1 Introduction

This lab continues the topic of Computational Geometry. Having studied tetrahedrons and how they are used to create a tetrahedral mesh or “tet mesh” of a region, we will now turn to the use of tetrahedrons to define the basis functions used in the finite element method (FEM).

The finite element method is a procedure for approximating and solving partial differential equations. Part of the finite element method involves constructing a mesh of the region, a topic which is discussed in other labs. Once the mesh is available, the finite element method uses this mesh to represent functions \( f(x, y, z) \). The representation is discrete, that is, it depends on just a finite number of values, but the resulting function is defined over the entire meshed region; with some restrictions, it can be evaluated, plotted, differentiated or integrated.

If you have ever used a finite difference method to solve differential equations, you will understand an important distinction between these two methods. The finite difference method works with values of a function at given points, but it does not try to “fill in the gaps” between the tabulated points. In contrast, the finite element method may only have exact knowledge of a function at specified points, but it builds a “model” of the function over the entire problem domain.

The key to this model building is the set of finite element basis functions. It is the purpose of this lab to understand how these basis functions are defined, evaluated and used to create the finite element functions.

2 Overview

This lab is one of a series on the finite element method. It may help to anticipate where we are going, so that the small results we achieve in this lab are understood to be leading to a much bigger result.

So we suppose that we are given a tet mesh \( \tau \) of some region \( \mathcal{R} \). The mesh is made up, of course, of points and tetrahedrons. We will assume there are \( NP \) points or “nodes”, with a typical point being identified as \( P \) or perhaps \( P_i \) or \( p \). If we wish to list the coordinates of \( p \), we might write \( p = \{ p.x, p.y, p.z \} \) or in some mathematical formulas, we may use the notation \( p = \{ p_x, p_y, p_z \} \).

The tet mesh is a set of \( NT \) tetrahedron, whose vertices are chosen from the set of points, with a typical tetrahedron being \( T \) or \( T_i \). If we wish to list the vertices, we may write \( T = \{ a, b, c, d \} \).

Let us suppose that we wish to come up with a formula for a function \( f(x, y, z) \), with the requirement that

\[
f(P_i) = f_i, \quad i = 1 \ldots NT,
\]

that is, we are going to specify in advance the value of this function at every node in the mesh.
Our goal is to somehow come up with a formula, or a procedure, which defines \( f(x, y, z) \) for every point \((x, y, z)\) in \( \mathbb{R} \), in such a way that the function is continuous, attains the specified values at the nodes, and is relatively simple to evaluate anywhere in the region. This is an example of what is called the interpolation problem.

Our progress in solving the interpolation problem on a tet mesh will start very simply. We will look at a ‘mesh that involves a single tetrahedron, called the reference tetrahedron. We will investigate how interpolation works in this very simple setting, and we will also “discover” the basis functions that make the answer simple to describe.

We will then transfer this formula to a general tetrahedron. Then we will consider what happens depending on which vertex is chosen to have the value 1 under the formula. When we have understood this problem, we will be able to handle the interpolation problem on the reference tetrahedron, or on any single general tetrahedron.

In later labs, we will consider the effect of setting up these formulas in every tetrahedron in the mesh simultaneously. This might seem to be a recipe for chaos. However, whenever two tetrahedron touch, they share three vertices, and the formula we develop for each tetrahedron will match up along their common boundary continuously, though not differentiably.

At this point, we will have developed all the machinery that the finite element requires in order to define a function \( f(x, y, z) \) over the finite element mesh with the desired values.

3 The Reference Tetrahedron

Our task is complicated, but we have to start somewhere. Instead of an entire tet mesh, we start with a single tetrahedron. Instead of an arbitrary tetrahedron, we start with the “reference tetrahedron”, whose definition is simply \( \text{Tref} = \{ \text{a, b, c, d} \} = \{ \{1,0,0\}, \{0,1,0\}, \{0,0,1\}, \{0,0,0\} \} \).

Now suppose we want to define a function \( f(x, y, z) \) over the entire tetrahedron, with the property that its value at each vertex is prescribed in advance:

\[
\begin{align*}
  f(a) &= fa \\
  f(b) &= fb \\
  f(c) &= fc \\
  f(d) &= fd
\end{align*}
\]

There are many ways to find such a function; if we make the natural choice that the function be the simplest polynomial possible, we will probably choose a form like:

\[
f(x, y, z) = c_1 + c_2x + c_3y + c_4z
\]
where the coefficients $c_1$, $c_2$, $c_3$ and $c_4$ may be chosen to fit our problem.

But the condition $f(d) = fd$ implies that $f(0,0,0) = c_1 = fd$. The condition $f(a) = fa$ then implies that $f(1,0,0) = fd + c_2 = fa$ which shows that $c_2 = fa - fd$, and similarly we have $c_3 = fb - fd$ and $c_4 = fc - fd$.

Thus, we have solved our interpolation problem for the reference tetrahedron. The function

$$f(x,y,z) = fd + (fa - fd)x + (fb - fd)y + (fc - fd)z$$

has the correct values at the vertices, is defined and continuous over the entire tetrahedron, and is simple to evaluate.

This certainly doesn’t solve our real problem, but it is a helpful guide as to how we want to proceed!

4 Program #1: Interpolation in the Reference Tetrahedron

For the reference tetrahedron $T_{\text{ref}} = \{a,b,c,d\} = \{(1,0,0), (0,1,0), (0,0,1), (0,0,0)\}$, write a program which:

- Reads four vertex function values $fa$, $fb$, $fc$ and $fd$;
- Reads the coordinates of a point $p$;
- Evaluates and prints the interpolation function $f(p)$.

Test your program with the vertex function values $(fa,fb,fc,fd) = (1,2,3,4)$.

As points $p$, use:

- $\{ 1, 0, 0 \}$
- $\{ 0, 1, 0 \}$
- $\{ 0, 0, 1 \}$
- $\{ 0.5, 0.5, 0.0 \}$
- $\{ 0.0, 0.5, 0.5 \}$
- $\{ 0.25, 0.0, 0.5 \}$
- $\{ 0.25, 0.25, 0.25 \}$
- $\{ 0.6, 0.7, 0.5 \}$
- $\{ 1.0, 2.0, 3.0 \}$

Prove: If a point $p$ is contained in the reference tetrahedron, then the value of the linear interpolation function $f(p)$ is bounded below by the minimum, and above by the maximum, of the data values $fa$, $fb$, $fc$, $fd$. Moreover, if $p$ is strictly contained within the reference tetrahedron, and if the data values are not all equal, then the value $f(p)$ is strictly between the given bounds.

5 Basis Functions for the Reference Tetrahedron

When we guessed that our interpolation function would be a linear function of the data values, we wrote out a symbolic formula, which we could regard as describing $f(x,y,z)$ as a combination of the basis functions $1, x, y$ and $z$. Any linear (actually, affine) function in the plane can be represented as such a combination.

However, there are many equivalent sets of basis functions. Notice how the formula for our solution uses the prescribed value $fd$ several times. What if we rearranged this formula so that each prescribed value showed up exactly once. We’d get something like this:

$$f(x,y,z) = fa \cdot x + fb \cdot y + fc \cdot z + fd \cdot (1 - x - y - z)$$
Now if we look at this formula, we can regard it as using a slightly different set of basis functions than before. Let’s actually rename each basis function:

\[
\begin{align*}
\phi_a(x, y, z) &= x \\
\phi_b(x, y, z) &= y \\
\phi_c(x, y, z) &= z \\
\phi_d(x, y, z) &= 1 - x - y - z
\end{align*}
\]

We can make some interesting statements about the value of basis function \(\phi_a(x, y, z)\) at various places in the tetrahedron:

- 1 at vertex \(a\);
- 0 at vertices \(b, c\) and \(d\);
- 0 along edges \{b,c\}, \{c,d\}, and \{d,b\};
- 0 on face \{b,c,d\};
- 0 < \(\phi_a(x, y, z)\) < 1 for points strictly inside the tetrahedron.

and by making the obvious changes, similar statements hold for the other basis functions.

We can also make some statements about the places in the tetrahedron:

- at vertex \(a\), \(\phi_a(x, y, z) = 1\);
- at vertex \(a\), \(\phi_b(x, y, z) = \phi_c(x, y, z) = \phi_d(x, y, z) = 0\);
- along edge \{a,b\}, \(\phi_c(x, y, z) = \phi_d(x, y, z) = 0\);
- on face \{a,b,c\}, \(\phi_d(x, y, z) = 0\);
- on interior point \((x, y, z)\), all basis functions are strictly between 0 and 1.

and by making obvious changes, similar statements hold on the other vertices, edges and faces.

We also note that

- at any point \((x, y, z)\), the sum of the four basis functions is exactly 1;
- at any point \((x, y, z)\), the sum of the derivatives of the four basis functions with respect to \(x\) is exactly 0; the same is true for derivatives with respect to \(y\) and \(z\). These facts follow from the previous property.

The property that each of the basis functions is 1 at its associated vertex, and 0 at the other three vertices means that the set of basis functions is a Lagrange interpolation basis for the vertices.

Using our basis function notation, the solution to the interpolation problem has the very nice form:

\[
f(x, y, z) = f_a \cdot \phi_a(x, y, z) + f_b \cdot \phi_b(x, y, z) + f_c \cdot \phi_c(x, y, z) + f_d \cdot \phi_d(x, y, z)
\]

If you can find a Lagrange interpolation basis for a set of points (which can be hard to do), then the interpolation problem becomes very easy. It should be clear now that, as we move to the problem of a general tetrahedron, we should hope to find a Lagrange interpolation basis there as well.

Finally, notice that the basis functions \((\phi_a(x, y, z), \phi_b(x, y, z), \phi_c(x, y, z), \phi_d(x, y, z))\) are really the same as considering the barycentric coordinates \((\xi_a, \xi_b, \xi_c, \xi_d)\) as functions of \(x, y\) and \(z\).
6 Program #2: Basis Functions for the Reference Tetrahedron

For the reference tetrahedron, write a program which

- reads a point \( p \);
- evaluates and prints the basis functions \( \phi_a, \phi_b, \phi_c \) and \( \phi_d \) at \( p \);
- prints the sum \( \phi_a(p) + \phi_b(p) + \phi_c(p) + \phi_d(p) \).

Test your program with the following points \( p \):

\[
\begin{align*}
\{ & 1, 0, 0 \} \\
\{ & 0, 1, 0 \} \\
\{ & 0, 0, 1 \} \\
\{ & 0, 0, 0 \} \\
\{ & 0.5, 0.5, 0.0 \} \\
\{ & 0.0, 0.5, 0.5 \} \\
\{ & 0.25, 0.0, 0.5 \} \\
\{ & 0.25, 0.25, 0.25 \} \\
\{ & 0.6, 0.7, 0.5 \} \\
\{ & 1.0, 2.0, 3.0 \}
\end{align*}
\]

Observe the property, stated earlier, that the basis functions can be used to indicate where the point \( p \) is relative to the reference tetrahedron.

7 Basis Functions for a General Tetrahedron

Now we are ready to consider the interpolation problem on a general tetrahedron, of the form \( T = \{a,b,c,d\} \). It should be clear that our best hope will be to find a set of basis functions \( \phi_a, \phi_b, \phi_c \) and \( \phi_d \) for this general tetrahedron that work like the ones we found in the reference tetrahedron.

We have seen earlier that a formula for the basis functions can be found as the ratio of two determinants. The determinant in the denominator is essentially the volume of the tetrahedron. The determinant in the numerator for \( \phi_a(p) \) is formed by starting with the same determinant, but replacing the coordinates of vertex \( a \) by the coordinates of the point \( p \). The result is an expression for the volume of the tetrahedron formed by the point \( p \) and the remaining vertices \( b, c \) and \( d \):

\[
\phi_a(p) = \phi_a(p.x, p.y, p.z) = \frac{| p_x \ b_x \ c_x \ d_x |}{| a_x \ b_x \ c_x \ d_x |}
\]

with corresponding formulas for \( \phi_b(p), \phi_c(p) \) and \( \phi_d(p) \).

Exercise: Evaluate the determinant for \( \phi_a(p) \), that is, write it out explicitly as an arithmetic formula and compare it to the formula we derived in the previous section.

Exercise: Show that if the tetrahedron \( T = \{a,b,c,d\} \) is actually the reference tetrahedron, then the determinant formulas for the basis functions give us \( x, y, z \) and \( 1-x-y-z \).
8 Program #3: Basis Functions for a General Triangle

Write a program which

- reads the definition of a general tetrahedron \( T = \{a, b, c, d\} \);
- reads the definition of a point \( p \);
- evaluates and prints the basis functions \( \phi_a, \phi_b, \phi_c \) and \( \phi_d \) at \( p \);
- prints the sum \( \phi_a(p) + \phi_b(p) + \phi_c(p) + \phi_d(p) \).

Test your program on tetrahedron \textbf{Tet3} defined by:

\[
\begin{align*}
\{ & \{ 1.0, 2.0, 3.0 \}, \\
& \{ 2.0, 2.0, 3.0 \}, \\
& \{ 1.0, 3.0, 3.0 \}, \\
& \{ 1.0, 2.0, 9.0 \} \}
\end{align*}
\]

For your points \( p \) try each of these:

\[
\begin{align*}
& \{ 1.25, 2.25, 4.50 \} \\
& \{ 1.00, 2.50, 4.00 \} \\
& \{ 1.00, 3.00, 3.00 \} \\
& \{ 1.00, 2.00, 7.80 \} \\
& \{ 0.80, 2.40, 6.60 \}
\end{align*}
\]

We have considered how to define and evaluate a set of basis functions on a single tetrahedron. This set of basis functions can be used to solve the interpolation problem on a single tetrahedron. In the following lab, we will consider the interpolation problem on a tetrahedron mesh, and for that lab we will need to use the results we have worked out here!