases.

For example, a degree 4 Lagrange finite element space defined on 64×64 unit square triangular mesh has about 66000 nodes. The full global matrix therefore has more that 4 billion entries and, at 8 bytes per matrix entry, will consume around 35 gigabytes of memory! However, there are actually only around 23 nonzeros per row, so more than 99.9% of the entries in the matrix are zeroes.

Instead of storing the complete matrix, sparse matrix formats store only those entries in the matrix which are nonzero. They also have to store some metadata to describe where in the matrix the non-zero entries are stored. There are various different sparse matrix formats available, which make different trade-offs between memory usage, insertion speed, and the speed of different matrix operations. However, if we make the (conservative) assumption that a sparse matrix takes 16 bytes to store each nonzero value, instead of 8 bytes, then we discover that in the example above, we would use less than 25 megabytes to store the matrix. The time taken to solving the matrix system will also be vastly reduced since operations on zeros are avoided.

Hint: The scipy.sparse package provides convenient interfaces which enable Python code to employ a variety of sparse matrix formats using essentially identical operations to the dense matrix case. The skeleton code already contains commands to construct empty sparse matrices and to solve the resulting linear system. You may, if you wish, experiment with choosing other sparse formats from scipy.sparse, but it is very strongly suggested that you do **not** switch to a dense numpy array; unless, that is, you particularly enjoy running out of memory on your computer!

6.3 The method of manufactured solutions

When the finite element method is employed to solve Helmholtz problems arising in science and engineering, the value forcing function f will come from the application data. However for the purpose of testing numerical methods and software, it is exceptionally useful to be able to find values of f such that an analytic solution to the partial differential equation is known. It turns out that there is a straightforward algorithm for this process. This algorithm is known as the *method of manufactured solutions*. It has but two steps:

1. Choose a function \tilde{u} which satisfies the boundary conditions of the PDE.

2. Substitute \tilde{u} into the left hand side of (6.1). Set f equal to the result of this calculation, and now \tilde{u} is a solution to (6.1).

To illustrate this algorithm, suppose we wish to construct f such that:

$$\tilde{u} = \cos(4\pi x_0)x_1^2(1 - x_1)^2 \tag{6.20}$$

is a solution to (6.1). It is simple to verify that \tilde{u} satisfies the boundary conditions. We then note that:

$$-\nabla^2 \tilde{u} + \tilde{u} = ((16\pi^2 + 1)(x_1 - 1)^2 x_1^2 - 12x_1^2 + 12x_1 - 2)\cos(4\pi x_0)$$
(6.21)

If we choose:

$$f = ((16\pi^2 + 1)(x_1 - 1)^2 x_1^2 - 12x_1^2 + 12x_1 - 2)\cos(4\pi x_0)$$
(6.22)

then \tilde{u} is a solution to (6.1).

6.4 Errors and convergence

6.4.1 The L^2 error

When studying finite element methods we are frequently concerned with convergence in the L^2 norm. That is to say, if V and W are finite element spaces defined over the same mesh, and $f \in V, g \in W$ then we need to calculate:

$$\sqrt{\int_{\Omega} (f-g)^2 dx} = \sqrt{\sum_{c} \int_{c} \left(\left(\sum_{i} f_{M_V(c,i)} \Phi_i \right) - \left(\sum_{j} g_{M_W(c,j)} \Psi_j \right) \right)^2 |J| dX}$$
 (6.23)

where M_V is the cell-node map for the space V and M_W is the cell-node map for the space W. Likewise $\{\Phi_i\}$ is the local basis for V and $\{\Psi_i\}$ is the local basis for W.

A complete quadrature rule for this integral will, due to the square in the integrand, require a degree of precision equal to twice the greater of the polynomial degrees of V and W.

6.4.2 Numerically estimating convergence rates

Using the approximation results from the theory part of the course, we know that the error term in the finite element solution of the Helmholtz equation is expected to have the form $\mathcal{O}(h^{p+1})$ where h is the mesh spacing and p is the polynomial degree of the finite element space employed. That is to say if \tilde{u} is the exact solution to our PDE and u_h is the solution to our finite element problem, then for sufficiently small h:

$$||u_h - \tilde{u}||_{L^2} < ch^{p+1} \tag{6.24}$$

for some c > 0 not dependent on h. Indeed, for sufficiently small h, there is a c such that we can write:

$$||u_h - \tilde{u}||_{L^2} \approx ch^{p+1} \tag{6.25}$$

Suppose we solve the finite element problem for two different (fine) mesh spacings, h_1 and h_2 . Then we have:

$$||u_{h_1} - \tilde{u}||_{L^2} \approx ch_1^{p+1} ||u_{h_2} - \tilde{u}||_{L^2} \approx ch_2^{p+1}$$
(6.26)

or equivalently:

$$\frac{\|u_{h_1} - \tilde{u}\|_{L^2}}{\|u_{h_2} - \tilde{u}\|_{L^2}} \approx \left(\frac{h_1}{h_2}\right)^{p+1} \tag{6.27}$$

By taking logarithms and rearranging this equation, we can produce a formula which, given the analytic solution and two numerical solutions, produces an estimate of the rate of convergence:

$$q = \frac{\ln\left(\frac{\|u_{h_1} - \tilde{u}\|_{L^2}}{\|u_{h_2} - \tilde{u}\|_{L^2}}\right)}{\ln\left(\frac{h_1}{h_2}\right)}$$
(6.28)

6.5 Implementing finite element problems

Exercise 204 fe_utils/solvers/helmholtz.py contains a partial implementation of the finite element method to solve (6.2) with f chosen as in (6.22). Your task is to implement the assemble() function using (6.12), and (6.18) or (6.19). The comments in the assemble() function provide some guidance as to the steps involved. You may also wish to consult the errornorm() function as a guide to the structure of the code required.

Run:

python fe_utils/solvers/helmholtz.py --help

for guidance on using the script to view the solution, the analytic solution and the error in your solution. In addition, $test/test_11_helmholtz_convergence.py$ contains tests that the helmholtz solver converges at the correct rate for degree 1, 2 and 3 polynomials.

Warning: test/test_12_helmholtz_convergence.py may take many seconds or even a couple of minutes to run, as it has to solve on some rather fine meshes in order to check convergence.

DIRICHLET BOUNDARY CONDITIONS

The Helmholtz problem we solved in the previous part was chosen to have homogeneous Neumann or *natural* boundary conditions, which can be implemented simply by cancelling the zero surface integral. We can now instead consider the case of Dirichlet, or *essential* boundary conditions. Instead of the Helmholtz problem we solved before, let us now specify a Poisson problem with homogeneous Dirichlet conditions, find u in some finite element space V such that:

$$-\nabla^2 u = f$$

$$u = 0 \text{ on } \Gamma$$
(7.1)

In order to implement the Dirichlet conditions, we need to decompose V into two parts:

$$V = V_0 \oplus V_{\Gamma} \tag{7.2}$$

where V_{Γ} is the space spanned by those functions in the basis of V which are non-zero on Γ , and V_0 is the space spanned by the remaining basis functions (i.e. those basis functions which vanish on Γ). It is a direct consequence of the nodal nature of the basis that the basis functions for V_{Γ} are those corresponding to the nodes on Γ while the basis for V_0 is composed of all the other functions.

We now write the weak form of (7.1), find $u = u_0 + u_\Gamma$ with $u_0 \in V_0$ and $u_\Gamma \in V_\Gamma$ such that:

$$\int_{\Omega} \nabla v_0 \cdot \nabla (u_0 + u_{\Gamma}) \, \mathrm{d}x - \underbrace{\int_{\Gamma} v_0 \nabla (u_0 + u_{\Gamma}) \cdot \mathbf{n} \, \mathrm{d}s}_{=0} = \int_{\Omega} v_0 f \, \mathrm{d}x \qquad \forall v_0 \in V_0$$

$$u_{\Gamma} = 0 \qquad \text{on } \Gamma$$

$$(7.3)$$

There are a number of features of this equation which require some explanation:

- 1. We only test with functions from V_0 . This is because it is only necessary that the differential equation is satisfied on the interior of the domain: on the boundary of the domain we need only satisfy the boundary conditions.
- 2. The surface integral now cancels because v_0 is guaranteed to be zero everywhere on the boundary.
- 3. The u_{Γ} definition actually implies that $u_{\Gamma} = 0$ everywhere, since all of the nodes in V_{Γ} lie on the boundary.

This means that the weak form is actually:

$$\int_{\Omega} \nabla v_0 \cdot \nabla u \, dx = \int_{\Omega} v_0 f \, dx \qquad \forall v_0 \in V_0$$

$$u_{\Gamma} = 0$$
(7.4)

7.1 An algorithm for homogeneous Dirichlet conditions

The implementation of homogeneous Dirichlet conditions is actually rather straightforward.

1. The system is assembled completely ignoring the Dirichlet conditions. This results in a global matrix and vector which are correct on the rows corresponding to test functions in V_0 , but incorrect on the V_{Γ} rows.

M345A47 Finite Elements: Analysis and Implementation, Edition 2020.0

- 2. The global vector rows corresponding to boundary nodes are set to 0.
- 3. The global matrix rows corresponding to boundary nodes are set to 0.
- 4. The diagonal entry on each matrix row corresponding to a boundary node is set to 1.

This has the effect of replacing the incorrect boundary rows of the system with the equation $u_i = 0$ for all boundary node numbers i.

Hint: This algorithm has the unfortunate side effect of making the global matrix non-symmetric. If a symmetric matrix is required (for example in order to use a symmetric solver), then forward substitution can be used to zero the boundary columns in the matrix, but that is beyond the scope of this module.

7.2 Implementing boundary conditions

Let:

$$f = (16\pi^2(x_1 - 1)^2x_1^2 - 2(x_1 - 1)^2 - 8(x_1 - 1)x_1 - 2x_1^2)\sin(4\pi x_0)$$

With this definition, (7.4) has solution:

$$u = \sin(4\pi x_0)(x_1 - 1)^2 x_1^2$$

Exercise 205 fe_utils/solvers/poisson.py contains a partial implementation of this problem. You need to implement the assemble() function. You should base your implementation on your fe_utils/solvers/helmholtz.py but take into account the difference in the equation, and the boundary conditions. The fe_utils.solvers.poisson.boundary_nodes() function in fe_utils/solvers/poisson.py is likely to be helpful in implementing the boundary conditions. As before, run:

```
python fe_utils/solvers/poisson.py --help
```

for instructions (they are the same as for fe_utils/solvers/helmholtz.py). Similarly, test/test_12_poisson_convergence.py contains convergence tests for this problem.

7.3 Inhomogeneous Dirichlet conditions

The algorithm described here can be extended to inhomogeneous systems by setting the entries in the global vector to the value of the boundary condition at the corresponding boundary node. This additional step is required for the mastery exercise, but will be explained in more detail in the next section.

NONLINEAR PROBLEMS

The finite element method may also be employed to numerically solve *nonlinear* PDEs. In order to do this, we can apply the classical technique for solving nonlinear systems: we employ an iterative scheme such as Newton's method to create a sequence of linear problems whose solutions converge to the correct solution to the nonlinear problem.

Note: This section is the mastery exercise for this module. This exercise is explicitly intended to test whether you can bring together what has been learned in the rest of the module in order to go beyond what has been covered in lectures and labs.

This exercise is not a part of the third year version of this module.

8.1 A model problem

As a simple case of a non-linear PDE, we can consider a steady non-linear diffusion equation. This is similar to the Poisson problem, except that the diffusion rate now depends on the value of the solution:

$$-\nabla \cdot ((u+1)\nabla u) = g$$

$$u = b \text{ on } \Gamma$$
(8.1)

where g and b are given functions defined over Ω and Γ respectively.

We can create the weak form of (8.1) by integrating by parts and taking the boundary conditions into account. The problem becomes, find $u \in V$ such that:

$$\int_{\Omega} \nabla v_0 \cdot (u+1) \nabla u \, dx = \int_{\Omega} v_0 g \, dx \qquad \forall v_0 \in V_0$$

$$u_{\Gamma} = b.$$
(8.2)

Once more, V_0 is the subspace of V spanned by basis functions which vanish on the boundary, $V=V_0\oplus V_{\Gamma}$, and $u=u_0+u_{\Gamma}$ with $u_0\in V_0$ and $u_{\Gamma}\in V_{\Gamma}$. This is corresponds directly with the weak form of the Poisson equation we already met. However, (8.2) is still nonlinear in u so we cannot simply substitute $u=u_i\phi_i$ in order to obtain a linear matrix system to solve.

8.2 Residual form

The general weak form of a non-linear problem is, find $u \in V$ such that:

$$f(u;v) = 0 \qquad \forall v \in V \tag{8.3}$$

The use of a semicolon is a common convention to indicate that f is assumed to be linear in the arguments after the semicolon, but might be nonlinear in the arguments before the semicolon. In this case, we observe that f may be nonlinear in u but is (by construction) linear in v.

The function f is called the *residual* of the nonlinear system. In essence, $f(u;v) = 0 \ \forall v \in V$ if and only if u is a weak solution to the PDE. Since the residual is linear in v, it suffices to define the residual for each ϕ_i in the basis of V. For $\phi_i \in V_0$, the residual is just the weak form of the equation, but what do we do for the boundary? The simple answer is that we need a linear functional which is zero if the boundary condition is satisfied at this test function, and nonzero otherwise. The simplest example of such a functional is:

$$f(u;\phi_i) = \phi_i^*(u) - \phi_i^*(b)$$
(8.4)

where ϕ_i^* is the node associated with basis function ϕ_i . For point evaluation nodes, $\phi_i^*(u)$ is the value of the proposed solution at node point i and $\phi_i^*(b)$ is just the boundary condition evaluated at that same point.

So for our model problem, we now have a full statement of the residual in terms of a basis function ϕ_i :

$$f(u;\phi_i) = \begin{cases} \int_{\Omega} \nabla \phi_i \cdot ((u+1)\nabla u) - \phi_i g \, \mathrm{d}x & \phi_i \in V_0 \\ \phi_i^*(u) - \phi_i^*(b) & \phi_i \in V_{\Gamma} \end{cases}$$
(8.5)

Hint: Evaluating the residual requires that the boundary condition be evaluated at the boundary nodes. A simple (if slightly inefficient) way to achieve this is to interpolate the boundary condition onto a function $\hat{b} \in V$.

8.3 Linearisation and Gâteaux Derivatives

Having stated our PDE in residual form, we now need to linearise the problem and thereby employ a technique such as Newton's method. In order to linearise the residual, we need to differentiate it with respect to u. Since u is not a scalar real variable, but is instead a function in V, the appropriate form of differentiation is the Gâteaux Derivative, given by:

$$J(u; v, \hat{u}) = \lim_{\epsilon \to 0} \frac{f(u + \epsilon \hat{u}; v) - f(u; v)}{\epsilon}.$$
 (8.6)

Here, the new argument $\hat{u} \in V$ indicates the "direction" in which the derivative is to be taken. Let's work through the Gâteaux Derivative for the residual of our model problem. Assume first that $v \in V_0$. Then:

$$J(u; v, \hat{u}) = \lim_{\epsilon \to 0} \frac{\int_{\Omega} \nabla v \cdot ((u + \epsilon \hat{u} + 1)\nabla(u + \epsilon \hat{u})) - vg \, dx - \int_{\Omega} \nabla v \cdot ((u + 1)\nabla u) - vg \, dx}{\epsilon}$$

$$= \lim_{\epsilon \to 0} \frac{\int_{\Omega} \nabla v \cdot (\epsilon \hat{u}\nabla u + (u + 1)\nabla(\epsilon \hat{u}) + \epsilon \hat{u}\nabla(\epsilon \hat{u})) \, dx}{\epsilon}$$

$$= \int_{\Omega} \nabla v \cdot (\hat{u}\nabla u + (u + 1)\nabla \hat{u}) \, dx.$$
(8.7)

Note that, as expected, J is linear in \hat{u} .

Next, we can work out the boundary case by assuming $v = \phi_i$, one of the basis functions of V_{Γ} :

$$\begin{split} J(u;\phi_i,\hat{u}) &= \lim_{\epsilon \to 0} \frac{\phi_i^*(u+\epsilon\hat{u}) - \phi_i^*(b) - (\phi_i^*(u) - \phi_i^*(b))}{\epsilon} \\ &= \phi_i^*(\hat{u}) \qquad \text{since } \phi_i^*(\cdot) \text{ is linear.} \end{split} \tag{8.8}$$

Once again, we can observe that J is linear in \hat{u} . Indeed, if we choose $\hat{u} = \phi_j$ for some ϕ_j in the basis if V then the definition of a nodal basis gives us:

$$J(u;\phi_i,\phi_j) = \delta_{ij} \tag{8.9}$$

8.4 A Taylor expansion and Newton's method

Since we now have the derivative of the residual with respect to a perturbation to the prospective solution u, we can write the first terms of a Taylor series approximation for the value of the residual at a perturbed solution $u + \hat{u}$:

$$f(u+\hat{u};v) = f(u;v) + J(u;v,\hat{u}) + \dots \qquad \forall v \in V.$$
(8.10)

Now, just as in the scalar case, Newton's method consists of approximating the function (the residual) by the first two terms and solving for the update that will set these terms to zero. In other words:

$$u^{n+1} = u^n + \hat{u} (8.11)$$

where $\hat{u} \in V$ is the solution to:

$$J(u^n; v, \hat{u}) = -f(u^n; v) \qquad \forall v \in V.$$
(8.12)

In fact, (8.12) is simply a linear finite element problem! To make this explicit, we can expand v and \hat{u} in terms of basis functions:

$$J(u^{n};\phi_{i},\phi_{j})\hat{u}_{j} = -f(u^{n};\phi_{i}). \tag{8.13}$$

For our nonlinear diffusion problem, the matrix J is given by:

$$J(u^n; \phi_i, \phi_j) = \begin{cases} \int_{\Omega} \nabla \phi_i \cdot (\phi_j \nabla u^n + (u^n + 1) \nabla \phi_j) \, dx & \phi_i \in V_0 \\ \delta_{ij} & \phi_i \in V_{\Gamma}, \end{cases}$$
(8.14)

and the right hand side vector f is given by (8.5). This matrix, J, is termed the *Jacobian matrix* of f.

8.4.1 Stopping criteria for Newton's method

Since Newton's method is an iterative algorithm, it creates a (hopefully convergent) sequence of approximations to the correct solution to the original nonlinear problem. How do we know when to accept the solution and terminate the algorithm?

The answer is that the update, \hat{u} which is calculated at each step of Newton's method is itself an approximation to the error in the solution. It is therefore appropriate to stop Newton's method when this error estimate becomes sufficiently small in the L^2 norm.

The observant reader will observe that \hat{u} is in fact an estimate of the error in the *previous* step. This is indeed true: the Newton step is both an estimate of the previous error and a correction to that error. However, having calculated the error estimate, it is utterly unreasonable to not apply the corresponding correction.

Note: Note!

Another commonly employed stopping mechanism is to consider the size of the residual f. However, the residual is not actually a function in V, but is actually a linear operator in V^* . Common practice would be to identify f with a function in V by simply taking the function whose coefficients match those of f. The L^2 or l^2 norm is then taken of this function and this value is used to determine when convergence has occurred.

This approach effectively assumes that the Riesz map on V is the trivial operator which identifies the basis function coefficients. This would be legitimate were the inner product on V the ℓ^2 dot product. However, since the inner product on V is defined by an integral, the mesh resolution is effectively encoded into f. This means that this approach produces convergence rates which depend on the level of mesh refinement.

Avoiding this mesh dependency requires the evaluation of an operator norm or, equivalently, the solution of a linear system in order to find the Riesz representer of f in V. However, since the error-estimator approach given above is both an actual estimate of the error in the solution, and requires no additional linear solves, it should be regarded as a preferable approach. For a full treatment of Newton methods, see [Deu11].

8.4.2 Stopping threshold values

What, then, qualifies as a sufficiently small value of our error estimate? There are two usual approaches:

relative tolerance Convergence is deemed to occur when the estimate becomes sufficiently small compared with the first error estimate calculated. This is generally the more defensible approach since it takes into account the overall scale of the solution. 10^{-6} would be a reasonably common relative tolerance.

absolute tolerance Computers employ finite precision arithmetic, so there is a limit to the accuracy which can ever be achieved. This is a difficult value to estimate, since it depends on the number and nature of operations undertaken in the algorithm. A common approach is to set this to a very small value (e.g. 10^{-50}) initially, in order to attempt to ensure that the relative tolerance threshold is hit. Only if it becomes apparent that the problem being solved is in a regime for which machine precision is a problem is a higher absolute tolerance set.

It is important to realise that both of these criteria involve making essentially arbitrary judgements about the scale of error which is tolerable. There is also a clear trade-off between the level of error tolerated and the cost of performing a large number of Newton steps. For realistic problems, it is therefore frequently expedient and/or necessary to tune the convergence criteria to the particular case.

In making these judgements, it is also important to remember that the error in the Newton solver is just one of the many sources of error in a calculation. It is pointless to expend computational effort in an attempt to drive the level of error in this component of the solver to a level which will be swamped by a larger error occurring somewhere else in the process.

8.4.3 Failure modes

Just as with the Newton method for scalar problems, Newton iteration is not guaranteed to converge for all non-linear problems or for all initial guesses. If Newton's method fails to converge, then the algorithm presented so far constitutes an infinite loop. It is therefore necessary to define some circumstances in which the algorithm should terminate having failed to find a solution. Two such circumstances are commonly employed:

maximum iterations It is a reasonable heuristic that Newton's method has failed if it takes a very large number of iterations. What constitutes "too many" is once again a somewhat arbitrary judgement, although if the approach takes many tens of iterations this should always be cause for reconsideration!

diverged error estimate Newton's method is not guaranteed to produce a sequence of iterations which monotonically decrease the error, however if the error estimate has increased to, say, hundreds or thousands of times its initial value, this would once again be grounds for the algorithm to fail.

Note that these failure modes are heuristic: having the algorithm terminate for these reasons is really an instruction to the user to think again about the problem, the solver, and the initial guess.

8.5 Implementing a nonlinear problem

Note: This problem is intentionally stated in more general terms than the previous ones. It is your responsibility to decide on a code structure, to derive a method of manufactured solutions answer, and to create the convergence tests which demonstrate that your solution is correct.

Exercise 206 The p-laplacian is a generalisation of the laplacian from a second derivative to an arbitrary derivative. It is nonlinear for $p \neq 2$.

Implement solve_mastery() so that it solves the following problem using degree 1 Lagrange elements over the unit square domain:

$$-\nabla \cdot (|\nabla u|^{p-2} \nabla u) = g$$

$$u = b \text{ on } \Gamma$$

$$p = 4$$
(8.15)

Select the solution $u = e^{xy}$ and compute the required forcing function g so that your solution solves the equations. Make sure your boundary condition function b is consistent with your chosen solution!

For this problem, it is not possible to use the zero function as an initial guess for Newton's method. A much better choice is to treat the 2-laplacian as an approximation to the 4-laplacian, and therefore to solve Poisson's equation first to obtain a good initial guess for the 4-laplacian problem.

Your submitted answer will consist of:

- 1. A written component containing your derivation of:
 - a. The weak form of (8.15); and
 - b. the Jacobian; and
 - c. the forcing term implied by the specified manufactured solution; and
 - d. an explanation of why the zero function cannot be used as an initial guess for the solution.

A neatly hand-written or a typed submission are equally acceptable.

2. The code to implement the solution. This should be in fe_utils.solvers.mastery. py in your implementation. A convergence test for your code is provided in test/test_12_mastery_convergence.py.

The submission of your mastery exercise, and indeed the entire implementation exercise will be on Black-board. You will submit a PDF containing the derivations above, and the git shal for the commit you would like to have marked.

Hint: It is an exceptionally useful aid to debugging to have your Newton iteration print out the value of the error norm and the iteration number for each iteration. If you wish to see the printed output while running the test, you can pass the -s option to py.test.

Hint: You could parametrise your code by p. By setting p=2, you reduce your problem to the linear case. You can use the linear case to test your code initially, before setting p=4 for the actual exercise. Note that, in the linear case, Newton's method will converge in exactly one iteration (although your algorithm will have to actually calculate two steps in order to know that convergence has occurred).

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