The Finite Element Basis for Simplices in Arbitrary Dimensions

John Burkardt
Department of Scientific Computing
Florida State University
http://people.sc.fsu.edu/~jburkardt/presentations/fem_basis.pdf

08 January 2011

1 Introduction

This informal technical report describes a procedure for defining and evaluating a finite element basis for simplices. The polynomial degree of the basis set and the spatial dimension of the simplex are both arbitrary.

The approach is a generalization of commonly-used families of Lagrange basis functions. These families typically are defined by selecting a certain set of special nodes inside the simplex, and then associating with each node a corresponding Lagrange polynomial. The resulting family has the property that each basis function is 1 when evaluated at its associated node, and 0 at all other nodes.

For a low spatial dimension and low polynomial degree, it is possible to construct such a family by inspection. However, as the spatial dimension or polynomial degree increases, it is impossible to generate a family of basis functions unless a systematic approach is available.

We begin the discussion with some technical details that are unnecessary to the specialist, who may proceed to the last two sections where the main material is presented.

2 Definition of a Triangle

The triangle is an elemental geometric shape. We think of the triangle as being defined by three points or "vertices". Depending on the situation, when we speak of a triangle, we might mean just those three points, or we might wish to include the lines that join them (called "edges"), or even all the points bounded by those lines as well.

It is this last idea that we wish to capture for this discussion, and we will need to formulate this mathematically. Therefore, we begin with three vertices, and try to describe a formula that captures the vertices, edges, and interior points of the triangle.

The edge between a pair of pair of vertices v_1 and v_2 is part of a line which extends infinitely far in both directions. We can describe this infinite line by the formula

$$p = a * v_1 + (1 - a) * v_2$$

The points that form the edge between v_1 and v_2 are the subset of the points on the line for which the coefficient a is between 0 and 1. We say that points on the edge are formed by a *convex combination* of the two vertices.

Generally, p is a convex combination of N objects $V = \{v_i \| i = 1, \dots N\}$, if p can be represented, using a coefficient vector $\vec{c}$, as

$$p = \sum_{i=1}^{N} c_i * v_i$$

with the conditions that every c_i is nonnegative, and $\sum_{i=1}^{N} c_i \leq 1$.

Now it should be obvious that any point p in the interior of the triangle can be regarded as a convex combination of some pair of points on the edges. In fact, if we draw any line through p, then this line must intersect the edges at two points which can be combined to form p. Thus, there might seem to be many ways of forming p. However, (as long as the triangle is not degenerate) it turns out that there is always a unique way to form p as a convex combination of all three vertices, and correspondingly, it is precisely these convex combinations which form the points in the triangle.

Thus, the triangle T may be described as the set of all points p which are convex combinations of the vertices, that is

$$T(v_1, v_2, v_3) = \{p : p = \xi_1 v_1 + \xi_2 v_2 + \xi_3 v_3; \quad 0 \leq \xi_i; \quad \xi_1 + \xi_2 + \xi_3 \leq 1\}$$

Thus, each point $p \in T$ corresponds to a set of values (ξ_1, ξ_2, ξ_3). These values, which represent weights applied to each vertex to produce the point, are called the *barycentric coordinates* of the point. The reader may consider, at this point, the facts that

- *vertices* have two zero barycentric coordinates,
- *edge points* have one zero coordinate,
- *interior points* are those with strictly positive coordinates,
- *exterior points* have at least one negative coordinate.

3 Definition of a Simplex

We wish to generalize the idea of a triangle; a reasonable approach begins from the fact that the triangle is an object in two dimensions that is described by three vertices. If we look for a similar object in one dimension, we would use two vertices and thereby describe an interval. In three dimensions, four vertices will specify a tetrahedron. The pattern suggested by these three cases makes it possible to generalize the idea to an arbitrary spatial dimension.

The *M-dimensional simplex* S is defined by a set V of **M**+1 vertices v_i (points in **M**-dimensional space), and includes all points p which are convex combinations of those vertices:

$$S(V) = \{p : p = \sum_{i=1}^{M+1} \xi_i v_i; 0 \leq \xi_i; \sum_{i=1}^{M+1} \xi_i \leq 1\}$$

We will always assume that the simplex is not degenerate, or equivalently, that the vertices lie in what is called "general position". In the case of the triangle, this means we assume the three vertices do not lie on a line, which would result in a "flat" (and uninteresting!) triangle of zero area. In **M** dimensions, this requirement is equivalent to the condition that the **M**-dimensional volume of the simplex is not zero.

The "volume" (area) of a triangle with vertices $V = \{v_1, v_2, v_3\} = \{(x_1, y_1), (x_2, y_2), (x_3, y_3)\}$ is

$$\frac{1}{2!} \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}$$

and the volume of a tetrahedron is

$$\frac{1}{3!} \begin{vmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \end{vmatrix}$$

This formula generalizes, in the obvious way, to produce the volume of a simplex in **M** dimensions.

From the definition of the simplex, it should be clear that any point p contained in the simplex can be identified either by its Cartesian coordinates $\vec{x}$, but also by its barycentric coordinates $\vec{\xi}$ as long as we also know the vertices V of the simplex. We will find both coordinates systems useful, and so it will be convenient to determine the computational relationship between them.

4 The Reference Simplex

Let us suppose that we are working in an **M**-dimensional space, and we define a special simplex E by choosing as vertices the **M** unit Cartesian basis vectors $\vec{e_i}$, for i from 1 to M, as well as the origin $\vec{0}$. This object is known as the **M**-*dimensional reference simplex.*

The volume formula tells us that the reference simplex will have volume $\frac{1}{M!}$.

If we list the vertices of the reference simplex in the natural order, followed by the origin, then it turns out that for any point in the simplex, the Cartesian and barycentric coordinate systems are essentially identical.

For instance, in 2D, the correspondence $\vec{x} \iff \vec{\xi}$ for the reference triangle is simply

$$
\begin{aligned}
&(x, y) \to (x, y, 1 - x - y) = (\xi_1, \xi_2, \xi_3) \\
&(x, y) = (\xi_1, \xi_2) \leftarrow (\xi_1, \xi_2, \xi_3)
\end{aligned}
$$

But now let us consider an arbitrary triangle T in 2D. Suppose we list its vertices as $V = (v_1, v_2, v_3)$ and associate these vertices, in this order, with the vertices of the reference triangle $(\vec{e_1}, \vec{e_2}, \vec{0})$. There is a unique linear mapping $\phi(v_1, v_2, v_3; \xi_1, \xi_2, \xi_3)$ which takes the vertices of the reference triangle to those of T, and its form is not hard to work out from the requirements that:

$$
\begin{aligned}
v_1 &= \phi(v_1, v_2, v_3; 1, 0, 0) \\
v_2 &= \phi(v_1, v_2, v_3; 0, 1, 0) \\
v_3 &= \phi(v_1, v_2, v_3; 0, 0, 0)
\end{aligned}
$$

However, this mapping also uniquely associates *every* point ξ in the reference triangle to a point p in T. Known as *the reference map*, it has the form:

$$
\begin{aligned}
p &= p(\xi_1, \xi_2, \xi_3) \\
&= \phi(v_1, v_2, v_3; \xi_1, \xi_2, \xi_3) \\
&= \xi_1 v_1 + \xi_2 v_2 + \xi_3 v_3 \\
&= V * \xi
\end{aligned}
$$

Assuming T is nondegenerate, this mapping is also invertible and so there is a corresponding function $\phi^{-1}(v_1, v_2, v_3; x, y)$ which maps points p in T to points ξ in the reference triangle.

Now the formula for ϕ is equivalent to the barycentric coordinates of the point p. This means that the barycentric coordinates of a point p are, at the same time, the coordinates of a representative point ξ in the reference triangle, and the coefficients that combine with the vertices of T to produce the point p.

These results extend to **M** dimensions, where there is a mapping $\phi(\mathbf{v}; \xi)$ from the reference simplex E to an arbitrary simplex S; if the simplex is nondegenerate, there is an inverse mapping as well.

5 Simplices in the Finite Element Method

An **M**-dimensional simplex is in some ways the natural geometrical element into which to decompose an arbitrary geometric object. Because of its flexibility and economy, it is very frequently used in finite element analysis.

Of course, most geometries of interest correspond to physical objects, and hence are likely to be 1-, 2- or 3-dimensional. However, there are always situations in which higher-dimensional geometries are of interest, and the main point of our discussion will be that formulas that are obvious in 2D can be extended not merely to the more involved case of 3D, but can be automatically generalized to the **M**-dimensional case.

A finite element analysis can be thought of as beginning with the definition of a geometric region to be studied. The region is then subdivided into numerous polygonal or polyhedral subregions, called *elements*. The most common choices for the element are rectangles or triangles and their higher dimensional generalizations. Our attention will focus on the case when a triangle, tetrahedron, or the general **M**-simplex is the element being used.

The finite element analysis takes advantage of the ideas of the reference element and the reference mapping. Although the calculation is intended to deal with the entire region, the majority of the computation occurs while considering only the reference simplex. This is accomplished by considering in turn each one of the elements that cover the region, and determining the inverse mapping that establishes its correspondence with the reference element. After computations are completed on the reference element, the forward reference mapping is used to transfer the results back to the element.

Thus, a prime feature of the finite element method is that complicated geometries can be handled, but that the calculations occur on a single, simple region, which in our case will be a simplex.

6 The Lagrange Polynomial Basis For Rectangles

We are not interested in using rectangles, but rather triangular elements and their generalizations. However, the rectangular case is a useful starting point, since the procedure for triangles begins in the same way, but then requires some special steps.

The finite element calculations require the definition of a set of basis functions $\psi_j(\xi)$, defined over the reference element. Generally, the basis functions are polynomials; moreover, it is usually the case that a nested family of such basis functions is available, indexed by the parameter d, with each succeeding member of the family being able to achieve a higher order of polynomial approximation.

When the element being used is a rectangle, or its higher-dimensional generalizations, the orderly definition of these polynomials is easy - the d-th member of the nested family is a set of polynomials for which no variable has an exponent exceeding d. Such a basis can be formed from $(d+1)^M$ monomials, but we are free to form an equivalent basis of that size in a form that is more convenient for the finite element method. For rectangles, we start by choosing $d+1$ equally spaced points along each unit coordinate axis, and forming the Cartesian product of all possible pairs (x_i, y_j). We call this the set of *grid points*. To define our d-th basis family, we identify an arbitrary element of that family by associating it with one of the grid points. Then the (i, j) element of the set, written $\psi_{i,j}(x, y)$ is a polynomial with the properties that

- for every monomial term in $\psi_{i,j}(x, y)$, the exponents of x and y are between 0 and d;
- $\psi_{i,j}(x_i, y_j) = 1$
- $\psi_{i,j}(x_k, y_l) = 0$ if (x_k, y_l) is any grid point other than (x_i, y_j).

Because of the use of the grid points, it should be clear that a formula for the (i, j) element of the d-th family of basis function is

$$\psi_{i,j}(x, y) = \frac{\prod_{k=0;k\neq i}^{d}(x - x_k)\prod_{l=0;l\neq j}^{d}(y - y_l)}{\prod_{k=0;k\neq i}^{d}(x_i - x_k)\prod_{l=0;l\neq j}^{d}(y_j - y_l)}$$

A set of polynomials and points with the property that each polynomial is identified with exactly one point, at which it attains the value 1, while being zero at all other points, is known as a *Lagrange polynomial basis*, and has an extensive history and wide application, particularly in the area of interpolation.

For rectangular elements in higher dimensions, the procedures outlined here are readily extensible, requiring nothing but the most obvious modifications.

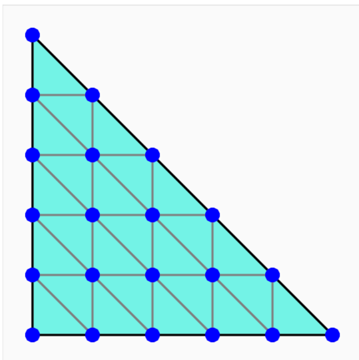

Figure 1: The reference triangle, with degree-5 gridlines.

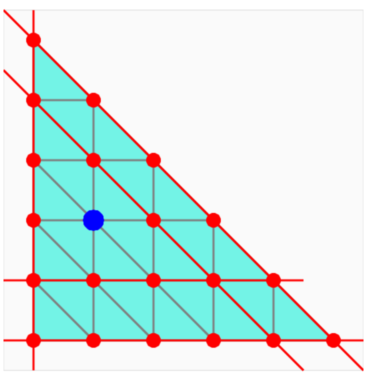

Figure 2: A node (in blue) and the 5 grid lines (in red) that each contribute a linear factor

7 The Lagrange Polynomial Basis For Triangles

In the case of triangles or general simplex elements, the natural way to nest a family of basis functions imposes the requirement that each member of the d-th family have *total degree* no more than d. This means that it is now the sum of the exponents of x and y that must be no more than d, rather than applying that limitation to each exponent separately.

To find these functions for the case of a triangle, in dimension $M = 2$, we again resort to choosing $d+1$ equally spaced points along each coordinate direction. We form the Cartesian product as before, but now many of the pairs will not be acceptable because they lie outside the triangle. We end up with $\binom{M+d}{M} = \frac{(d+1)(d+2)}{2}$ acceptable grid points compared to the $(d+1)^2$ points in the case of the corresponding calculation for a rectangle.

The rationale for producing the basis functions from the grid points is the same as in the rectangular case. Each basis function is to be associated with a grid point; it is 1 there and 0 at the other grid points; it has a total degree of d. The problem now is that coming up with formulas for these functions is significantly less obvious than it was for the rectangular case.

However, we will now find it convenient to index the nodes with a sort of *barycentric index*, that corresponds with the barycentric coordinate system. That is, given the value **d**, which represents the index of the polynomial basis family we are generating, we assign indices i and j to the nodes in the obvious way, but then add an auxiliary index $k = d - i - j$. Thus, the barycentric indices are nonnegative, and add to d. Moreover, a node whose barycentric indices are (i, j, k) has barycentric coordinates $(\frac{i}{d}, \frac{j}{d}, \frac{k}{d})$.

With this understanding, we can now write a formula for the polynomial basis function associated with the node whose barycentric index is (i, j, k):

$$L(i,j,k)(x,y) = \prod_{p=0}^{i-1}(x - \frac{p}{d}) \prod_{p=0}^{j-1}(y - \frac{p}{d}) \prod_{p=0}^{k-1}((1-x-y) - \frac{p}{d})$$

but then we have to normalize by computing the value of this polynomial at the associated node.

$$\psi(i,j,k)(x,y) = \frac{L(i,j,k)(x,y)}{L(i,j,k)(x_{i,j,k}, y_{i,j,k})}$$

8 The Lagrange Polynomial Basis For Tetrahedrons

The procedure outlined in the previous section for triangles was framed in terms of scaled barycentric coordinates. To extend these results to dimension $M = 3$, where the simplex is the tetrahedron, it is enough to note that the same scaled barycentric coordinate system can be defined, once we have added another coordinate index to account for the higher spatial dimension.

Thus, in 3D, the scaled barycentric coordinate system for the tetrahedron involves a vector whose typical entries are represented by (i, j, k, l) and a scaled factor d. If a point is contained in the tetrahedron, its scaled barycentric coordinates must be nonnegative and their sum must lie between 0 and d. Moreover, there will be $\binom{M+d}{M}$ nodes, namely, the tetrahedral points whose scaled barycentric coordinates are all integers, and the same number of Lagrange basis functions.

We index a given Lagrange basis function using the scaled barycentric coordinates of its associated node. Thus, a typical Lagrange basis function could be represented as $L(i, j, k, l)(x, y, z)$.

For a given index (i, j, k, l), we can evaluate the Lagrange basis function as follows:

$$L(i,j,k,l)(x,y,z) = \prod_{p=0}^{i-1}(x - \frac{p}{d}) \prod_{p=0}^{j-1}(y - \frac{p}{d}) \prod_{p=0}^{k-1}(z - \frac{p}{d}) \prod_{p=0}^{l-1}((1-x-y-z) - \frac{p}{d})$$

but then we have to normalize by dividing by the value of this polynomial at the associated node.

9 The Lagrange Polynomial Basis For Simplices

One of the primary advantages of the approach presented here is that we can now see how to generate the basis functions for an arbitrary degree d, and in a reference simplex of arbitrary dimension M.

To begin with, we know that the number of basis functions to be generated will be $\binom{M+d}{M}$. We choose $d + 1$ equally spaced points along each of the **M** coordinate axes to generate the grid points. We define the $M + 1$-dimensional barycentric grid index $\mathbf{i}$ in the corresponding way. For a point $\mathbf{x}$, we evaluate the Lagrange basis function by:

$$L(\mathbf{i};\mathbf{x}) = \prod_{p=0}^{\mathbf{i}_1-1}(\mathbf{x}_1 - \frac{p}{d}) \prod_{p=0}^{\mathbf{i}_2-1}(\mathbf{x}_2 - \frac{p}{d}) \dots \prod_{p=0}^{\mathbf{i}_M-1}(\mathbf{x}_M - \frac{p}{d}) \prod_{p=0}^{\mathbf{i}_{M+1}-1}((1 - \mathbf{x}_1 - \mathbf{x}_2 \dots - \mathbf{x}_M) - \frac{p}{d})$$

or, if we extend the vector $\mathbf{x}$ by an $\mathbf{M}$+1-th component, so that $\mathbf{x}_{M+1} = 1 - \sum_{i=1}^{M} \mathbf{x}_i$, we have

$$L(\mathbf{i};\mathbf{x}) = \prod_{j=1}^{M+1} \prod_{p=0}^{\mathbf{i}_j - 1} (\mathbf{x}_j - \frac{p}{d})$$

and we normalize by dividing by the value of this polynomial at the associated node to get $\phi(\mathbf{i};\mathbf{x})$.

10 MATLAB Code

The web page http://people.sc.fsu.edu/∼jburkardt/m_src/fem_basis.html makes available MATLAB implementations of the various versions of the finite element basis function formulas. (Versions in C++ and FORTRAN90 are also available.) Here is the text for the function which handles the case of an $\mathbf{M}$-dimensional simplex.

```
function l = fem_basis_md ( m, i, x )

%*****************************************************************************80
%
%% FEM_BASIS_MD evaluates an arbitrary M-dimensional basis function.
%
%  Licensing:
%
%    This code is distributed under the GNU LGPL license.
%
%  Modified:
%
%    08 January 2011
%
%  Author:
%
%    John Burkardt
%
%  Parameters:
%
%    Input, integer M, the spatial dimension.
%
%    Input, integer I(M+1), the integer barycentric
%    coordinates of the basis function, 0 <= I(1:M+1).
%    The polynomial degree D = sum(I(1:M+1)).
%
%    Input, real X(M), the evaluation point.
%
%    Output, real L, the value at X of the basis function designated by I.
%

%
%  Augment the X vector.
%
  x(m+1) = 1.0 - sum ( x(1:m) );
%
```

```
%  Determine the degree.
%
  d = sum ( i(1:m+1) );

  l = 1.0;

  for q = 1 : m + 1
   for p = 0 : i(q) - 1
      l = l * ( d * x(q) - p ) / ( i(q) - p );
    end
  end

  return
end
```