

Approximation of functions with finite elements

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The finite element method is a powerful tool for solving differential equations. The method can easily deal with complex geometries and higher-order approximations of the solution. Figure 1 shows a two-dimensional domain with a non-trivial geometry. The idea is to divide the domain into triangles (elements) and seek a polynomial approximations to the unknown functions on each triangle. The method glues these piecewise approximations together to find a global solution. Linear and quadratic polynomials over the triangles are particularly popular.

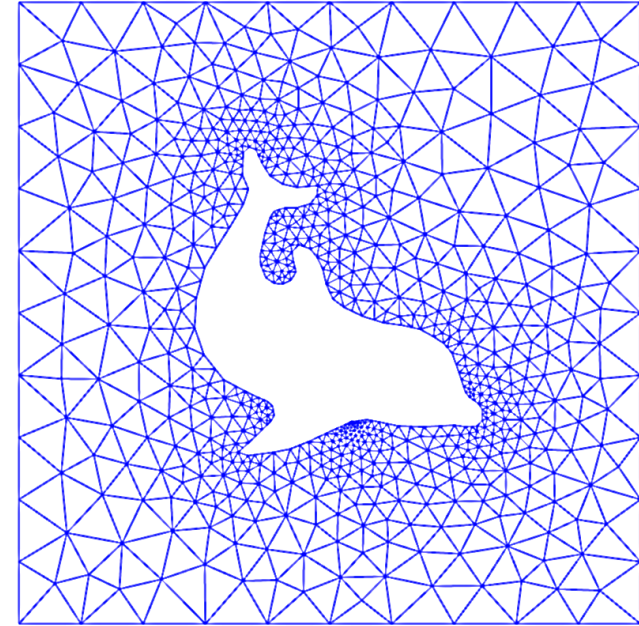


Figure 1: Domain for flow around a dolphin.

Many successful numerical methods for differential equations, including the finite element method, aim at approximating the unknown function by a sum

$$u(x) = \sum_{i=0}^N c_i \psi_i(x), \quad (1)$$

where $\psi_i(x)$ are prescribed functions and c_0, \dots, c_N are unknown coefficients to be determined. Solution methods for differential equations utilizing (1) must have a *principle* for constructing $N + 1$ equations to determine c_0, \dots, c_N . Then there is a *machinery* regarding the actual constructions of the equations for c_0, \dots, c_N , in a particular problem. Finally, there is a *solve* phase for computing the solution c_0, \dots, c_N of the $N + 1$ equations.

Especially in the finite element method, the machinery for constructing the discrete equations to be implemented on a computer is quite comprehensive, with many mathematical and implementational details entering the scene at the same time. From an ease-of-learning perspective it can therefore be wise to introduce the computational machinery for a trivial equation: $u = f$. Solving this equation with f given and u on the form (1) means that we seek an approximation u to f . This approximation problem has the advantage of introducing most of the finite element toolbox, but with postponing demanding topics related to differential equations (e.g., integration by parts, boundary conditions, and coordinate mappings). This is the reason why we shall first become familiar with finite element *approximation* before addressing finite element methods for differential equations.

First, we refresh some linear algebra concepts about approximating vectors in vector spaces. Second, we extend these concepts to approximating functions in function spaces, using the same principles and the same notation. We present examples on approximating functions by global basis functions with support throughout the entire domain. Third, we introduce the finite element type of local basis functions and explain the computational algorithms for working with such functions. Three types of approximation principles are covered: 1) the least squares method, 2) the L_2 projection or Galerkin method, and 3) interpolation or collocation.

1 Approximation of vectors

We shall start with introducing two fundamental methods for determining the coefficients c_i in (1) and illustrate the methods on approximation of vectors, because vectors in vector spaces give a more intuitive understanding than starting directly with approximation of functions in function spaces. The extension from vectors to functions will be trivial as soon as the fundamental ideas are understood.

The first method of approximation is called the *least squares method* and consists in finding c_i such that the difference $u - f$, measured in some norm, is minimized. That is, we aim at finding the best approximation u to f (in some norm). The second method is not as intuitive: we find u such that the error $u - f$ is orthogonal to the space where we seek u . This is known as *projection*, or we may also call it a *Galerkin method*. When approximating vectors and functions, the two methods are equivalent, but this is no longer the case when applying the principles to differential equations.

1.1 Approximation of planar vectors

Suppose we have given a vector $\mathbf{f} = (3, 5)$ in the xy plane and that we want to approximate this vector by a vector aligned in the direction of the vector (a, b) . Figure 2 depicts the situation.

We introduce the vector space V spanned by the vector $\psi_0 = (a, b)$:

$$V = \text{span} \{ \psi_0 \}. \quad (2)$$

We say that ψ_0 is a basis vector in the space V . Our aim is to find the vector $\mathbf{u} = c_0 \psi_0 \in V$ which best approximates the given vector $\mathbf{f} = (3, 5)$. A reasonable criterion for a best approximation could be to minimize the length of the difference between the approximate \mathbf{u} and the given \mathbf{f} . The difference, or error $\mathbf{e} = \mathbf{f} - \mathbf{u}$, has its length given by the *norm*

$$\|\mathbf{e}\| = (\mathbf{e}, \mathbf{e})^{\frac{1}{2}},$$

where (\mathbf{e}, \mathbf{e}) is the *inner product* of \mathbf{e} and itself. The inner product, also called *scalar product* or *dot product*, of two vectors $\mathbf{u} = (u_0, u_1)$ and $\mathbf{v} = (v_0, v_1)$ is defined as

$$(\mathbf{u}, \mathbf{v}) = u_0 v_0 + u_1 v_1. \quad (3)$$

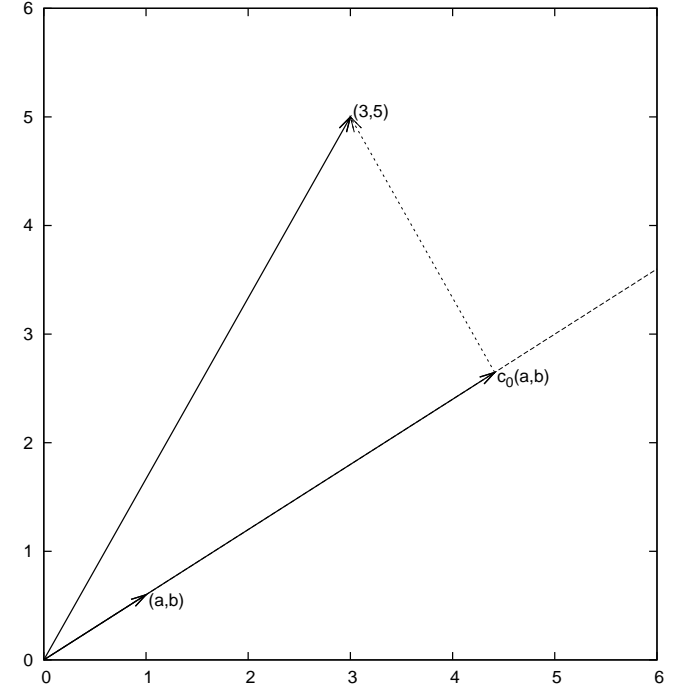


Figure 2: Approximation of a two-dimensional vector by a one-dimensional vector.

Remark 1. We should point out that we use the notation (\cdot, \cdot) for two different things: (a, b) for scalar quantities a and b means the vector starting in the origin and ending in the point (a, b) , while (\mathbf{u}, \mathbf{v}) with vectors \mathbf{u} and \mathbf{v} means the inner product of these vectors. Since vectors are here written in boldface font there should be no confusion. We may add that the norm associated with this inner product is the usual Euclidean length of a vector.

Remark 2. It might be wise to refresh some basic linear algebra by consulting a textbook. Exercises 1 and 2 suggest specific tasks to regain familiarity with fundamental operations on inner product vector spaces.

The least squares method. We now want to find c_0 such that it minimizes $\|\mathbf{e}\|$. The algebra is simplified if we minimize the square of the norm, $\|\mathbf{e}\|^2 = (\mathbf{e}, \mathbf{e})$, instead of the norm itself. Define the function

$$E(c_0) = (\mathbf{e}, \mathbf{e}) = (\mathbf{f} - c_0 \psi_0, \mathbf{f} - c_0 \psi_0). \quad (4)$$

We can rewrite the expressions of the right-hand side in a more convenient form for further work:

$$E(c_0) = (\mathbf{f}, \mathbf{f}) - 2c_0(\mathbf{f}, \psi_0) + c_0^2(\psi_0, \psi_0). \quad (5)$$

The rewrite results from using the following fundamental rules for inner product spaces:

$$(\alpha \mathbf{u}, \mathbf{v}) = \alpha(\mathbf{u}, \mathbf{v}), \quad \alpha \in \mathbb{R}, \quad (6)$$

$$(\mathbf{u} + \mathbf{v}, \mathbf{w}) = (\mathbf{u}, \mathbf{w}) + (\mathbf{v}, \mathbf{w}), \quad (7)$$

$$(\mathbf{u}, \mathbf{v}) = (\mathbf{v}, \mathbf{u}). \quad (8)$$

Minimizing $E(c_0)$ implies finding c_0 such that

$$\frac{\partial E}{\partial c_0} = 0.$$

Differentiating (5) with respect to c_0 gives

$$\frac{\partial E}{\partial c_0} = -2(\mathbf{f}, \psi_0) + 2c_0(\psi_0, \psi_0). \quad (9)$$

Setting the above expression equal to zero and solving for c_0 gives

$$c_0 = \frac{(\mathbf{f}, \psi_0)}{(\psi_0, \psi_0)}, \quad (10)$$

which in the present case with $\psi_0 = (a, b)$ results in

$$c_0 = \frac{3a + 5b}{a^2 + b^2}. \quad (11)$$

For later, it is worth mentioning that setting the key equation (9) to zero can be rewritten as

$$(\mathbf{f} - c_0\psi_0, \psi_0) = 0,$$

or

$$(\mathbf{e}, \psi_0) = 0. \quad (12)$$

The projection method. We shall now show that minimizing $\|\mathbf{e}\|^2$ implies that \mathbf{e} is orthogonal to *any* vector \mathbf{v} in the space V . This result is visually quite clear from Figure 2 (think of other vectors along the line (a, b) : all of them will lead to a larger distance between the approximation and \mathbf{f}). To see this result mathematically, we express any $\mathbf{v} \in V$ as $\mathbf{v} = s\psi_0$ for any scalar parameter s , recall that two vectors are orthogonal when their inner product vanishes, and

calculate the inner product

$$\begin{aligned} (\mathbf{e}, s\psi_0) &= (\mathbf{f} - c_0\psi_0, s\psi_0) \\ &= (\mathbf{f}, s\psi_0) - (c_0\psi_0, s\psi_0) \\ &= s(\mathbf{f}, \psi_0) - sc_0(\psi_0, \psi_0) \\ &= s(\mathbf{f}, \psi_0) - s \frac{(\mathbf{f}, \psi_0)}{(\psi_0, \psi_0)} (\psi_0, \psi_0) \\ &= s((\mathbf{f}, \psi_0) - (\mathbf{f}, \psi_0)) \\ &= 0. \end{aligned}$$

Therefore, instead of minimizing the square of the norm, we could demand that \mathbf{e} is orthogonal to any vector in V . This method is known as *projection*, because it is the same as projecting the vector onto the subspace. (The approach can also be referred to as a Galerkin method as explained at the end of Section ??.)

Mathematically the projection method is stated by the equation

$$(\mathbf{e}, \mathbf{v}) = 0, \quad \forall \mathbf{v} \in V. \quad (13)$$

An arbitrary $\mathbf{v} \in V$ can be expressed as $s\psi_0$, $s \in \mathbb{R}$, and therefore (13) implies

$$(\mathbf{e}, s\psi_0) = s(\mathbf{e}, \psi_0) = 0,$$

which means that the error must be orthogonal to the basis vector in the space V :

$$(\mathbf{e}, \psi_0) = 0 \quad \text{or} \quad (\mathbf{f} - c_0\psi_0, \psi_0) = 0.$$

The latter equation gives (10) and it also arose from least squares computations in (12).

1.2 Approximation of general vectors

Let us generalize the vector approximation from the previous section to vectors in spaces with arbitrary dimension. Given some vector \mathbf{f} , we want to find the best approximation to this vector in the space

$$V = \text{span}\{\psi_0, \dots, \psi_N\}.$$

We assume that the *basis vectors* ψ_0, \dots, ψ_N are linearly independent so that none of them are redundant and the space has dimension $N + 1$. Any vector $\mathbf{u} \in V$ can be written as a linear combination of the basis vectors,

$$\mathbf{u} = \sum_{j=0}^N c_j \psi_j,$$

where $c_j \in \mathbb{R}$ are scalar coefficients to be determined.

The least squares method. Now we want to find c_0, \dots, c_N , such that \mathbf{u} is the best approximation to \mathbf{f} in the sense that the distance (error) $\mathbf{e} = \mathbf{f} - \mathbf{u}$ is minimized. Again, we define the squared distance as a function of the free parameters c_0, \dots, c_N ,

$$\begin{aligned}
E(c_0, \dots, c_N) &= (\mathbf{e}, \mathbf{e}) = (\mathbf{f} - \sum_j c_j \boldsymbol{\psi}_j, \mathbf{f} - \sum_j c_j \boldsymbol{\psi}_j) \\
&= (\mathbf{f}, \mathbf{f}) - 2 \sum_{j=0}^N c_j (\mathbf{f}, \boldsymbol{\psi}_j) + \sum_{p=0}^N \sum_{q=0}^N c_p c_q (\boldsymbol{\psi}_p, \boldsymbol{\psi}_q).
\end{aligned} \tag{14}$$

Minimizing this E with respect to the independent variables c_0, \dots, c_N is obtained by requiring

$$\frac{\partial E}{\partial c_i} = 0, \quad i = 0, \dots, N.$$

The second term in (14) is differentiated as follows:

$$\frac{\partial}{\partial c_i} \sum_{j=0}^N c_j (\mathbf{f}, \boldsymbol{\psi}_j) = (\mathbf{f}, \boldsymbol{\psi}_i), \tag{15}$$

since the expression to be differentiated is a sum and only one term, $c_i (\mathbf{f}, \boldsymbol{\psi}_i)$, contains c_i and this term is linear in c_i . To understand this differentiation in detail, write out the sum specifically for, e.g. $N = 3$ and $i = 1$.

The last term in (14) is more tedious to differentiate. We start with

$$\frac{\partial}{\partial c_i} c_p c_q = \begin{cases} 0, & \text{if } p \neq i \text{ and } q \neq i, \\ c_q, & \text{if } p = i \text{ and } q \neq i, \\ c_p, & \text{if } p \neq i \text{ and } q = i, \\ 2c_i, & \text{if } p = q = i, \end{cases} \tag{16}$$

Then

$$\frac{\partial}{\partial c_i} \sum_{p=0}^N \sum_{q=0}^N c_p c_q (\boldsymbol{\psi}_p, \boldsymbol{\psi}_q) = \sum_{p=0, p \neq i}^N c_p (\boldsymbol{\psi}_p, \boldsymbol{\psi}_i) + \sum_{q=0, q \neq i}^N c_q (\boldsymbol{\psi}_q, \boldsymbol{\psi}_i) + 2c_i (\boldsymbol{\psi}_i, \boldsymbol{\psi}_i).$$

The last term can be included in the other two sums, resulting in

$$\frac{\partial}{\partial c_i} \sum_{p=0}^N \sum_{q=0}^N c_p c_q (\boldsymbol{\psi}_p, \boldsymbol{\psi}_q) = 2 \sum_{j=0}^N c_j (\boldsymbol{\psi}_j, \boldsymbol{\psi}_i). \tag{17}$$

It then follows that setting

$$\frac{\partial E}{\partial c_i} = 0, \quad i = 0, \dots, N,$$

leads to a linear system for c_0, \dots, c_N :

$$\sum_{j=0}^N A_{i,j} c_j = b_i, \quad i = 0, \dots, N, \tag{18}$$

where

$$A_{i,j} = (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j), \tag{19}$$

$$b_i = (\boldsymbol{\psi}_i, \mathbf{f}). \tag{20}$$

We have changed the order of the two vectors in the inner product according to (1.1):

$$A_{i,j} = (\boldsymbol{\psi}_j, \boldsymbol{\psi}_i) = (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j),$$

simply because the sequence i - j looks more aesthetic.

The Galerkin or projection method. In analogy with the "one-dimensional" example in Section 1.1, it holds also here in the general case that minimizing the distance (error) \mathbf{e} is equivalent to demanding that \mathbf{e} is orthogonal to all $\mathbf{v} \in V$:

$$(\mathbf{e}, \mathbf{v}) = 0, \quad \forall \mathbf{v} \in V. \tag{21}$$

Since any $\mathbf{v} \in V$ can be written as $\mathbf{v} = \sum_{i=0}^N c_i \boldsymbol{\psi}_i$, the statement (21) is equivalent to saying that

$$(\mathbf{e}, \sum_{i=0}^N c_i \boldsymbol{\psi}_i) = 0,$$

for any choice of coefficients c_0, \dots, c_N . The latter equation can be rewritten as

$$\sum_{i=0}^N c_i (\mathbf{e}, \boldsymbol{\psi}_i) = 0.$$

If this is to hold for arbitrary values of c_0, \dots, c_N we must require that each term in the sum vanishes,

$$(\mathbf{e}, \boldsymbol{\psi}_i) = 0, \quad i = 0, \dots, N. \tag{22}$$

These $N + 1$ equations result in the same linear system as (18):

$$(\mathbf{f} - \sum_{j=0}^N c_j \boldsymbol{\psi}_j, \boldsymbol{\psi}_i) = (\mathbf{f}, \boldsymbol{\psi}_i) - \sum_{j \in I} (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j) c_j = 0,$$

and hence

$$\sum_{j=0}^N (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j) c_j = (\mathbf{f}, \boldsymbol{\psi}_i), \quad i = 0, \dots, N.$$

So, instead of differentiating the $E(c_0, \dots, c_N)$ function, we could simply use (21) as the principle for determining c_0, \dots, c_N , resulting in the $N + 1$ equations (22).

The names *least squares method* or *least squares approximation* are natural since the calculation consists of minimizing $\|\mathbf{e}\|^2$, and $\|\mathbf{e}\|^2$ is a sum of squares of differences between the components in \mathbf{f} and \mathbf{u} . We find \mathbf{u} such that this sum of squares is minimized.

The principle (21), or the equivalent form (22), is known as *projection*. Almost the same mathematical idea was used by the Russian mathematician Boris Galerkin¹ to solve differential equations, resulting in what is widely known as *Galerkin's method*.

¹http://en.wikipedia.org/wiki/Boris_Galerkin

2 Approximation of functions

Let V be a function space spanned by a set of *basis functions* ψ_0, \dots, ψ_N ,

$$V = \text{span} \{ \psi_0, \dots, \psi_N \},$$

such that any function $u \in V$ can be written as a linear combination of the basis functions:

$$u = \sum_{j \in I} c_j \psi_j. \quad (23)$$

The index set I is defined as $I = \{0, \dots, N\}$ and is used both for compact notation and for flexibility in the numbering of elements in sequences.

For now, in this introduction, we shall look at functions of a single variable x : $u = u(x)$, $\psi_i = \psi_i(x)$, $i \in I$. Later, we will almost trivially extend the mathematical details to functions of two- or three-dimensional physical spaces. The approximation (23) is typically used to discretize a problem in space. Other methods, most notably finite differences, are common for time discretization, although the form (23) can be used in time as well.

2.1 The least squares method

Given a function $f(x)$, how can we determine its best approximation $u(x) \in V$? A natural starting point is to apply the same reasoning as we did for vectors in Section 1.2. That is, we minimize the distance between u and f . However, this requires a norm for measuring distances, and a norm is most conveniently defined through an inner product. Viewing a function as a vector of infinitely many point values, one for each value of x , the inner product could intuitively be defined as the usual summation of pairwise components, with summation replaced by integration:

$$(f, g) = \int f(x)g(x) \, dx.$$

To fix the integration domain, we let $f(x)$ and $\psi_i(x)$ be defined for a domain $\Omega \subset \mathbb{R}$. The inner product of two functions $f(x)$ and $g(x)$ is then

$$(f, g) = \int_{\Omega} f(x)g(x) \, dx. \quad (24)$$

The distance between f and any function $u \in V$ is simply $f - u$, and the squared norm of this distance is

$$E = (f(x) - \sum_{j \in I} c_j \psi_j(x), f(x) - \sum_{j \in I} c_j \psi_j(x)). \quad (25)$$

Note the analogy with (14): the given function f plays the role of the given vector \mathbf{f} , and the basis function ψ_i plays the role of the basis vector ψ_i . We can rewrite (25), through similar steps as used for the result (14), leading to

$$E(c_i, \dots, c_N) = (f, f) - 2 \sum_{j \in I} c_j (f, \psi_j) + \sum_{p \in I} \sum_{q \in I} c_p c_q (\psi_p, \psi_q). \quad (26)$$

Minimizing this function of $N + 1$ scalar variables $\{c_i\}_{i \in I}$, requires differentiation with respect to c_i , for all $i \in I$. The resulting equations are very similar to those we had in the vector case, and we hence end up with a linear system of the form (18), with basically the same expressions:

$$A_{i,j} = (\psi_i, \psi_j), \quad (27)$$

$$b_i = (f, \psi_i). \quad (28)$$

2.2 The projection (or Galerkin) method

As in Section 1.2, the minimization of (e, e) is equivalent to

$$(e, v) = 0, \quad \forall v \in V. \quad (29)$$

This is known as a projection of a function f onto the subspace V . We may also call it a Galerkin method for approximating functions. Using the same reasoning as in (21)-(22), it follows that (29) is equivalent to

$$(e, \psi_i) = 0, \quad i \in I. \quad (30)$$

Inserting $e = f - u$ in this equation and ordering terms, as in the multi-dimensional vector case, we end up with a linear system with a coefficient matrix (27) and right-hand side vector (28).

Whether we work with vectors in the plane, general vectors, or functions in function spaces, the least squares principle and the projection or Galerkin method are equivalent.

2.3 Example: linear approximation

Let us apply the theory in the previous section to a simple problem: given a parabola $f(x) = 10(x - 1)^2 - 1$ for $x \in \Omega = [1, 2]$, find the best approximation $u(x)$ in the space of all linear functions:

$$V = \text{span} \{1, x\}.$$

With our notation, $\psi_0(x) = 1$, $\psi_1(x) = x$, and $N = 1$. We seek

$$u = c_0 \psi_0(x) + c_1 \psi_1(x) = c_0 + c_1 x,$$

where c_0 and c_1 are found by solving a 2×2 the linear system. The coefficient matrix has elements

$$A_{0,0} = (\psi_0, \psi_0) = \int_1^2 1 \cdot 1 \, dx = 1, \quad (31)$$

$$A_{0,1} = (\psi_0, \psi_1) = \int_1^2 1 \cdot x \, dx = 3/2, \quad (32)$$

$$A_{1,0} = A_{0,1} = 3/2, \quad (33)$$

$$A_{1,1} = (\psi_1, \psi_1) = \int_1^2 x \cdot x \, dx = 7/3. \quad (34)$$

The corresponding right-hand side is

$$b_1 = (f, \psi_0) = \int_1^2 (10(x - 1)^2 - 1) \cdot 1 \, dx = 7/3, \quad (35)$$

$$b_2 = (f, \psi_1) = \int_1^2 (10(x - 1)^2 - 1) \cdot x \, dx = 13/3. \quad (36)$$

Solving the linear system results in

$$c_0 = -38/3, \quad c_1 = 10, \quad (37)$$

and consequently

$$u(x) = 10x - \frac{38}{3}. \quad (38)$$

Figure 3 displays the parabola and its best approximation in the space of all linear functions.

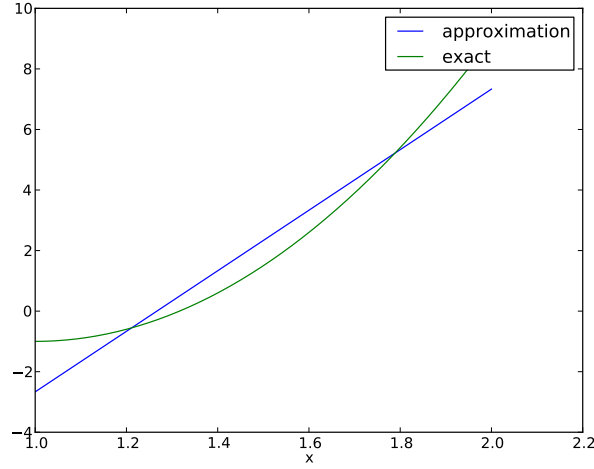


Figure 3: Best approximation of a parabola by a straight line.

2.4 Implementation of the least squares method

The linear system can be computed either symbolically or numerically (a numerical integration rule is needed in the latter case). Here is a function for symbolic computation of the linear system, where $f(x)$ is given as a sympy expression `f` involving the symbol `x`, `psi` is a list of expressions for $\{\psi_i\}_{i \in I}$, and `Omega` is a 2-tuple/list holding the limits of the domain Ω :

```
import sympy as sm

def least_squares(f, psi, Omega):
    N = len(psi) - 1
    A = sm.zeros((N+1, N+1))
    b = sm.zeros((N+1, 1))
    x = sm.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
```

```
A[i,j] = sm.integrate(psi[i]*psi[j],
                      (x, Omega[0], Omega[1]))
A[j,i] = A[i,j]
b[i,0] = sm.integrate(psi[i]*f, (x, Omega[0], Omega[1]))
c = A.LUsolve(b)
u = 0
for i in range(len(psi)):
    u += c[i,0]*psi[i]
return u
```

Observe that we exploit the symmetry of the coefficient matrix: only the upper triangular part is computed. Symbolic integration in `sympy` is often time consuming, and (roughly) halving the work has noticeable effect on the waiting time for the function to finish execution.

Comparing the given $f(x)$ and the approximate $u(x)$ visually is done by the following function, which with the aid of `sympy`'s `lambdify` tool converts a `sympy` expression to a Python function for numerical computations:

```
def comparison_plot(f, u, Omega, filename='tmp.pdf'):
    x = sm.Symbol('x')
    f = sm.lambdify([x], f, modules="numpy")
    u = sm.lambdify([x], u, modules="numpy")
    resolution = 401 # no of points in plot
    xcoor = linspace(Omega[0], Omega[1], resolution)
    exact = f(xcoor)
    approx = u(xcoor)
    plot(xcoor, approx)
    hold('on')
    plot(xcoor, exact)
    legend(['approximation', 'exact'])
    savefig(filename)
```

The `modules='numpy'` argument to `lambdify` is important if there are mathematical functions, such as `sin` or `exp` in the symbolic expressions in `f` or `u`, and these mathematical functions are to be used with vector arguments, like `xcoor` above.

Both the `least_squares` and `comparison_plot` are found and coded in the file `approx1D.py`². The forthcoming examples on their use appear in `ex_approx1D.py`.

2.5 Perfect approximation

Let us use the code above to recompute the problem from Section 2.3 where we want to approximate a parabola. What happens if we add an element x^2 to the basis and test what the best approximation is if V is the space of all parabolic functions? The answer is quickly found by running

```
>>> from approx1D import *
>>> x = sm.Symbol('x')
>>> f = 10*(x-1)**2-1
>>> u = least_squares(f=f, psi=[1, x, x**2], Omega=[1, 2])
>>> print u
10*x**2 - 20*x + 9
>>> print sm.expand(f)
10*x**2 - 20*x + 9
```

Now, what if we use $\psi_i(x) = x^i$ for $i = 0, 1, \dots, N = 40$? The output from `least_squares` gives $c_i = 0$ for $i > 2$, which means that the method finds the perfect approximation.

In fact, we have a general result that if $f \in V$, the least squares and Galerkin/projection methods compute the exact solution $u = f$. The proof is straightforward: if $f \in V$, f can be

²<http://tinyurl.com/jvzzcfn/fem/approx1D.py>

expanded in terms of the basis functions, $f = \sum_{j \in I} d_j \psi_j$, for some coefficients $\{d_i\}_{i \in I}$, and the right-hand side then has entries

$$b_i = (f, \psi_i) = \sum_{j \in I} d_j (\psi_j, \psi_i) = \sum_{j \in I} d_j A_{i,j}.$$

The linear system $\sum_j A_{i,j} c_j = b_i$, $i \in I$, is then

$$\sum_{j \in I} c_j A_{i,j} = \sum_{j \in I} d_j A_{i,j}, \quad i \in I,$$

which implies that $c_i = d_i$ for $i \in I$.

2.6 Ill-conditioning

The computational example in Section 2.5 applies the `least_squares` function which invokes symbolic methods to calculate and solve the linear system. The correct solution $c_0 = 9, c_1 = -20, c_2 = 10, c_i = 0$ for $i \geq 3$ is perfectly recovered.

Suppose we convert the matrix and right-hand side to floating-point arrays and then solve the system using finite-precision arithmetics, which is what one will (almost) always do in real life. This time we get astonishing results! Up to about $N = 7$ we get a solution that is reasonably close to the exact one. Increasing N shows that seriously wrong coefficients are computed. Below is a table showing the solution of the linear system arising from approximating a parabola by functions on the form $u(x) = c_0 + c_1 x + c_2 x^2 + \dots + c_{10} x^{10}$. Analytically, we know that $c_j = 0$ for $j > 2$, but numerically we may get $c_j \neq 0$ for $j > 2$.

exact	sympy	numpy32	numpy64
9	9.62	5.57	8.98
-20	-23.39	-7.65	-19.93
10	17.74	-4.50	9.96
0	-9.19	4.13	-0.26
0	5.25	2.99	0.72
0	0.18	-1.21	-0.93
0	-2.48	-0.41	0.73
0	1.81	-0.013	-0.36
0	-0.66	0.08	0.11
0	0.12	0.04	-0.02
0	-0.001	-0.02	0.002

The exact value of c_j , $j = 0, 1, \dots, 10$, appears in the first column while the other columns correspond to results obtained by three different methods:

- Column 2: The matrix and vector are converted to the data structure `sympy.mpmath.fp.matrix` and the `sympy.mpmath.fp.lu_solve` function is used to solve the system.
- Column 3: The matrix and vector are converted to `numpy` arrays with data type `numpy.float32` (single precision floating-point number) and solved by the `numpy.linalg.solve` function.
- Column 4: As column 3, but the data type is `numpy.float64` (double precision floating-point number).

We see from the numbers in the table that double precision performs much better than single precision. Nevertheless, when plotting all these solutions the curves cannot be visually distinguished

(!). This means that the approximations look perfect, despite the partially very wrong values of the coefficients.

Increasing N to 12 makes the numerical solver in `numpy` abort with the message: "matrix is numerically singular". A matrix has to be non-singular to be invertible, which is a requirement when solving a linear system. Already when the matrix is close to singular, it is *ill-conditioned*, which here implies that the numerical solution algorithms are sensitive to round-off errors and may produce (very) inaccurate results.

The reason why the coefficient matrix is nearly singular and ill-conditioned is that our basis functions $\psi_i(x) = x^i$ are nearly linearly dependent for large i . That is, x^i and x^{i+1} are very close for i not very small. This phenomenon is illustrated in Figure 4. There are 15 lines in this figure, but only half of them are visually distinguishable. Almost linearly dependent basis functions give rise to an ill-conditioned and almost singular matrix. This fact can be illustrated by computing the determinant, which is indeed very close to zero (recall that a zero determinant implies a singular and non-invertible matrix): 10^{-65} for $N = 10$ and 10^{-92} for $N = 12$. Already for $N = 28$ the numerical determinant computation returns a plain zero.

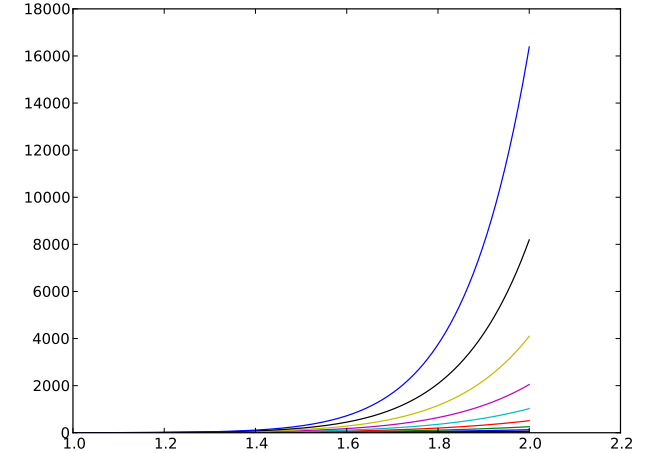


Figure 4: The 15 first basis functions x^i , $i = 0, \dots, 14$.

On the other hand, the double precision `numpy` solver do run for $N = 100$, resulting in answers that are not significantly worse than those in the table above, and large powers are associated with small coefficients (e.g., $c_j < 10^{-2}$ for $10 \leq j \leq 20$ and $c < 10^{-5}$ for $j > 20$). Even for $N = 100$ the approximation still lies on top of the exact curve in a plot (!).

The conclusion is that visual inspection of the quality of the approximation may not uncover fundamental numerical problems with the computations. However, numerical analysts have studied approximations and ill-conditioning for decades, and it is well known that the basis

$\{1, x, x^2, x^3, \dots\}$ is a bad basis. The best basis from a matrix conditioning point of view is to have orthogonal functions such that $(\psi_i, \psi_j) = 0$ for $i \neq j$. There are many known sets of orthogonal polynomials and other functions. The functions used in the finite element methods are almost orthogonal, and this property helps to avoid problems with solving matrix systems. Almost orthogonal is helpful, but not enough when it comes to partial differential equations, and ill-conditioning of the coefficient matrix is a theme when solving large-scale matrix systems arising from finite element discretizations.

2.7 Fourier series

A set of sine functions is widely used for approximating functions (the sines are also orthogonal as explained more in Section 2.6). Let us take

$$V = \text{span} \{ \sin \pi x, \sin 2\pi x, \dots, \sin(N+1)\pi x \}.$$

That is,

$$\psi_i(x) = \sin((i+1)\pi x), \quad i \in I.$$

An approximation to the $f(x)$ function from Section 2.3 can then be computed by the `least_squares` function from Section 2.4:

```
N = 3
from sympy import sin, pi
x = sm.Symbol('x')
psi = [sin(pi*(i+1)*x) for i in range(N+1)]
f = 10*(x-1)**2 - 1
Omega = [0, 1]
u = least_squares(f, psi, Omega)
comparison_plot(f, u, Omega)
```

Figure 5 (left) shows the oscillatory approximation of $\sum_{j=0}^N c_j \sin((j+1)\pi x)$ when $N = 3$. Changing N to 11 improves the approximation considerably, see Figure 5 (right).

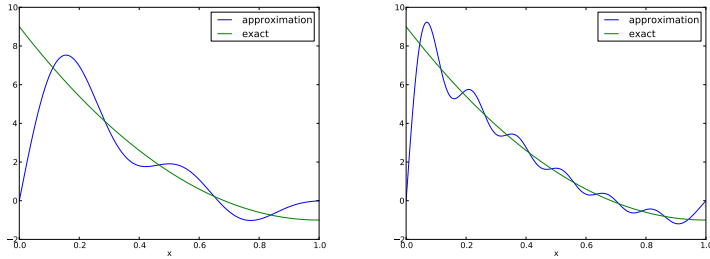


Figure 5: Best approximation of a parabola by a sum of 3 (left) and 11 (right) sine functions.

There is an error $f(0) - u(0) = 9$ at $x = 0$ in Figure 5 regardless of how large N is, because all $\psi_i(0) = 0$ and hence $u(0) = 0$. We may help the approximation to be correct at $x = 0$ by seeking

$$u(x) = f(0) + \sum_{j \in I} c_j \psi_j(x). \quad (39)$$

However, this adjustment introduces a new problem at $x = 1$ since we now get an error $f(1) - u(1) = f(1) - 0 = -1$ at this point. A more clever adjustment is to replace the $f(0)$ term by a term that is $f(0)$ at $x = 0$ and $f(1)$ at $x = 1$. A simple linear combination $f(0)(1-x) + xf(1)$ does the job:

$$u(x) = f(0)(1-x) + xf(1) + \sum_{j \in I} c_j \psi_j(x). \quad (40)$$

This adjustment of u alters the linear system slightly as we get an extra term $-(f(0)(1-x) + xf(1), \psi_i)$ on the right-hand side. Figure 6 shows the result of this technique for ensuring right boundary values: even 3 sines can now adjust the $f(0)(1-x) + xf(1)$ term such that u approximates the parabola really well, at least visually.

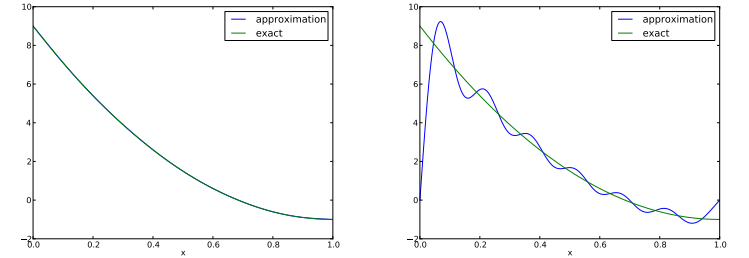


Figure 6: Best approximation of a parabola by a sum of 3 (left) and 11 (right) sine functions with a boundary term.

2.8 Orthogonal basis functions

The choice of sine functions $\psi_i(x) = \sin((i+1)\pi x)$ has a great computational advantage: on $\Omega = [0, 1]$ these basis functions are *orthogonal*, implying that $A_{i,j} = 0$ if $i \neq j$. This result is realized by trying

```
integrate(sin(j*pi*x)*sin(k*pi*x), x, 0, 1)
```

in [WolframAlpha](http://wolframalpha.com)³ (avoid i in the integrand as this symbol means the imaginary unit $\sqrt{-1}$). Also by asking WolframAlpha about $\int_0^1 \sin^2(j\pi x) dx$, we find it to equal $1/2$. With a diagonal matrix we can easily solve for the coefficients by hand:

$$c_i = 2 \int_0^1 f(x) \sin((i+1)\pi x) dx, \quad i \in I, \quad (41)$$

which is nothing but the classical formula for the coefficients of the Fourier sine series of $f(x)$ on $[0, 1]$. In fact, when V contains the basic functions used in a Fourier series expansion, the approximation method derived in Section 2 results in the classical Fourier series for $f(x)$ (see Exercise 6 for details).

With orthogonal basis functions we can make the `least_squares` function (much) more efficient since we know that the matrix is diagonal and only the diagonal elements need to be computed:

³<http://wolframalpha.com>

```
def least_squares_orth(f, psi, Omega):
    N = len(psi) - 1
    A = [0]*(N+1)
    b = [0]*(N+1)
    x = sm.Symbol('x')
    for i in range(N+1):
        A[i] = sm.integrate(psi[i]**2, (x, Omega[0], Omega[1]))
        b[i] = sm.integrate(psi[i]*f, (x, Omega[0], Omega[1]))
    c = [b[i]/A[i] for i in range(len(b))]
    u = 0
    for i in range(len(psi)):
        u += c[i]*psi[i]
    return u
```

This function is found in the file `approx1D.py`.

2.9 The interpolation (or collocation) method

The principle of minimizing the distance between u and f is an intuitive way of computing a best approximation $u \in V$ to f . However, there are other approaches as well. One is to demand that $u(x_i) = f(x_i)$ at some selected points x_i , $i \in I$:

$$u(x_i) = \sum_{j \in I} c_j \psi_j(x_i) = f(x_i), \quad i \in I. \quad (42)$$

This criterion also gives a linear system with $N + 1$ unknown coefficients $\{c_i\}_{i \in I}$:

$$\sum_{j \in I} A_{i,j} c_j = b_i, \quad i \in I, \quad (43)$$

with

$$A_{i,j} = \psi_j(x_i), \quad (44)$$

$$b_i = f(x_i). \quad (45)$$

This time the coefficient matrix is not symmetric because $\psi_j(x_i) \neq \psi_i(x_j)$ in general. The method is often referred to as an *interpolation method* since some point values of f are given ($f(x_i)$) and we fit a continuous function u that goes through the $f(x_i)$ points. In this case the x_i points are called *interpolation points*. When the same approach is used to approximate differential equations, one usually applies the name *collocation method* and x_i are known as *collocation points*.

Given f as a sympy symbolic expression `f`, $\{\psi_i\}_{i \in I}$ as a list `psi`, and a set of points $\{x_i\}_{i \in I}$ as a list or array `points`, the following Python function sets up and solves the matrix system for the coefficients $\{c_i\}_{i \in I}$:

```
def interpolation(f, psi, points):
    N = len(psi) - 1
    A = sm.zeros((N+1, N+1))
    b = sm.zeros((N+1, 1))
    x = sm.Symbol('x')
    # Turn psi and f into Python functions
    psi = [sm.lambdify([x], psi[i]) for i in range(N+1)]
    f = sm.lambdify([x], f)
    for i in range(N+1):
        for j in range(N+1):
            A[i,j] = psi[j](points[i])
        b[i,0] = f(points[i])
    c = A.LUsolve(b)
```

```
u = 0
for i in range(len(psi)):
    u += c[i,0]*psi[i](x)
return u
```

The interpolation function is a part of the `approx1D` module.

We found it convenient in the above function to turn the expressions `f` and `psi` into ordinary Python functions of `x`, which can be called with `float` values in the list `points` when building the matrix and the right-hand side. The alternative is to use the `subs` method to substitute the `x` variable in an expression by an element from the `points` list. The following session illustrates both approaches in a simple setting:

```
>>> from sympy import *
>>> x = Symbol('x')
>>> e = x**2                # symbolic expression involving x
>>> p = 0.5                  # a value of x
>>> v = e.subs(x, p)         # evaluate e for x=p
>>> v
0.2500000000000000
>>> type(v)
sympy.core.numbers.Float
>>> e = lambdify([x], e)     # make Python function of e
>>> type(e)
>>> function
>>> v = e(p)                 # evaluate e(x) for x=p
>>> v
0.25
>>> type(v)
float
```

A nice feature of the interpolation or collocation method is that it avoids computing integrals. However, one has to decide on the location of the x_i points. A simple, yet common choice, is to distribute them uniformly throughout Ω .

Example. Let us illustrate the interpolation or collocation method by approximating our parabola $f(x) = 10(x-1)^2 - 1$ by a linear function on $\Omega = [1, 2]$, using two collocation points $x_0 = 1 + 1/3$ and $x_1 = 1 + 2/3$:

```
f = 10*(x-1)**2 - 1
psi = [1, x]
Omega = [1, 2]
points = [1 + sm.Rational(1,3), 1 + sm.Rational(2,3)]
u = interpolation(f, psi, points)
comparison_plot(f, u, Omega)
```

The resulting linear system becomes

$$\begin{pmatrix} 1 & 4/3 \\ 1 & 5/3 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} 1/9 \\ 31/9 \end{pmatrix}$$

with solution $c_0 = -119/9$ and $c_1 = 10$. Figure 7 (left) shows the resulting approximation $u = -119/9 + 10x$. We can easily test other interpolation points, say $x_0 = 1$ and $x_1 = 2$. This changes the line quite significantly, see Figure 7 (right).

2.10 Lagrange polynomials

In Section 2.7 we explain the advantage with having a diagonal matrix: formulas for the coefficients $\{c_i\}_{i \in I}$ can then be derived by hand. For an interpolation/collocation method a diagonal matrix implies that $\psi_j(x_i) = 0$ if $i \neq j$. One set of basis functions $\psi_i(x)$ with this property is the

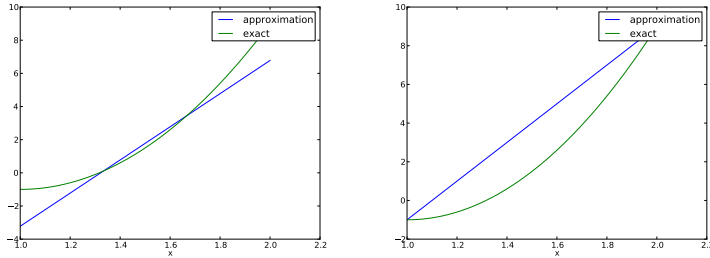


Figure 7: Approximation of a parabola by linear functions computed by two interpolation points: 4/3 and 5/3 (left) versus 1 and 2 (right).

Lagrange interpolating polynomials, or just *Lagrange polynomials*. (Although the functions are named after Lagrange, they were first discovered by Waring in 1779, rediscovered by Euler in 1783, and published by Lagrange in 1795.) The Lagrange polynomials have the form

$$\psi_i(x) = \prod_{j=0, j \neq i}^N \frac{x - x_j}{x_i - x_j} = \frac{x - x_0}{x_i - x_0} \dots \frac{x - x_{i-1}}{x_i - x_{i-1}} \frac{x - x_{i+1}}{x_i - x_{i+1}} \dots \frac{x - x_N}{x_i - x_N}, \quad (46)$$

for $i \in I$. We see from (46) that all the ψ_i functions are polynomials of degree N which have the property

$$\psi_i(x_s) = \begin{cases} 1, & i = s, \\ 0, & i \neq s, \end{cases} \quad (47)$$

when x_s is an interpolation/collocation point. This property implies that $A_{i,j} = 0$ for $i \neq j$ and $A_{i,j} = 1$ when $i = j$. The solution of the linear system is then simply

$$c_i = f(x_i), \quad i \in I, \quad (48)$$

and

$$u(x) = \sum_{j \in I} f(x_j) \psi_j(x). \quad (49)$$

The following function computes the Lagrange interpolating polynomial $\psi_i(x)$, given the interpolation points x_0, \dots, x_N in the list or array **points**:

```
def Lagrange_polynomial(x, i, points):
    p = 1
    for k in range(len(points)):
        if k != i:
            p *= (x - points[k]) / (points[i] - points[k])
    return p
```

The next function computes a complete basis using equidistant points throughout Ω :

```
def Lagrange_polynomials_01(x, N):
    if isinstance(x, sm.Symbol):
        h = sm.Rational(1, N-1)
    else:
        h = 1.0/(N-1)
    points = [i*h for i in range(N)]
    psi = [Lagrange_polynomial(x, i, points) for i in range(N)]
    return psi, points
```

When x is an `sm.Symbol` object, we let the spacing between the interpolation points, h , be a `sympy` rational number for nice end results in the formulas for ψ_i . The other case, when x is a plain Python float, signifies numerical computing, and then we let h be a floating-point number. Observe that the `Lagrange_polynomial` function works equally well in the symbolic and numerical case - just think of x being an `sm.Symbol` object or a Python float. A little interactive session illustrates the difference between symbolic and numerical computing of the basis functions and points:

```
>>> import sympy as sm
>>> x = sm.Symbol('x')
>>> psi, points = Lagrange_polynomials_01(x, N=3)
>>> points
[0, 1/2, 1]
>>> psi
[(1 - x)*(1 - 2*x), 2*x*(2 - 2*x), -x*(1 - 2*x)]

>>> x = 0.5 # numerical computing
>>> psi, points = Lagrange_polynomials_01(x, N=3)
>>> points
[0.0, 0.5, 1.0]
>>> psi
[-0.0, 1.0, 0.0]
```

The Lagrange polynomials are very much used in finite element methods because of their property (47).

Successful example. Trying out the Lagrange polynomial basis for approximating $f(x) = \sin 2\pi x$ on $\Omega = [0, 1]$ with the least squares and the interpolation techniques can be done by

```
x = sm.Symbol('x')
f = sm.sin(2*sm.pi*x)
psi, points = Lagrange_polynomials_01(x, N)
Omega=[0, 1]
u = least_squares(f, psi, Omega)
comparison_plot(f, u, Omega)
u = interpolation(f, psi, points)
comparison_plot(f, u, Omega)
```

Figure 8 shows the results. There is little difference between the least squares and the interpolation technique. Increasing N gives visually better approximations.

Less successful example. The next example concerns interpolating $f(x) = |1 - 2x|$ on $\Omega = [0, 1]$ using Lagrange polynomials. Figure 9 shows a peculiar effect: the approximation starts to oscillate more and more as N grows. This numerical artifact is not surprising when looking at the individual Lagrange polynomials. Figure 10 shows two such polynomials, $\psi_2(x)$ and $\psi_7(x)$, both of degree 11 and computed from uniformly spaced points $x_{x_i} = i/11$, $i = 0, \dots, 11$, marked with circles. We clearly see the property of Lagrange polynomials: $\psi_2(x_i) = 0$ and $\psi_7(x_i) = 0$ for all i , except $\psi_2(x_2) = 1$ and $\psi_7(x_7) = 1$. The most striking feature, however, is the significant oscillation near the boundary. The reason is easy to understand: since we force the functions to

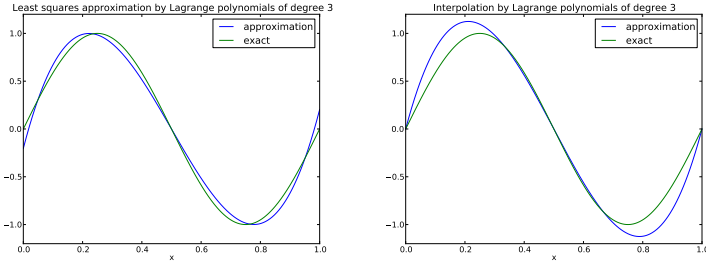


Figure 8: Approximation via least squares (left) and interpolation (right) of a sine function by Lagrange interpolating polynomials of degree 3.

zero at so many points, a polynomial of high degree is forced to oscillate between the points. The phenomenon is named *Runge's phenomenon* and you can read a more detailed explanation on Wikipedia⁴.

Remedy for strong oscillations. The oscillations can be reduced by a more clever choice of interpolation points, called the *Chebyshev nodes*:

$$x_i = \frac{1}{2}(a+b) + \frac{1}{2}(b-a) \cos\left(\frac{2i+1}{2(N+1)}\pi\right), \quad i = 0 \dots, N, \quad (50)$$

on the interval $\Omega = [a, b]$. Here is a flexible version of the `Lagrange_polynomials_01` function above, valid for any interval $\Omega = [a, b]$ and with the possibility to generate both uniformly distributed points and Chebyshev nodes:

```
def Lagrange_polynomials(x, N, Omega, point_distribution='uniform'):
    if point_distribution == 'uniform':
        if isinstance(x, sm.Symbol):
            h = sm.Rational(Omega[1] - Omega[0], N)
        else:
            h = (Omega[1] - Omega[0])/float(N)
        points = [Omega[0] + i*h for i in range(N+1)]
    elif point_distribution == 'Chebyshev':
        points = Chebyshev_nodes(Omega[0], Omega[1], N)
    psi = [Lagrange_polynomial(x, i, points) for i in range(N+1)]
    return psi, points

def Chebyshev_nodes(a, b, N):
    from math import cos, pi
    return [0.5*(a+b) + 0.5*(b-a)*cos(float(2*i+1)/(2*(N+1))*pi) \
            for i in range(N+1)]
```

All the functions computing Lagrange polynomials listed above are found in the module file `Lagrange.py`. Figure 11 shows the improvement of using Chebyshev nodes (compared with Figure 9).

Another cure for undesired oscillation of higher-degree interpolating polynomials is to use lower-degree Lagrange polynomials on many small patches of the domain, which is the idea pursued in the finite element method. For instance, linear Lagrange polynomials on $[0, 1/2]$ and

⁴http://en.wikipedia.org/wiki/Runge%27s_phenomenon

$[1/2, 1]$ would yield a perfect approximation to $f(x) = |1 - 2x|$ on $\Omega = [0, 1]$ since f is piecewise linear.

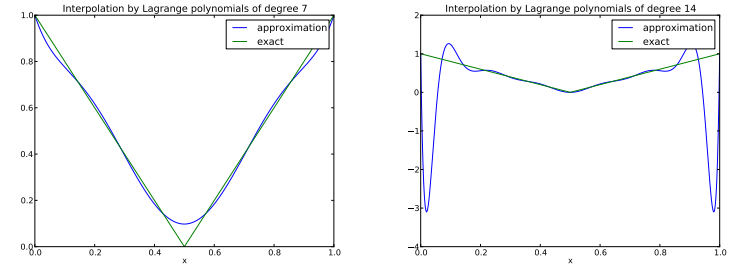


Figure 9: Interpolation of an absolute value function by Lagrange polynomials and uniformly distributed interpolation points: degree 7 (left) and 14 (right).

How does the least squares or projection methods work with Lagrange polynomials? Unfortunately, `sympy` has problems integrating the $f(x) = |1 - 2x|$ function times a polynomial. Other choices of $f(x)$ can also make the symbolic integration fail. Therefore, we should extend the `least_squares` function such that it falls back on numerical integration if the symbolic integration is unsuccessful. In the latter case, the returned value from `sympy`'s `integrate` function is an object of type `Integral`. We can test on this type and utilize the `mpmath` module in `sympy` to perform numerical integration of high precision. Here is the code:

```
def least_squares(f, psi, Omega):
    N = len(psi) - 1
    A = sm.zeros((N+1, N+1))
    b = sm.zeros((N+1, 1))
    x = sm.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            integrand = psi[i]*psi[j]
            I = sm.integrate(integrand, (x, Omega[0], Omega[1]))
            if isinstance(I, sm.Integral):
                # Could not integrate symbolically, fallback
                # on numerical integration with mpmath.quad
                integrand = sm.lambdify([x], integrand)
                I = sm.mpmath.quad(integrand, [Omega[0], Omega[1]])
            A[i,j] = A[j,i] = I
        integrand = psi[i]*f
        I = sm.integrate(integrand, (x, Omega[0], Omega[1]))
        if isinstance(I, sm.Integral):
            integrand = sm.lambdify([x], integrand)
            I = sm.mpmath.quad(integrand, [Omega[0], Omega[1]])
        b[i,0] = I
    c = A.LUsolve(b)
    u = 0
    for i in range(len(psi)):
        u += c[i,0]*psi[i]
    return u
```

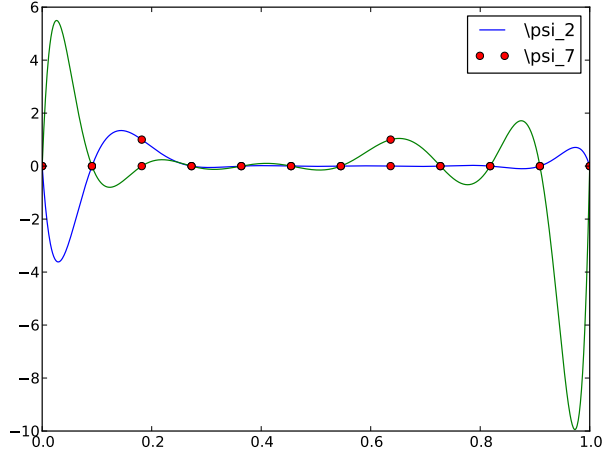


Figure 10: Illustration of the oscillatory behavior of two Lagrange polynomials based on 12 uniformly spaced points (marked by circles).

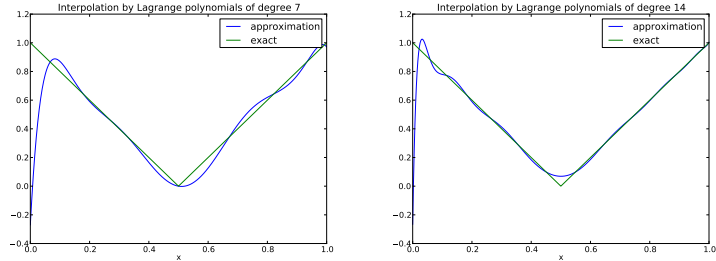


Figure 11: Interpolation of an absolute value function by Lagrange polynomials and Chebyshev nodes as interpolation points: degree 7 (left) and 14 (right).

3 Finite element basis functions

The specific basis functions exemplified in Section 2 are in general nonzero on the entire domain Ω , see Figure 12 for an example where we plot $\psi_0(x) = \sin \frac{1}{2}\pi x$ and $\psi_1(x) = \sin 2\pi x$ together with a possible sum $u(x) = 4\psi_0(x) - \frac{1}{2}\psi_1(x)$. We shall now turn the attention to basis functions that have *compact support*, meaning that they are nonzero on only a small portion of Ω . Moreover, we shall restrict the functions to be *piecewise polynomials*. This means that the domain is split into subdomains and the function is a polynomial on one or more subdomains, see Figure 13 for a sketch involving locally defined hat functions that make $u = \sum_j c_j \psi_j$ piecewise linear. At the boundaries between subdomains one normally forces continuity of the function only so that when connecting two polynomials from two subdomains, the derivative becomes discontinuous. These type of basis functions are fundamental in the finite element method.

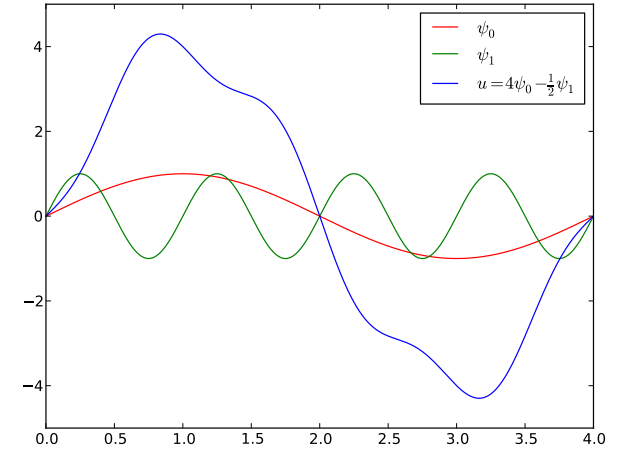


Figure 12: A function resulting from adding two sine basis functions.

We first introduce the concepts of elements and nodes in a simplistic fashion as often met in the literature. Later, we shall generalize the concept of an element, which is a necessary step to treat a wider class of approximations within the family of finite element methods. The generalization is also compatible with the concepts used in the FEniCS⁵ finite element software.

3.1 Elements and nodes

Let us divide the interval Ω on which f and u are defined into non-overlapping subintervals $\Omega^{(e)}$, $e = 0, \dots, N_e$:

⁵<http://fenicsproject.org>

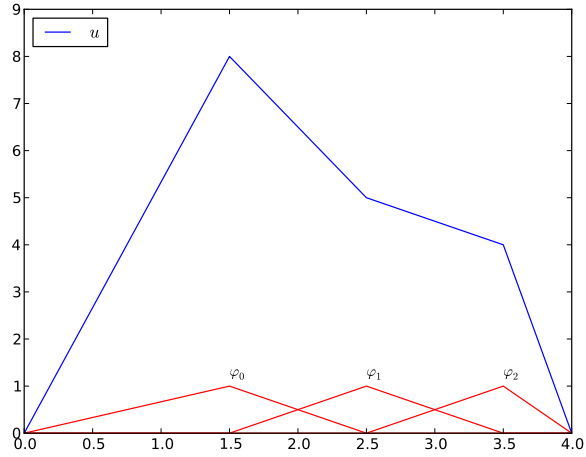


Figure 13: A function resulting from adding three local piecewise linear (hat) functions.

$$\Omega = \Omega^{(0)} \cup \dots \cup \Omega^{(N_e)}. \quad (51)$$

We shall for now refer to $\Omega^{(e)}$ as an *element*, having number e . On each element we introduce a set of points called *nodes*. For now we assume that the nodes are uniformly spaced throughout the element and that the boundary points of the elements are also nodes. The nodes are given numbers both within an element and in the global domain. These are referred to as *local* and *global* node numbers, respectively. Figure 14 shows element boundaries with small vertical lines, nodes as small disks, element numbers in circles, and global node numbers under the nodes.

Nodes and elements uniquely define a *finite element mesh*, which is our discrete representation of the domain in the computations. A common special case is that of a *uniformly partitioned mesh* where each element has the same length and the distance between nodes is constant.

Example. On $\Omega = [0, 1]$ we may introduce two elements, $\Omega^{(0)} = [0, 0.4]$ and $\Omega^{(1)} = [0.4, 1]$. Furthermore, let us introduce three nodes per element, equally spaced within each element. Figure 15 shows the mesh. The three nodes in element number 0 are $x_0 = 0$, $x_1 = 0.2$, and $x_2 = 0.4$. The local and global node numbers are here equal. In element number 1, we have the local nodes $x_0 = 0.4$, $x_1 = 0.7$, and $x_2 = 1$ and the corresponding global nodes $x_2 = 0.4$, $x_3 = 0.7$, and $x_4 = 1$. Note that the global node $x_2 = 0.4$ is shared by the two elements.

For the purpose of implementation, we introduce two lists or arrays: **nodes** for storing the coordinates of the nodes, with the global node numbers as indices, and **elements** for holding the global node numbers in each element, with the local node numbers as indices. The **nodes** and **elements** lists for the sample mesh above take the form

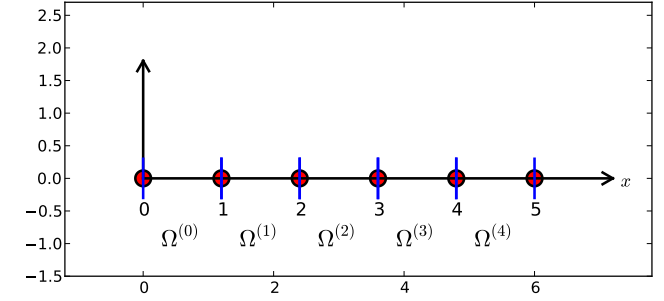


Figure 14: Finite element mesh with 5 elements and 6 nodes.

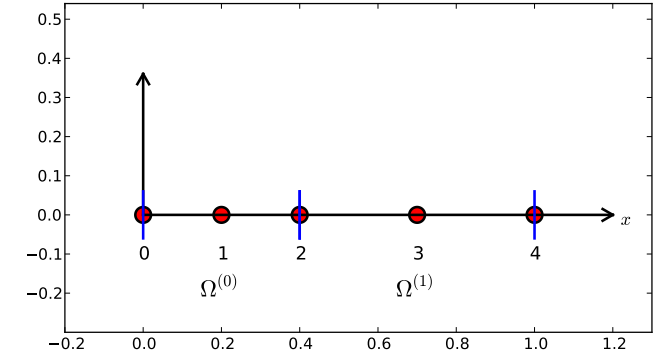


Figure 15: Finite element mesh with 2 elements and 5 nodes.

```
nodes = [0, 0.2, 0.4, 0.7, 1]
elements = [[0, 1, 2], [2, 3, 4]]
```

Looking up the coordinate of local node number 2 in element 1 is here done by `nodes[elements[1][2]]` (recall that nodes and elements start their numbering at 0).

The numbering of elements and nodes does not need to be regular. Figure 16 shows and example corresponding to

```
nodes = [1.5, 5.5, 4.2, 0.3, 2.2, 3.1]
elements = [[2, 1], [4, 5], [0, 4], [3, 0], [5, 2]]
```

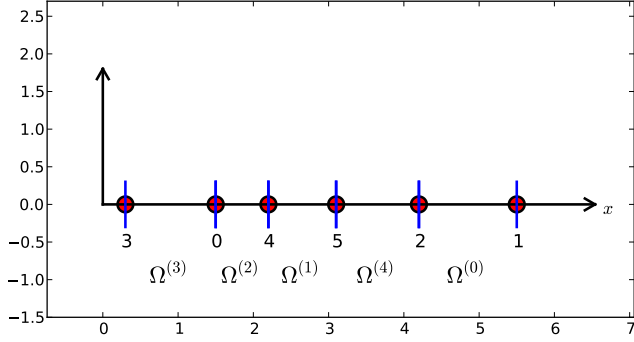


Figure 16: Example on irregular numbering of elements and nodes.

3.2 The basis functions

Construction principles. Finite element basis functions are in this text recognized by the notation $\varphi_i(x)$, where the index now in the beginning corresponds to a global node number. In the current approximation problem we shall simply take $\psi_i = \varphi_i$.

Let i be the global node number corresponding to local node r in element number e . The finite element basis functions φ_i are now defined as follows.

- If local node number r is not on the boundary of the element, take $\varphi_i(x)$ to be the Lagrange polynomial that is 1 at the local node number r and zero at all other nodes in the element. On all other elements, $\varphi_i = 0$.
- If local node number r is on the boundary of the element, let φ_i be made up of the Lagrange polynomial that is 1 at this node in element number e and its neighboring element. On all other elements, $\varphi_i = 0$.

A visual impression of three such basis functions are given in Figure 18.

Properties of φ_i . The construction of basis functions according to the principles above lead to two important properties of $\varphi_i(x)$. First,

$$\varphi_i(x_j) = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \quad (52)$$

when x_j is a node in the mesh with global node number j . This result arises because the Lagrange polynomials are constructed to have exactly this property. The property also implies a convenient interpretation of c_i as the value of u at node i . To show this, we expand u in the usual way as $\sum_j c_j \psi_j$ and choose $\psi_i = \varphi_i$:

$$u(x_i) = \sum_{j \in I} c_j \psi_j(x_i) = \sum_{j \in I} c_j \varphi_j(x_i) = c_i \varphi_i(x_i) = c_i.$$

Because of this interpretation, the coefficient c_i is by many named u_i or U_i .

Second, $\varphi_i(x)$ is mostly zero throughout the domain:

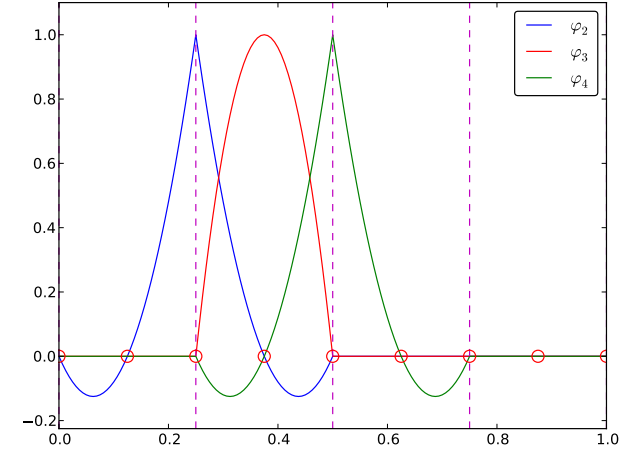


Figure 17: Illustration of the piecewise quadratic basis functions associated with nodes in element 1.

- $\varphi_i(x) \neq 0$ only on those elements that contain global node i ,
- $\varphi_i(x)\varphi_j(x) \neq 0$ if and only if i and j are global node numbers in the same element.

Since $A_{i,j}$ is the integral of $\varphi_i \varphi_j$ it means that *most of the elements in the coefficient matrix will be zero*. We will come back to these properties and use them actively in computations to save memory and CPU time.

We let each element have $d + 1$ nodes, resulting in local Lagrange polynomials of degree d . It is not a requirement to have the same d value in each element, but for now we will assume so.

3.3 Example on piecewise quadratic finite element functions

Figure 18 illustrates how piecewise quadratic basis functions can look like ($d = 2$). We work with the domain $\Omega = [0, 1]$ divided into four equal-sized elements, each having three nodes. The **nodes** and **elements** lists in this particular example become

```
nodes = [0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1.0]
elements = [[0, 1, 2], [2, 3, 4], [4, 5, 6], [6, 7, 8]]
```

Figure 19 sketches the mesh and the numbering. Nodes are marked with circles on the x axis and element boundaries are marked with vertical dashed lines in Figure 18.

Let us explain in detail how the basis functions are constructed according to the principles. Consider element number 1 in Figure 18, $\Omega^{(1)} = [0.25, 0.5]$, with local nodes 0, 1, and 2

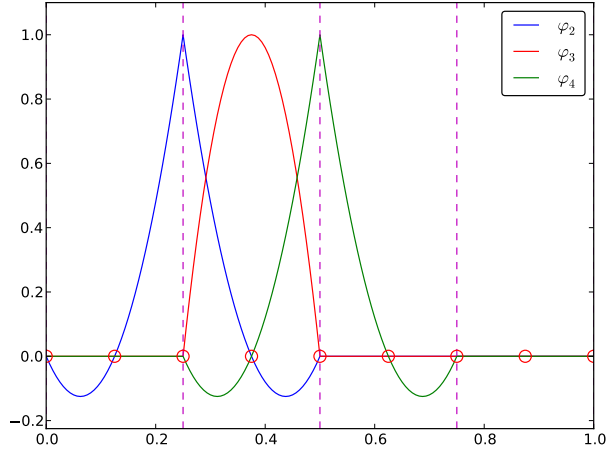


Figure 18: Illustration of the piecewise quadratic basis functions associated with nodes in element 1.

corresponding to global nodes 2, 3, and 4. The coordinates of these nodes are 0.25, 0.375, and 0.5, respectively. We define three Lagrange polynomials on this element:

1. The polynomial that is 1 at local node 1 ($x = 0.375$, global node 3) makes up the basis function $\varphi_3(x)$ over this element, with $\varphi_3(x) = 0$ outside the element.
2. The Lagrange polynomial that is 1 at local node 0 is the "right part" of the global basis function $\varphi_2(x)$. The "left part" of $\varphi_2(x)$ consists of a Lagrange polynomial associated with local node 2 in the neighboring element $\Omega^{(0)} = [0, 0.25]$.
3. Finally, the polynomial that is 1 at local node 2 (global node 4) is the "left part" of the global basis function $\varphi_4(x)$. The "right part" comes from the Lagrange polynomial that is 1 at local node 0 in the neighboring element $\Omega^{(2)} = [0.5, 0.75]$.

As mentioned earlier, any global basis function $\varphi_i(x)$ is zero on elements that do not contain the node with global node number i .

The other global functions associated with internal nodes, φ_1 , φ_5 , and φ_7 , are all of the same shape as the drawn φ_3 , while the global basis functions associated with shared nodes also have the same shape, provided the elements are of the same length.

3.4 Example on piecewise linear finite element functions

Figure 20 shows piecewise linear basis functions ($d = 1$). Also here we have four elements on $\Omega = [0, 1]$. Consider the element $\Omega^{(1)} = [0.25, 0.5]$. Now there are no internal nodes in the

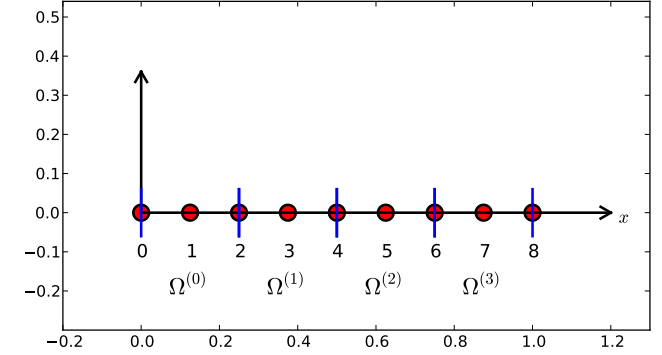


Figure 19: Sketch of mesh with 4 elements and 3 nodes per element.

elements so that all basis functions are associated with nodes at the element boundaries and hence made up of two Lagrange polynomials from neighboring elements. For example, $\varphi_1(x)$ results from the Lagrange polynomial in element 0 that is 1 at local node 1 and 0 at local node 0, combined with the Lagrange polynomial in element 1 that is 1 at local node 0 and 0 at local node 1. The other basis functions are constructed similarly.

Explicit mathematical formulas are needed for $\varphi_i(x)$ in computations. In the piecewise linear case, one can show that

$$\varphi_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ (x - x_{i-1})/(x_i - x_{i-1}), & x_{i-1} \leq x < x_i, \\ 1 - (x - x_i)/(x_{i+1} - x_i), & x_i \leq x < x_{i+1}, \\ 0, & x \geq x_{i+1}. \end{cases} \quad (53)$$

Here, x_j , $j = i - 1, i, i + 1$, denotes the coordinate of node j . For elements of equal length h the formulas can be simplified to

$$\varphi_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ (x - x_{i-1})/h, & x_{i-1} \leq x < x_i, \\ 1 - (x - x_i)/h, & x_i \leq x < x_{i+1}, \\ 0, & x \geq x_{i+1} \end{cases} \quad (54)$$

3.5 Example on piecewise cubic finite element basis functions

Piecewise cubic basis functions can be defined by introducing four nodes per element. Figure 21 shows examples on $\varphi_i(x)$, $i = 3, 4, 5, 6$, associated with element number 1. Note that φ_4 and φ_5 are nonzero on element number 1, while φ_3 and φ_6 are made up of Lagrange polynomials on two neighboring elements.

We see that all the piecewise linear basis functions have the same "hat" shape. They are naturally referred to as *hat functions*, also called *chapeau functions*. The piecewise quadratic functions in Figure 18 are seen to be of two types. "Rounded hats" associated with internal nodes in the elements and some more "sombbrero" shaped hats associated with element boundary

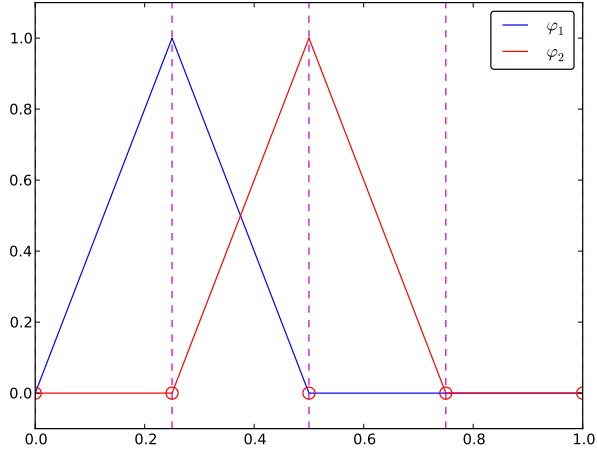


Figure 20: Illustration of the piecewise linear basis functions associated with nodes in element 1.

nodes. Higher-order basis functions also have hat-like shapes, but the functions have pronounced oscillations in addition, as illustrated in Figure 21.

A common terminology is to speak about *linear elements* as elements with two local nodes associated with piecewise linear basis functions. Similarly, *quadratic elements* and *cubic elements* refer to piecewise quadratic or cubic functions over elements with three or four local nodes, respectively. Alternative names, frequently used later, are P1 elements for linear elements, P2 for quadratic elements, and so forth: *Pd* signifies degree *d* of the polynomial basis functions.

3.6 Calculating the linear system

The elements in the coefficient matrix and right-hand side are given by the formulas (27) and (28), but now the choice of ψ_i is φ_i . Consider P1 elements where $\varphi_i(x)$ piecewise linear. Nodes and elements numbered consecutively from left to right in a uniformly partitioned mesh imply the nodes

$$x_i = ih, \quad i = 0, \dots, N,$$

and the elements

$$\Omega^{(i)} = [x_i, x_{i+1}] = [ih, (i+1)h], \quad i = 0, \dots, N_e = N-1. \quad (55)$$

We have in this case N elements and $N+1$ nodes, and $\Omega = [x_0, x_N]$. The formula for $\varphi_i(x)$ is given by (54) and a graphical illustration is provided in Figures 20 and 23. First we clearly

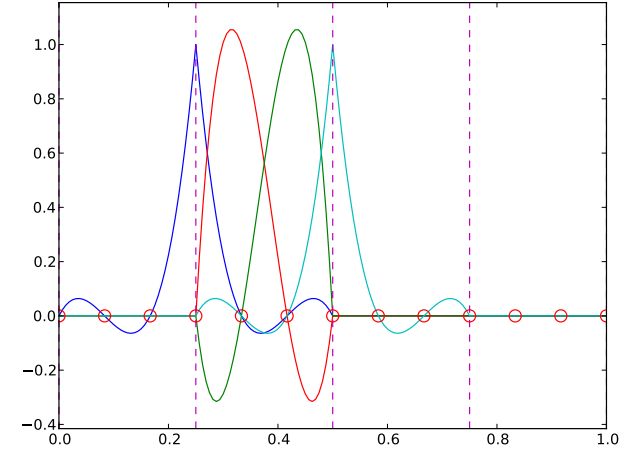


Figure 21: Illustration of the piecewise cubic basis functions associated with nodes in element 1.

see from the figures the very important property $\varphi_i(x)\varphi_j(x) \neq 0$ if and only if $j = i-1$, $j = i$, or $j = i+1$, or alternatively expressed, if and only if i and j are nodes in the same element. Otherwise, φ_i and φ_j are too distant to have an overlap and consequently their product vanishes.

Calculating a specific matrix entry. Let us calculate the specific matrix entry $A_{2,3} = \int_{\Omega} \varphi_2 \varphi_3 dx$. Figure 22 shows how φ_2 and φ_3 look like. We realize from this figure that the product $\varphi_2 \varphi_3 \neq 0$ only over element 2, which contains node 2 and 3. The particular formulas for $\varphi_2(x)$ and $\varphi_3(x)$ on $[x_2, x_3]$ are found from (54). The function φ_3 has positive slope over $[x_2, x_3]$ and corresponds to the interval $[x_{i-1}, x_i]$ in (54). With $i = 3$ we get

$$\varphi_3(x) = (x - x_2)/h,$$

while $\varphi_2(x)$ has negative slope over $[x_2, x_3]$ and corresponds to setting $i = 2$ in (54),

$$\varphi_2(x) = 1 - (x - x_2)/h.$$

We can now easily integrate,

$$A_{2,3} = \int_{\Omega} \varphi_2 \varphi_3 dx = \int_{x_2}^{x_3} \left(1 - \frac{x - x_2}{h}\right) \frac{x - x_2}{h} dx = \frac{h}{6}.$$

The diagonal entry in the coefficient matrix becomes

$$A_{2,2} = \int_{x_1}^{x_2} \left(\frac{x - x_1}{h}\right)^2 dx + \int_{x_2}^{x_3} \left(1 - \frac{x - x_2}{h}\right)^2 dx = \frac{h}{3}.$$

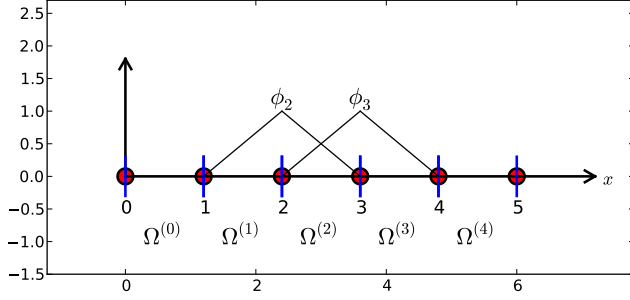


Figure 22: Illustration of the piecewise linear basis functions corresponding to global node 2 and 3.

The entry $A_{2,1}$ has the integral that is geometrically similar to the situation in Figure 22, so we get $A_{2,1} = h/6$.

Calculating a general row in the matrix. We can now generalize the calculation of matrix entries to a general row number i . The entry $A_{i,i-1} = \int_{\Omega} \varphi_i \varphi_{i-1} dx$ involves hat functions as depicted in Figure 23. Since the integral is geometrically identical to the situation with specific nodes 2 and 3, we realize that $A_{i,i-1} = A_{i,i+1} = h/6$ and $A_{i,i} = h/3$. However, we can compute the integral directly too:

$$\begin{aligned} A_{i,i-1} &= \int_{\Omega} \varphi_i \varphi_{i-1} dx = \underbrace{\int_{x_{i-2}}^{x_{i-1}} \varphi_i \varphi_{i-1} dx}_{\varphi_i=0} + \int_{x_i}^{x_{i+1}} \varphi_i \varphi_{i-1} dx + \underbrace{\int_{x_i}^{x_{i+1}} \varphi_i \varphi_{i-1} dx}_{\varphi_{i-1}=0} \\ &= \int_{x_{i-1}}^{x_i} \underbrace{\frac{x - x_i}{h}}_{\varphi_i(x)} \underbrace{\left(1 - \frac{x - x_{i-1}}{h}\right)}_{\varphi_{i-1}(x)} dx = \frac{h}{6}. \end{aligned}$$

The particular formulas for $\varphi_{i-1}(x)$ and $\varphi_i(x)$ on $[x_{i-1}, x_i]$ are found from (54): φ_i is the linear function with positive slope, corresponding to the interval $[x_{i-1}, x_i]$ in (54), while φ_{i-1} has a negative slope so the definition in interval $[x_i, x_{i+1}]$ in (54) must be used. (The appearance of i in (54) and the integral might be confusing, as we speak about two different i indices.)

The first and last row of the coefficient matrix lead to slightly different integrals:

$$A_{0,0} = \int_{\Omega} \varphi_0^2 dx = \int_{x_0}^{x_1} \left(1 - \frac{x - x_0}{h}\right)^2 dx = \frac{h}{3}.$$

Similarly, $A_{N,N}$ involves an integral over only one element and equals hence $h/3$.

The general formula for b_i , see Figure 24, is now easy to set up

$$b_i = \int_{\Omega} \varphi_i(x) f(x) dx = \int_{x_{i-1}}^{x_i} \frac{x - x_{i-1}}{h} f(x) dx + \int_{x_i}^{x_{i+1}} \left(1 - \frac{x - x_i}{h}\right) f(x) dx. \quad (56)$$

We need a specific $f(x)$ function to compute these integrals. With two equal-sized elements in $\Omega = [0, 1]$ and $f(x) = x(1 - x)$, one gets

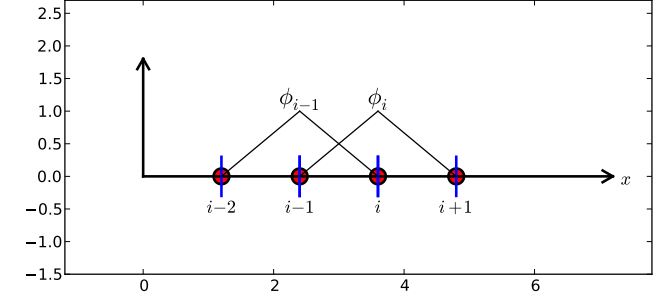


Figure 23: Illustration of two neighboring linear (hat) functions with general node numbers.

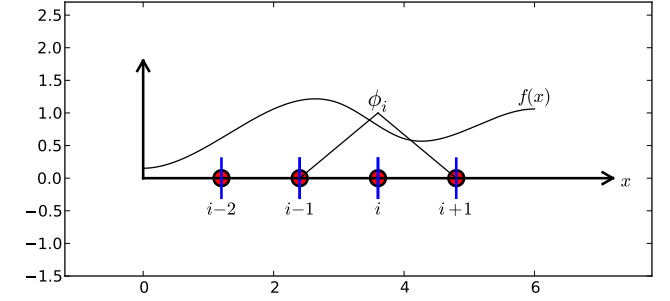


Figure 24: Right-hand side integral with the product of a basis function and the given function to approximate.

$$A = \frac{h}{6} \begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{pmatrix}, \quad b = \frac{h^2}{12} \begin{pmatrix} 2 - 3h \\ 12 - 14h \\ 10 - 17h \end{pmatrix}.$$

The solution becomes

$$c_0 = \frac{h^2}{6}, \quad c_1 = h - \frac{5}{6}h^2, \quad c_2 = 2h - \frac{23}{6}h^2.$$

The resulting function

$$u(x) = c_0 \varphi_0(x) + c_1 \varphi_1(x) + c_2 \varphi_2(x)$$

is displayed in Figure 25 (left). Doubling the number of elements to four leads to the improved approximation in the right part of Figure 25.

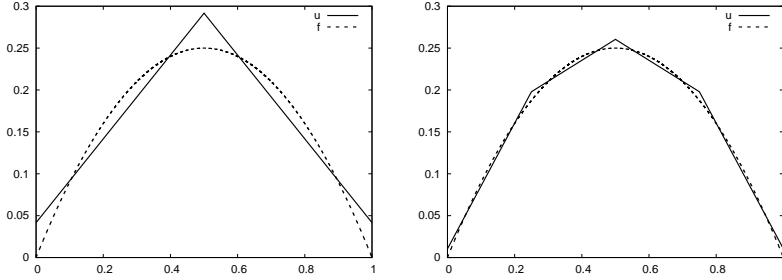


Figure 25: Least squares approximation using 2 (left) and 4 (right) P1 elements.

3.7 Assembly of elementwise computations

The integrals are naturally split into integrals over individual elements since the formulas change with the elements. This idea of splitting the integral is fundamental in all practical implementations of the finite element method.

Let us split the integral over Ω into a sum of contributions from each element:

$$A_{i,j} = \int_{\Omega} \varphi_i \varphi_j \, dx = \sum_e A_{i,j}^{(e)}, \quad A_{i,j}^{(e)} = \int_{\Omega^{(e)}} \varphi_i \varphi_j \, dx. \quad (57)$$

Now, $A_{i,j}^{(e)} \neq 0$ if and only if i and j are nodes in element e . Introduce $i = q(e, r)$ as the mapping of local node number r in element e to the global node number i . This is just a short mathematical notation for the expression `i=elements[e][r]` in a program. Let r and s be the local node numbers corresponding to the global node numbers $i = q(e, r)$ and $j = q(e, s)$. With d nodes per element, all the nonzero elements in $A_{i,j}^{(e)}$ arise from the integrals involving basis functions with indices corresponding to the global node numbers in element number e :

$$\int_{\Omega^{(e)}} \varphi_{q(e,r)} \varphi_{q(e,s)} \, dx, \quad r, s = 0, \dots, d.$$

These contributions can be collected in a $(d+1) \times (d+1)$ matrix known as the *element matrix*. We introduce the notation

$$\tilde{A}^{(e)} = \{\tilde{A}_{r,s}^{(e)}\}, \quad r, s \in I_d = \{0, 1, \dots, d\},$$

for the element matrix. For the case $d = 2$ we have

$$\tilde{A}^{(e)} = \begin{bmatrix} \tilde{A}_{0,0}^{(e)} & \tilde{A}_{0,1}^{(e)} & \tilde{A}_{0,2}^{(e)} \\ \tilde{A}_{1,0}^{(e)} & \tilde{A}_{1,1}^{(e)} & \tilde{A}_{1,2}^{(e)} \\ \tilde{A}_{2,0}^{(e)} & \tilde{A}_{2,1}^{(e)} & \tilde{A}_{2,2}^{(e)} \end{bmatrix}.$$

Given the numbers $\tilde{A}_{r,s}^{(e)}$, we should according to (57) add the contributions to the global coefficient matrix by

$$A_{q(e,r),q(e,s)} := A_{q(e,r),q(e,s)} + \tilde{A}_{r,s}^{(e)}, \quad r, s \in I_d. \quad (58)$$

This process of adding in elementwise contributions to the global matrix is called *finite element assembly* or simply *assembly*. Figure 26 illustrates how element matrices for elements with two nodes are added into the global matrix. More specifically, the figure shows how the element matrix associated with elements 2 and 3 assembled, assuming that global nodes are numbered from left to right in the domain.

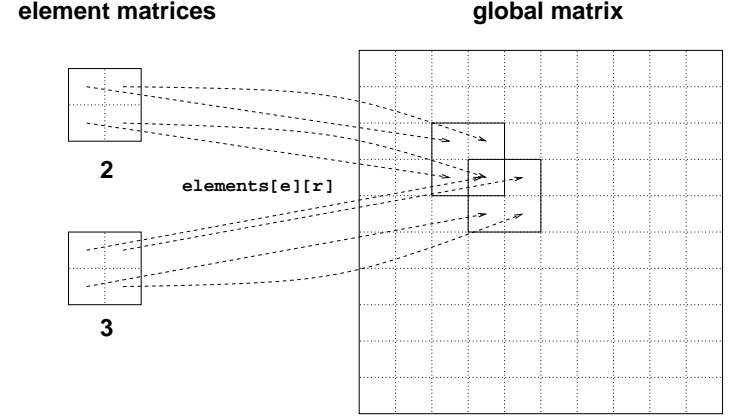


Figure 26: Illustration of matrix assembly.

The right-hand side of the linear system is also computed elementwise:

$$b_i = \int_{\Omega} \varphi_i \varphi_j \, dx = \sum_e b_i^{(e)}, \quad b_i^{(e)} = \int_{\Omega^{(e)}} f(x) \varphi_i(x) \, dx. \quad (59)$$

We observe that $b_i^{(e)} \neq 0$ if and only if global node i is a node in element e . With d nodes per element we can collect the $d+1$ nonzero contributions $b_i^{(e)}$, for $i = q(e, r)$, $r \in I_d$, in an *element vector*

$$\tilde{b}_r^{(e)} = \{b_i^{(e)}\}, \quad r \in I_d.$$

These contributions are added to the global right-hand side by an assembly process similar to that for the element matrices:

$$b_{q(e,r)} := b_{q(e,r)} + \tilde{b}_r^{(e)}, \quad r, s \in I_d. \quad (60)$$

3.8 Mapping to a reference element

Instead of computing the integrals

$$\tilde{A}_{r,s}^{(e)} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}(x) \varphi_{q(e,s)}(x) \, dx$$

over some element $\Omega^{(e)} = [x_L, x_R]$, it is convenient to map the element domain $[x_L, x_R]$ to a standardized reference element domain $[-1, 1]$. (We have now introduced x_L and x_R as the

left and right boundary points of an arbitrary element. With a natural numbering of nodes and elements from left to right through the domain, $x_L = x_e$ and $x_R = x_{e+1}$.) Let X be the coordinate in the reference element. A linear or *affine mapping* from X to x reads

$$x = \frac{1}{2}(x_L + x_R) + \frac{1}{2}(x_R - x_L)X. \quad (61)$$

This relation can alternatively be expressed by

$$x = x_m + \frac{1}{2}hX, \quad (62)$$

where we have introduced the element midpoint $x_m = (x_L + x_R)/2$ and the element length $h = x_R - x_L$.

Integrating on the reference element is a matter of just changing the integration variable from x to X . Let

$$\tilde{\varphi}_r(X) = \varphi_{q(e,r)}(x(X)) \quad (63)$$

be the basis function associated with local node number r in the reference element. The integral transformation reads

$$\tilde{A}_{r,s}^{(e)} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}(x) \varphi_{q(e,s)}(x) dx = \int_{-1}^1 \tilde{\varphi}_r(X) \tilde{\varphi}_s(X) \frac{dx}{dX} dX. \quad (64)$$

The stretch factor dx/dX between the x and X coordinates becomes the determinant of the Jacobian matrix of the mapping between the coordinate systems in 2D and 3D. To obtain a uniform notation for 1D, 2D, and 3D problems we therefore replace dx/dX by $\det J$ already now. In 1D, $\det J = dx/dX = h/2$. The integration over the reference element is then written as

$$\tilde{A}_{r,s}^{(e)} = \int_{-1}^1 \tilde{\varphi}_r(X) \tilde{\varphi}_s(X) \det J dX. \quad (65)$$

The corresponding formula for the element vector entries becomes

$$\tilde{b}_r^{(e)} = \int_{\Omega^{(e)}} f(x) \varphi_{q(e,r)}(x) dx = \int_{-1}^1 f(x(X)) \tilde{\varphi}_r(X) \det J dX. \quad (66)$$

Since we from now on will work in the reference element, we need explicit mathematical formulas for the basis functions $\varphi_i(x)$ in the reference element only, i.e., we only need to specify formulas for $\tilde{\varphi}_r(X)$. This is a very convenient simplification compared to specifying piecewise polynomials in the physical domain.

The $\tilde{\varphi}_r(x)$ functions are simply the Lagrange polynomials defined through the local nodes in the reference element. For $d = 1$ and two nodes per element, we have the linear Lagrange polynomials

$$\tilde{\varphi}_0(X) = \frac{1}{2}(1 - X) \quad (67)$$

$$\tilde{\varphi}_1(X) = \frac{1}{2}(1 + X) \quad (68)$$

Quadratic polynomials, $d = 2$, have the formulas

$$\tilde{\varphi}_0(X) = \frac{1}{2}(X - 1)X \quad (69)$$

$$\tilde{\varphi}_1(X) = 1 - X^2 \quad (70)$$

$$\tilde{\varphi}_2(X) = \frac{1}{2}(X + 1)X \quad (71)$$

In general,

$$\tilde{\varphi}_r(x) = \prod_{s=0, s \neq r}^d \frac{X - X_{(s)}}{X_{(r)} - X_{(s)}}, \quad (72)$$

where $X_{(0)}, \dots, X_{(d)}$ are the coordinates of the local nodes in the reference element. These are normally uniformly spaced: $X_{(r)} = -1 + 2r/d$, $r \in I_d$.

3.9 Integration over a reference element

To illustrate the concepts from the previous section in a specific example, we now consider calculation of the element matrix and vector for a specific choice of d and $f(x)$. A simple choice is $d = 1$ and $f(x) = x(1 - x)$ on $\Omega = [0, 1]$. We have the general expressions (65) and (66) for $\tilde{A}_{r,s}^{(e)}$ and $\tilde{b}_r^{(e)}$. Writing these out for the choices (67) and (68), and using that $\det J = h/2$, we get

$$\begin{aligned} \tilde{A}_{0,0}^{(e)} &= \int_{-1}^1 \tilde{\varphi}_0(X) \tilde{\varphi}_0(X) \frac{h}{2} dX \\ &= \int_{-1}^1 \frac{1}{2}(1 - X) \frac{1}{2}(1 - X) \frac{h}{2} dX = \frac{h}{8} \int_{-1}^1 (1 - X)^2 dX = \frac{h}{3}, \end{aligned} \quad (73)$$

$$\begin{aligned} \tilde{A}_{1,0}^{(e)} &= \int_{-1}^1 \tilde{\varphi}_1(X) \tilde{\varphi}_0(X) \frac{h}{2} dX \\ &= \int_{-1}^1 \frac{1}{2}(1 + X) \frac{1}{2}(1 - X) \frac{h}{2} dX = \frac{h}{8} \int_{-1}^1 (1 - X^2) dX = \frac{h}{6}, \end{aligned} \quad (74)$$

$$\tilde{A}_{0,1}^{(e)} = \tilde{A}_{1,0}^{(e)}, \quad (75)$$

$$\begin{aligned} \tilde{A}_{1,1}^{(e)} &= \int_{-1}^1 \tilde{\varphi}_1(X) \tilde{\varphi}_1(X) \frac{h}{2} dX \\ &= \int_{-1}^1 \frac{1}{2}(1 + X) \frac{1}{2}(1 + X) \frac{h}{2} dX = \frac{h}{8} \int_{-1}^1 (1 + X)^2 dX = \frac{h}{3}. \end{aligned} \quad (76)$$

$$\begin{aligned}
\tilde{b}_0^{(e)} &= \int_{-1}^1 f(x(X)) \tilde{\varphi}_0(X) \frac{h}{2} dX \\
&= \int_{-1}^1 (x_m + \frac{1}{2}hX)(1 - (x_m + \frac{1}{2}hX)) \frac{1}{2}(1 - X) \frac{h}{2} dX \\
&= -\frac{1}{24}h^3 + \frac{1}{6}h^2x_m - \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m
\end{aligned} \tag{77}$$

$$\begin{aligned}
\tilde{b}_1^{(e)} &= \int_{-1}^1 f(x(X)) \tilde{\varphi}_1(X) \frac{h}{2} dX \\
&= \int_{-1}^1 (x_m + \frac{1}{2}hX)(1 - (x_m + \frac{1}{2}hX)) \frac{1}{2}(1 + X) \frac{h}{2} dX \\
&= -\frac{1}{24}h^3 - \frac{1}{6}h^2x_m + \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m
\end{aligned} \tag{78}$$

In the last two expressions we have used the element midpoint x_m .

Integration of lower-degree polynomials above is tedious, and higher-degree polynomials that very much more algebra, but `sympy` may help. For example,

```
>>> import sympy as sm
>>> x, x_m, h, X = sm.symbols('x x_m h X')
>>> sm.integrate(h/8*(1-X)**2, (X, -1, 1))
h/3
>>> sm.integrate(h/8*(1+X)*(1-X), (X, -1, 1))
h/6
>>> x = x_m + h/2*X
>>> b_0 = sm.integrate(h/4*x*(1-x)*(1-X), (X, -1, 1))
>>> print b_0
-h**3/24 + h**2*x_m/6 - h**2/12 - h*x_m**2/2 + h*x_m/2
```

For inclusion of formulas in documents (like the present one), `sympy` can print expressions in \LaTeX format:

```
>>> print sm.latex(b_0, mode='plain')
- \frac{1}{24} h^3 + \frac{1}{6} h^2 x_m - \frac{1}{12} h^2 - \frac{1}{2} h x_m^2 + \frac{1}{2} h x_m
```

4 Implementation

Based on the experience from the previous example, it makes sense to write some code to automate the integration process for any choice of finite element basis functions. In addition, we can automate the assembly process and linear system solution. Appropriate functions for this purpose document all details of all steps in the finite element computations and can found in the module file `fe_approx1D.py`⁶. Some of the functions are explained below.

4.1 Integration

First we need a Python function for defining $\tilde{\varphi}_r(X)$ in terms of a Lagrange polynomial of degree d :

```
import sympy as sm
import numpy as np

def phi_r(r, X, d):
    if isinstance(X, sm.Symbol):
        h = sm.Rational(1, d) # node spacing
        nodes = [2*i*h - 1 for i in range(d+1)]
    else:
        # assume X is numeric: use floats for nodes
        nodes = np.linspace(-1, 1, d+1)
    return Lagrange_polynomial(X, r, nodes)

def Lagrange_polynomial(x, i, points):
    p = 1
    for k in range(len(points)):
        if k != i:
            p *= (x - points[k])/(points[i] - points[k])
    return p
```

Observe how we construct the `phi_r` function to be a symbolic expression for $\tilde{\varphi}_r(X)$ if X is a `Symbol` object from `sympy`. Otherwise, we assume that X is a `float` object and compute the corresponding floating-point value of $\tilde{\varphi}_r(X)$. The `Lagrange_polynomial` function, copied here from Section 2.7, works with both symbolic and numeric `x` and `points` variables.

The complete basis $\tilde{\varphi}_0(X), \dots, \tilde{\varphi}_d(X)$ on the reference element is constructed by

```
def basis(d=1):
    X = sm.Symbol('X')
    phi = [phi_r(r, X, d) for r in range(d+1)]
    return phi
```

Now we are in a position to write the function for computing the element matrix:

```
def element_matrix(phi, Omega_e, symbolic=True):
    n = len(phi)
    A_e = sm.zeros((n, n))
    X = sm.Symbol('X')
    if symbolic:
        h = sm.Symbol('h')
    else:
        h = Omega_e[1] - Omega_e[0]
    detJ = h/2 # dx/dX
    for r in range(n):
        for s in range(r, n):
            A_e[r,s] = sm.integrate(phi[r]*phi[s]*detJ, (X, -1, 1))
            A_e[s,r] = A_e[r,s]
    return A_e
```

In the symbolic case (`symbolic` is `True`), we introduce the element length as a symbol `h` in the computations. Otherwise, the real numerical value of the element interval `Omega_e` is used and the final matrix elements are numbers, not symbols. This functionality can be demonstrated:

```
>>> from fe_approx1D import *
>>> phi = basis(d=1)
>>> phi
[1/2 - X/2, 1/2 + X/2]
>>> element_matrix(phi, Omega_e=[0.1, 0.2], symbolic=True)
[h/3, h/6]
[h/6, h/3]
>>> element_matrix(phi, Omega_e=[0.1, 0.2], symbolic=False)
[0.0333333333333333, 0.0166666666666667]
[0.0166666666666667, 0.0333333333333333]
```

⁶http://tinyurl.com/jvzzcfn/fe/fe_approx1D.py

The computation of the element vector is done by a similar procedure:

```
def element_vector(f, phi, Omega_e, symbolic=True):
    n = len(phi)
    b_e = sm.zeros((n, 1))
    # Make f a function of X
    X = sm.Symbol('X')
    if symbolic:
        h = sm.Symbol('h')
    else:
        h = Omega_e[1] - Omega_e[0]
    x = (Omega_e[0] + Omega_e[1])/2 + h/2*X # mapping
    f = f.subs('x', x) # substitute mapping formula for x
    detJ = h/2 # dx/dX
    for r in range(n):
        b_e[r] = sm.integrate(f*phi[r]*detJ, (X, -1, 1))
    return b_e
```

Here we need to replace the symbol x in the expression for f by the mapping formula such that f contains the variable X .

The integration in the element matrix function involves only products of polynomials, which `sympy` can easily deal with, but for the right-hand side `sympy` may face difficulties with certain types of expressions f . The result of the integral is then an `Integral` object and not a number as when symbolic integration is successful. It may therefore be wise to introduce a fallback on numerical integration. The symbolic integration can also take much time before an unsuccessful conclusion so we may introduce a parameter `symbolic` and set it to `False` to avoid symbolic integration:

```
def element_vector(f, phi, Omega_e, symbolic=True):
    ...
    if symbolic:
        I = sm.integrate(f*phi[r]*detJ, (X, -1, 1))
    if not symbolic or isinstance(I, sm.Integral):
        h = Omega_e[1] - Omega_e[0] # Ensure h is numerical
        detJ = h/2
        integrand = sm.lambdify([X], f*phi[r]*detJ)
        I = sm.mpmath.quad(integrand, [-1, 1])
    b_e[r] = I
    ...
```

Successful numerical integration requires that the symbolic integrand is converted to a plain Python function (`integrand`) and that the element length h is a real number.

4.2 Linear system assembly and solution

The complete algorithm for computing and assembling the elementwise contributions takes the following form

```
def assemble(nodes, elements, phi, f, symbolic=True):
    N_n, N_e = len(nodes), len(elements)
    if symbolic:
        A = sm.zeros((N_n, N_n))
        b = sm.zeros((N_n, 1)) # note: (N_n, 1) matrix
    else:
        A = np.zeros((N_n, N_n))
        b = np.zeros(N_n)
    for e in range(N_e):
        Omega_e = [nodes[elements[e][0]], nodes[elements[e][-1]]]
        A_e = element_matrix(phi, Omega_e, symbolic)
```

```
b_e = element_vector(f, phi, Omega_e, symbolic)

for r in range(len(elements[e])):
    for s in range(len(elements[e])):
        A[elements[e][r], elements[e][s]] += A_e[r, s]
        b[elements[e][r]] += b_e[r]
return A, b
```

The `nodes` and `elements` variables represent the finite element mesh as explained earlier.

Given the coefficient matrix A and the right-hand side b , we can compute the coefficients $\{c_i\}_{i \in I}$ in the expansion $u(x) = \sum_j c_j \varphi_j$ as the solution vector c of the linear system:

```
if symbolic:
    c = A.LUsolve(b)
else:
    c = np.linalg.solve(A, b)
```

When A and b are `sympy` arrays, solution procedure implied by `A.LUsolve` is symbolic, otherwise, when A and b are `numpy` arrays, a standard numerical solver is called. The symbolic version is suited for small problems only (small N values) since the calculation time becomes prohibitively large otherwise. Normally, the symbolic integration will be more time consuming in small problems than the symbolic solution of the linear system.

4.3 Example on computing approximations

We can exemplify the use of `assemble` on the computational case from Section 3.6 with two P1 elements (linear basis functions) on the domain $\Omega = [0, 1]$. Let us first work with a symbolic element length:

```
>>> h, x = sm.symbols('h x')
>>> nodes = [0, h, 2*h]
>>> elements = [[0, 1], [1, 2]]
>>> phi = basis(d=1)
>>> f = x*(1-x)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=True)
>>> A
[h/3, h/6, 0]
[h/6, 2*h/3, h/6]
[ 0, h/6, h/3]
>>> b
[ h**2/6 - h**3/12]
[ h**2 - 7*h**3/6]
[5*h**2/6 - 17*h**3/12]
>>> c = A.LUsolve(b)
>>> c
[ h**2/6]
[12*(7*h**2/12 - 35*h**3/72)/(7*h)]
[ 7*(4*h**2/7 - 23*h**3/21)/(2*h)]
```

We may, for comparison, compute the c vector for an interpolation/collocation method, taking the nodes as collocation points. This is carried out by evaluating f numerically at the nodes:

```
>>> fn = sm.lambdify([x], f)
>>> c = [fn(xc) for xc in nodes]
>>> c
[0, h*(1 - h), 2*h*(1 - 2*h)]
```

The corresponding numerical computations, as done by `sympy` and still based on symbolic integration, goes as follows:

```

>>> nodes = [0, 0.5, 1]
>>> elements = [[0, 1], [1, 2]]
>>> phi = basis(d=1)
>>> x = sm.Symbol('x')
>>> f = x*(1-x)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=False)
>>> A
[ 0.166666666666667, 0.0833333333333333, 0]
[0.0833333333333333, 0.333333333333333, 0.0833333333333333]
[ 0, 0.0833333333333333, 0.166666666666667]
>>> b
[ 0.03125]
[0.104166666666667]
[ 0.03125]
>>> c = A.LUsolve(b)
>>> c
[0.0416666666666666]
[ 0.291666666666667]
[0.0416666666666666]

```

The `fe_approx1D` module contains functions for generating the `nodes` and `elements` lists for equal-sized elements with any number of nodes per element. The coordinates in `nodes` can be expressed either through the element length symbol `h` or by real numbers. There is also a function

```
def approximate(f, symbolic=False, d=1, N_e=4, filename='tmp.pdf'):
```

which computes a mesh with `N_e` elements, basis functions of degree `d`, and approximates a given symbolic expression `f` by a finite element expansion $u(x) = \sum_j c_j \varphi_j(x)$. When `symbolic` is `False`, $u(x)$ can be computed at a (large) number of points and plotted together with $f(x)$. The construction of u points from the solution vector `c` is done elementwise by evaluating $\sum_r c_r \tilde{\varphi}_r(X)$ at a (large) number of points in each element, and the discrete (x, u) values on each element are stored in arrays that are finally concatenated to form global arrays with the x and u coordinates for plotting. The details are found in the `u_glob` function in `fe_approx1D.py`.

4.4 The structure of the coefficient matrix

Let us first see how the global matrix looks like if we assemble symbolic element matrices, expressed in terms of `h`, from several elements:

```

>>> d=1; N_e=8; Omega=[0,1] # 8 linear elements on [0,1]
>>> phi = basis(d)
>>> f = x*(1-x)
>>> nodes, elements = mesh_symbolic(N_e, d, Omega)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=True)
>>> A
[h/3, h/6, 0, 0, 0, 0, 0, 0]
[h/6, 2*h/3, h/6, 0, 0, 0, 0, 0]
[ 0, h/6, 2*h/3, h/6, 0, 0, 0, 0]
[ 0, 0, h/6, 2*h/3, h/6, 0, 0, 0]
[ 0, 0, 0, h/6, 2*h/3, h/6, 0, 0]
[ 0, 0, 0, 0, h/6, 2*h/3, h/6, 0]
[ 0, 0, 0, 0, 0, h/6, 2*h/3, h/6]
[ 0, 0, 0, 0, 0, 0, h/6, 2*h/3]

```

(The reader is encouraged to assemble the element matrices by hand and verify this result, as this exercise will give a hands-on understanding of what the assembly is about.) In general we have a coefficient matrix that is tridiagonal:

$$A = \frac{h}{6} \begin{pmatrix} 2 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1 & 4 & 1 & \ddots & & & & \vdots \\ 0 & 1 & 4 & 1 & \ddots & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & 0 & 1 & 4 & 1 & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & 1 & 4 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 1 & 2 \end{pmatrix} \quad (79)$$

The structure of the right-hand side is more difficult to reveal since it involves an assembly of elementwise integrals of $f(x(X))\tilde{\varphi}_r(X)h/2$, which obviously depend on the particular choice of $f(x)$. It is easier to look at the integration in x coordinates, which gives the general formula (56). For equal-sized elements of length h , we can apply the Trapezoidal rule at the global node points to arrive at a somewhat more specific expression than (56):

$$b_i = h \left(\frac{1}{2} \varphi_i(x_0) f(x_0) + \frac{1}{2} \varphi_i(x_N) f(x_N) + \sum_{j=1}^{N-1} \varphi_i(x_j) f(x_j) \right) \quad (80)$$

$$= \begin{cases} \frac{1}{2} h f(x_i), & i = 0 \text{ or } i = N, \\ h f(x_i), & 1 \leq i \leq N-1 \end{cases} \quad (81)$$

The reason for this simple formula is simply that φ_i is either 0 or 1 at the nodes and 0 at all but one of them.

Going to P2 elements (`d=2`) leads to the element matrix

$$A^{(e)} = \frac{h}{30} \begin{pmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{pmatrix} \quad (82)$$

and the following global assembled matrix from four elements:

$$A = \frac{h}{30} \begin{pmatrix} 4 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 16 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & 8 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 16 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & 4 \end{pmatrix} \quad (83)$$

In general, for i odd we have the nonzeros

$$A_{i,i-2} = -1, \quad A_{i,i-1} = 2, \quad A_{i,i} = 8, \quad A_{i,i+1} = 2, \quad A_{i,i+2} = -1,$$

multiplied by $h/30$, and for i even we have the nonzeros

$$A_{i-1,i} = 2, \quad A_{i,i} = 16, \quad A_{i+1,i} = 2,$$

multiplied by $h/30$. The rows with odd numbers correspond to nodes at the element boundaries and get contributions from two neighboring elements in the assembly process, while the even numbered rows correspond to internal nodes in the elements where the only one element contributes to the values in the global matrix.

4.5 Applications

With the aid of the `approximate` function in the `fe_approx1D` module we can easily investigate the quality of various finite element approximations to some given functions. Figure 27 shows how linear and quadratic elements approximates the polynomial $f(x) = x(1-x)^8$ on $\Omega = [0, 1]$, using equal-sized elements. The results arise from the program

```
import sympy as sm
from fe_approx1D import approximate
x = sm.Symbol('x')

approximate(f=x*(1-x)**8, symbolic=False, d=1, N_e=4)
approximate(f=x*(1-x)**8, symbolic=False, d=2, N_e=2)
approximate(f=x*(1-x)**8, symbolic=False, d=1, N_e=8)
approximate(f=x*(1-x)**8, symbolic=False, d=2, N_e=4)
```

The quadratic functions are seen to be better than the linear ones for the same value of N , as we increase N . This observation has some generality: higher degree is not necessarily better on a coarse mesh, but it is as we refined the mesh.

4.6 Sparse matrix storage and solution

Some of the examples in the preceding section took several minutes to compute, even on small meshes consisting of up to eight elements. The main explanation for slow computations is unsuccessful symbolic integration: `sympy` may use a lot of energy on integrals like $\int f(x(X))\tilde{\varphi}_r(X)h/2dx$ before giving up, and the program resorts to numerical integration. Codes that can deal with a large number of basis functions and accept flexible choices of $f(x)$ should compute all integrals numerically and replace the matrix objects from `sympy` by the far more efficient array objects from `numpy`.

A matrix whose majority of entries are zeros, are known as a *sparse* matrix. We know beforehand that matrices from finite element approximations are sparse. The sparsity should be utilized in software as it dramatically decreases the storage demands and the CPU-time needed to compute the solution of the linear system. This optimization is not critical in 1D problems where modern computers can afford computing with all the zeros in the complete square matrix, but in 2D and especially in 3D, sparse matrices are fundamental for feasible finite element computations.

For one-dimensional finite element approximation problems, using a numbering of nodes and elements from left to right over the domain, the assembled coefficient matrix has only a few diagonals different from zero. More precisely, $2d + 1$ diagonals are different from zero. With a different numbering of global nodes, say a random ordering, the diagonal structure is lost, but the number of nonzero elements is unaltered. Figures 28 and 29 exemplifies sparsity patterns.

The `scipy.sparse` library supports creation of sparse matrices and linear system solution.

- `scipy.sparse.diags` for matrix defined via diagonals
- `scipy.sparse.lil_matrix` for creation via setting elements
- `scipy.sparse.dok_matrix` for creation via setting elements

Examples to come....

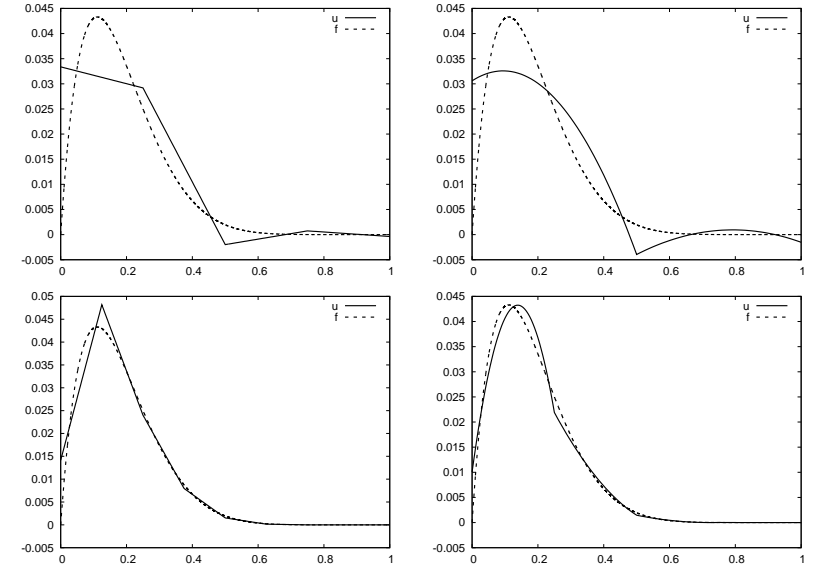


Figure 27: Comparison of the finite element approximations: 4 P1 elements with 5 nodes (upper left), 2 P2 elements with 5 nodes (upper right), 8 P1 elements with 9 nodes (lower left), and 4 P2 elements with 9 nodes (lower right).



Figure 28: Matrix sparsity pattern for left-to-right numbering (left) and random numbering (right) of nodes in P1 elements.



Figure 29: Matrix sparsity pattern for left-to-right numbering (left) and random numbering (right) of nodes in P3 elements.

5 Comparison of finite element and finite difference approximation

The previous sections on approximating f by a finite element function u utilize the projection/-Galerkin or least squares approaches to minimize the approximation error. We may, alternatively, use the collocation/interpolation method. Here we shall compare these three approaches with what one does in the finite difference method when representing a given function on a mesh.

5.1 Collocation or interpolation

Let $x_i, i \in I$, be the nodes in the mesh. Collocation means

$$u(x_i) = f(x_i), \quad i \in I. \quad (84)$$

With $u(x) \approx \sum_{j \in I} c_j \psi_j(x)$ and ψ_j chosen as φ_j , we get

$$\sum_{j \in I} c_j \varphi_j(x_i) = f(x_i),$$

but $\varphi_j(x_i) = 0$ if $i \neq j$ so the sum collapses to one term $c_i \varphi_i(x_i) = c_i$, and we have the result

$$c_i = f(x_i). \quad (85)$$

That is, u *interpolates* f at the node points (the values coincide at these points, but the variation between the points is dictated by the type of polynomials used in the expansion for u). The collocation/interpolation approach is obviously much simpler and faster to use than the least squares or projection/Galerkin approach.

Remark. When dealing with approximation of functions via finite elements, all the three methods are in use, while the least squares and collocation methods are used to only a small extent when solving differential equations.

5.2 Finite difference approximation of given functions

Approximating a given function $f(x)$ on a mesh in a finite difference context will typically just sample f at the grid points. That is, the discrete version of $f(x)$ is the set of point values $f(x_i)$, $i \in I$, where x_i denotes a mesh point. The collocation/interpolation method above gives exactly the same representation.

How does a finite element Galerkin or least squares approximation differ from this straightforward interpolation of f ? This is the question to be addressed next.

5.3 Finite difference interpretation of a finite element approximation

We now limit the scope to P1 elements since this is the element type that gives formulas closest to what one gets from the finite difference method.

The linear system arising from a Galerkin or least squares approximation reads in general

$$\sum_{j \in I} c_j (\psi_i, \psi_j) = (f, \psi_i), \quad i \in I.$$

In the finite element approximation we choose $\psi_i = \varphi_i$. With φ_i corresponding to P1 elements and a uniform mesh of element length h we have in Section 3.6 calculated the matrix with entries (φ_i, φ_j) . Equation number i reads

$$\frac{h}{6} (u_{i-1} + 4u_i + u_{i+1}) = (f, \varphi_i). \quad (86)$$

The finite difference counterpart of this equation is just $u_i = f_i$. (The first and last equation, corresponding to $i = 0$ and $i = N$ are slightly different, see Section 4.4.)

The left-hand side of (86) can be manipulated to equal

$$h(u_i - \frac{1}{6}(-u_{i-1} + 2u_i - u_{i+1})). \quad (87)$$

Thinking in terms of finite differences, we can write this expression using finite difference operator notation:

$$[h(u - \frac{h^2}{6}D_x D_x u)]_i,$$

which is nothing but the standard discretization of

$$h(u - \frac{h^2}{6}u'').$$

Before interpreting the approximation procedure as solving a differential equation, we need to work out what the right-hand side is in the context of P1 elements. Since φ_i is the linear function that is 1 at x_i and zero at all other nodes, only the interval $[x_{i-1}, x_{i+1}]$ contributes to the integral on the right-hand side. This integral is naturally split into two parts according to (54):

$$(f, \varphi_i) = \int_{x_{i-1}}^{x_i} f(x) \frac{1}{h}(x - x_{i-1})dx + \int_{x_i}^{x_{i+1}} f(x) \frac{1}{h}(1 - (x - x_i))dx.$$

However, if f is not known we cannot do much else with this expression. It is clear that many values of f around x_i contributes to the right-hand side, not just the single point value $f(x_i)$ as in the finite difference method.

To proceed with the right-hand side, we turn to numerical integration schemes. Let us say we use the Trapezoidal method for (f, φ_i) , based on the node points $x_i = ih$:

$$(f, \varphi_i) = \int_{\Omega} f \varphi_i dx \approx h \frac{1}{2}(f(x_0)\varphi_i(x_0) + f(x_N)\varphi_i(x_N)) + h \sum_{j=1}^{N-1} f(x_j)\varphi_i(x_j).$$

Since φ_i is zero at all these points, except at x_i , the Trapezoidal rule collapses to one term:

$$(f, \varphi_i) \approx hf(x_i), \quad (88)$$

for $i = 1, \dots, N-1$, which is the same result as with collocation/interpolation, and of course the same result as in the finite difference method. For $i = 0$ and $i = N$ we get contribution from only one element so

$$(f, \varphi_i) \approx \frac{1}{2}hf(x_i), \quad i = 0, i = N. \quad (89)$$

Turning to Simpson's rule with sample points also in the middle of the elements, $x_i = ih/2$, $i = 0, \dots, 2N$, it reads in general

$$\int_{\Omega} f(x)dx \approx \frac{\tilde{h}}{3} \left(f(x_0) + 2 \sum_{j=2,4,6,\dots} f(x_j) + 4 \sum_{j=1,3,5,\dots} f(x_j) + f(x_{2N}) \right),$$

where $\tilde{h} = x_i - x_{i-1} = h/2$ is the spacing between the sample points. We see that the midpoints with odd numbers have the weight $2h/3$ while the node points with even numbers have the weight

$h/3$. Since $\varphi_i = 0$ at the even numbers, except for $x_{2i} = x_i$, and $\varphi_i = 0$ at all the midpoints, on the midpoints and $4h/3$ on the node points. Since φ_i vanishes at all the node points, except ξi , and except $x_{2i-1} = \xi i - h/2$ and $x_{2i+1} = \xi i + h/2$, where $\varphi_i = 1/2$, we get

$$(f, \varphi_i) \approx \frac{h}{3}(f(x_i - \frac{1}{2}h) + f(x_i) + f(x_i + \frac{1}{2}h)). \quad (90)$$

In a finite difference context we would typically express this formula as

$$\frac{h}{3}(f_{i-\frac{1}{2}} + f_i + f_{i+\frac{1}{2}}).$$

This shows that, with Simpson's rule, the finite element method operates with the average of f over three points, while the finite difference method just applies f at one point. We may interpret this as a "smearing" or smoothing of f by the finite element method.

We can now summarize our findings. With the approximation of (f, φ_i) by the Trapezoidal rule, P1 elements give rise to equations that can be expressed as a finite difference discretization of

$$u + \frac{h^2}{6}u'' = f, \quad u'(0) = u'(L) = 0, \quad (91)$$

expressed with operator notation as

$$[u + \frac{h^2}{6}D_x D_x u = f]_i. \quad (92)$$

As $h \rightarrow 0$, the extra term proportional to u'' goes to zero, and the two methods are then equal.

With the Simpson's rule, we may say that we solve

$$[u + \frac{h^2}{6}D_x D_x u = \bar{f}]_i, \quad (93)$$

where \bar{f}_i means the average $\frac{1}{3}(f_{i-1/2} + f_i + f_{i+1/2})$.

The extra term $\frac{h^2}{6}u''$ represents a smoothing: with just this term, we would find u by integrating f twice and thereby smooth f considerably. In addition, the finite element representation of f involves an average, or a smoothing, of f on the right-hand side of the equation system. If f is a noisy function, direct interpolation $u_i = f_i$ may result in a noisy u too, but with a Galerkin or least squares formulation and P1 elements, we should expect that u is smoother than f unless h is very small.

The interpretation that finite elements tend to smooth the solution is valid in applications far beyond approximation of 1D function.

5.4 Making finite elements behave as finite differences

With a simple trick, using numerical integration, we can easily produce the same result $u_i = f_i$ with the Galerkin or least square formulation with P1 elements. This is useful in many occasions when we deal with more difficult differential equations and want the finite element method to have properties like the finite difference method (solving standard linear wave equations is one primary example).

We have already seen that applying the Trapezoidal rule to the right-hand side (f, φ_i) simply gives f sampled at x_i . Using the Trapezoidal rule on the matrix entries (φ_i, φ_j) involves a sum

$$\sum_k \varphi_i(x_k)\varphi_j(x_k),$$

but $\varphi_i(x_k) = 0$ for all k , except $k = i$, and $\varphi_j(x_k) = 0$ for all k , except $k = j$. The product $\varphi_i\varphi_j$ is then different from zero only when sampled at x_i and $i = j$. The approximation to the integral is then

$$(\varphi_i, \varphi_j) \approx h, \quad i = j,$$

and zero if $i \neq j$. This means that we have obtained a diagonal matrix! The first and last diagonal elements, (φ_0, φ_0) and (φ_N, φ_N) get contribution only from the first and last element, respectively, resulting in the approximate integral value $h/2$. The corresponding right-hand side also has a factor $1/2$ for $i = 0$ and $i = N$. Therefore, the least squares or Galerkin approach with P1 elements and *Trapezoidal* integration results in

$$c_i = f_i.$$

Simpson's rule can be used to achieve a similar result for P2 elements, i.e, a diagonal coefficient matrix, but with the previously derived average of f on the right-hand side.

Elementwise computations. Identical results to those above will arise if we perform elementwise computations. The idea is to use the Trapezoidal rule on the reference element for computing the element matrix and vector. When assembled, the same equations $c_i = f(x_i)$ arise. Exercise 16 encourages you to carry out the details.

Terminology. The matrix with entries (φ_i, φ_j) typically arises from terms proportional to u in a differential equation where u is the unknown function. This matrix is often called the *mass matrix*, because in the early days of the finite element method, the matrix arose from the mass times acceleration term in Newton's second law of motion. Making the mass matrix diagonal by, e.g., numerical integration, as demonstrated above, is a widely used technique and is called *mass lumping*. In time-dependent problems it can enhance the numerical accuracy and computational efficiency of the finite element method. However, there are also examples where mass lumping destroys accuracy.

6 A generalized element concept

So far, finite element computing has employed the **nodes** and **element** lists together with the definition of the basis functions in the reference element. Suppose we want to introduce a piecewise constant approximation with one basis function $\tilde{\varphi}_0(x) = 1$ in the reference element. Although we could associate the function value with a node in the middle of the elements, there are no nodes at the ends, and the previous code snippets will not work because we cannot find the element boundaries from the **nodes** list.

6.1 Cells, vertices, and degrees of freedom

We now introduce *cells* as the subdomains $\Omega^{(e)}$ previously referred as elements. The cell boundaries are denoted as *vertices*. The reason for this name is that cells are recognized by their vertices in 2D and 3D. Then we define a set of *degrees of freedom*, which are the quantities we aim to compute. The most common type of degree of freedom is the value of the unknown function u at some point. For example, we can introduce nodes as before and say the degrees of freedom are the values of u at the nodes. The basis functions are constructed so that they equal unity for one particular degree of freedom and zero for the rest. This property ensures that when we evaluate $u = \sum_j c_j \varphi_j$ for degree of freedom number i , we get $u = c_i$. Integrals are performed over cells, usually by mapping the cell of interest to a *reference cell*.

With the concepts of cells, vertices, and degrees of freedom we increase the decoupling the geometry (cell, vertices) from the space of basis functions. We can associate different sets of

basis functions with a cell. In 1D, all cells are intervals, while in 2D we can have cells that are triangles with straight sides, or any polygon, or in fact any two-dimensional geometry. Triangles and quadrilaterals are most common, though. The popular cell types in 3D are tetrahedra and hexahedra.

6.2 Extended finite element concept

The concept of a *finite element* is now

- a *reference cell* in a local reference coordinate system;
- a set of *basis functions* $\tilde{\varphi}_i$ defined on the cell;
- a set of *degrees of freedom* that uniquely determine the basis functions such that $\tilde{\varphi}_i = 1$ for degree of freedom number i and $\tilde{\varphi}_i = 0$ for all other degrees of freedom;
- a mapping between local and global degree of freedom numbers;
- a *mapping* of the reference cell onto to cell in the physical domain.

There must be a geometric description of a cell. This is trivial in 1D since the cell is an interval and is described by the interval limits, here called vertices. If the cell is $\Omega^{(e)} = [x_L, x_R]$, vertex 0 is x_L and vertex 1 is x_R . The reference cell in 1D is $[-1, 1]$ in the reference coordinate system X .

Our previous P1, P2, etc., elements are defined by introducing $d + 1$ equally spaced nodes in the reference cell and saying that the degrees of freedom are the $d + 1$ function values at these nodes. The basis functions must be 1 at one node and 0 at the others, and the Lagrange polynomials have exactly this property. The nodes can be numbered from left to right with associated degrees of freedom that are numbered in the same way. The degree of freedom mapping becomes what was previously represented by the **elements** lists. The cell mapping is the same affine mapping (61) as before.

The expansion of u over one cell is often used. In terms of reference coordinates we have

$$u(x) = \sum_r c_r \tilde{\varphi}_r(X), \quad (94)$$

where the sum is taken over the numbers of the degrees of freedom and c_r is the value of u for degree of freedom number r .

6.3 Implementation

Implementationwise,

- we replace **nodes** by **vertices**;
- we introduce **cells** such that **cell[e][r]** gives the mapping from local vertex **r** in cell **e** to the global vertex number in **vertices**;
- we replace **elements** by **dof_map** (the contents are the same).

Consider the example from Section 3.1 where $\Omega = [0, 1]$ is divided into two cells, $\Omega^{(0)} = [0, 0.4]$ and $\Omega^{(1)} = [0.4, 1]$. The vertices are $[0, 0.4, 1]$. Local vertex 0 and 1 are 0 and 0.4 in cell 0 and 0.4 and 1 in cell 1. A P2 element means that the degrees of freedom are the value of u at three equally spaced points (nodes) in each cell. The data structures become

```
vertices = [0, 0.4, 1]
cells = [[0, 1], [1, 2]]
dof_map = [[0, 1, 2], [1, 2, 3]]
```

If we would approximate f by piecewise constants, we simply introduce one point or node in an element, preferably $X = 0$, and choose $\tilde{\varphi}_0(X) = 1$. Only the `dof_map` is altered:

```
dof_map = [[0], [1], [2]]
```

We use the `cells` and `vertices` lists to retrieve information on the geometry of a cell, while `dof_map` is used in the assembly of element matrices and vectors. For example, the `Omega_e` variable (representing the cell interval) in previous code snippets must now be computed as

```
Omega_e = [vertices[cells[e][0], vertices[cells[e][1]]]
```

The assembly is done by

```
A[dof_map[e][r], dof_map[e][s]] += A_e[r,s]
b[dof_map[e][r]] += b_e[r]
```

We will hereafter work with `cells`, `vertices`, and `dof_map`.

6.4 Cubic Hermite polynomials

The finite elements considered so far represent u as piecewise polynomials with discontinuous derivatives at the cell boundaries. Sometimes it is desired to have continuous derivatives. A primary examples is the solution of differential equations with fourth-order derivatives where standard finite element formulations lead to a need for basis functions with continuous first-order derivatives. The most common type of such basis functions in 1D is the cubic Hermite polynomials.

There are ready-made formulas for the cubic Hermite polynomials, but it is instructive to apply the principles for constructing basis functions in detail. Given a reference cell $[-1, 1]$, we seek cubic polynomials with the values of the *function* and its *first-order derivative* at $X = -1$ and $X = 1$ as the four degrees of freedom. Let us number the degrees of freedom as

- 0: value of function at $X = -1$
- 1: value of first derivative at $X = -1$
- 2: value of function at $X = 1$
- 3: value of first derivative at $X = 1$

By having the derivatives as unknowns, we ensure that the derivative of a basis function in two neighboring elements is the same at the node points.

The four basis functions can be written in a general form

$$\tilde{\varphi}_i(X) = \sum_{j=0}^3 C_{i,j} X^j,$$

with four coefficients $C_{i,j}$, $j = 0, 1, 2, 3$, to be determined for each i . The constraints that basis function number i must be 1 for degree of freedom number i and zero for the other three degrees

of freedom, gives four equations to determine $C_{i,j}$ for each i . In mathematical detail,

$$\begin{aligned} \tilde{\varphi}_0(-1) &= 1, & \tilde{\varphi}_0(1) &= \tilde{\varphi}'_0(-1) = \tilde{\varphi}'_0(1) = 0, \\ \tilde{\varphi}'_1(-1) &= 1, & \tilde{\varphi}_1(-1) &= \tilde{\varphi}_1(1) = \tilde{\varphi}'_1(1) = 0, \\ \tilde{\varphi}_2(1) &= 1, & \tilde{\varphi}_2(-1) &= \tilde{\varphi}'_2(-1) = \tilde{\varphi}'_2(1) = 0, \\ \tilde{\varphi}'_3(1) &= 1, & \tilde{\varphi}_3(-1) &= \tilde{\varphi}'_3(-1) = \tilde{\varphi}_3(1) = 0. \end{aligned}$$

These four 4×4 linear equations can be solved, yielding these formulas for the cubic basis functions:

$$\tilde{\varphi}_0(X) = 1 - \frac{3}{4}(X+1)^2 + \frac{1}{4}(X+1)^3 \quad (95)$$

$$\tilde{\varphi}_1(X) = -(X+1)(1 - \frac{1}{2}(X+1))^2 \quad (96)$$

$$\tilde{\varphi}_2(X) = \frac{3}{4}(X+1)^2 - \frac{1}{2}(X+1)^3 \quad (97)$$

$$\tilde{\varphi}_3(X) = -\frac{1}{2}(X+1)(\frac{1}{2}(X+1)^2 - (X+1)) \quad (98)$$

$$(99)$$

Remaining tasks:

- Global numbering of the dofs
- `dof_map`
- 4×4 element matrix

7 Numerical integration

Finite element codes usually apply numerical approximations to integrals. Since the integrands in the coefficient matrix often are (lower-order) polynomials, integration rules that can integrate polynomials exactly are popular.

The numerical integration rules can be expressed in a common form,

$$\int_{-1}^1 g(X) dX \approx \sum_{j=0}^M w_j \bar{X}_j, \quad (100)$$

where \bar{X}_j are *integration points* and w_j are *integration weights*, $j = 0, \dots, M$. Different rules correspond to different choices of points and weights.

The very simplest method is the *Midpoint rule*,

$$\int_{-1}^1 g(X) dX \approx 2g(0), \quad \bar{X}_0 = 0, \quad w_0 = 2, \quad (101)$$

which integrates linear functions exactly.

7.1 Newton-Cotes rules

The *Newton-Cotes*⁷ rules are based on a fixed uniform distribution of the points. The first two formulas in this family is the well-known *Trapezoidal rule*,

$$\int_{-1}^1 g(X) dX \approx g(-1) + g(1), \quad \bar{X}_0 = -1, \bar{X}_1 = 1, w_0 = w_1 = 1, \quad (102)$$

and *Simpson's rule*,

$$\int_{-1}^1 g(X) dX \approx \frac{1}{3} (g(-1) + 4g(0) + g(1)), \quad (103)$$

where

$$\bar{X}_0 = -1, \bar{X}_1 = 0, \bar{X}_2 = 1, w_0 = w_2 = \frac{1}{3}, w_1 = \frac{4}{3}. \quad (104)$$

Newton-Cotes rules up to five points is supported in the module file `numint.py`⁸.

For higher accuracy one can divide the reference cell into a set of subintervals and use the rules above on each subinterval. This approach results in *composite* rules, well-known from basic introductions to numerical integration of $\int_a^b f(x) dx$.

7.2 Gauss-Legendre rules with optimized points

All these rules apply equally spaced points. More accurate rules, for a given M , arise if the location of the points are optimized for polynomial integrands. The *Gauss-Legendre rules*⁹ (also known as Gauss-Legendre quadrature or Gaussian quadrature) constitute one such class of integration methods. Two widely applied Gauss-Legendre rules in this family have the choice

$$M = 1: \quad \bar{X}_0 = -\frac{1}{\sqrt{3}}, \bar{X}_1 = \frac{1}{\sqrt{3}}, w_0 = w_1 = 1 \quad (105)$$

$$M = 2: \quad \bar{X}_0 = -\sqrt{\frac{3}{5}}, \bar{X}_1 = 0, \bar{X}_2 = \sqrt{\frac{3}{5}}, w_0 = w_2 = \frac{5}{9}, w_1 = \frac{8}{9}. \quad (106)$$

These rules integrate 3rd and 5th degree polynomials exactly. In general, an M -point Gauss-Legendre rule integrates a polynomial of degree $2M + 1$ exactly. The code `numint.py`¹⁰ contains a large collection of Gauss-Legendre rules.

8 Approximation of functions in 2D

All the concepts and algorithms developed for approximation of 1D functions $f(x)$ can readily be extended to 2D functions $f(x, y)$ and 3D functions $f(x, y, z)$. Basically, the extensions consists of defining basis functions $\varphi_i(x, y)$ or $\varphi_i(x, y, z)$ over some domain Ω , and for the least squares and Galerkin methods, the integration is done over Ω .

⁷http://en.wikipedia.org/wiki/Newton%E2%80%93Cotes_formulas

⁸<http://tinyurl.com/jvzzcfn/fem/numint.py>

⁹http://en.wikipedia.org/wiki/Gaussian_quadrature

¹⁰<http://tinyurl.com/jvzzcfn/fem/numint.py>

8.1 Global basis functions

An example will demonstrate the necessary extensions to use global basis functions and the least squares, Galerkin/projection, or interpolation/collocation methods in 2D. The former two lead to linear systems

$$\sum_{j \in I} A_{i,j} c_j = b_i, \quad i \in I, \\ A_{i,j} = (\varphi_i, \varphi_j), \\ b_i = (f, \varphi_i),$$

where the inner product of two functions $f(x, y)$ and $g(x, y)$ is defined completely analogously to the 1D case (24):

$$(f, g) = \int_{\Omega} f(x, y) g(x, y) dx dy \quad (107)$$

Constructing 2D basis functions from 1D functions. One straightforward way to construct a basis in 2D is to combine 1D basis functions. Say we have the 1D basis

$$\{\hat{\varphi}_0(x), \dots, \hat{\varphi}_{N_x}(x)\}.$$

We can now form 2D basis functions as products of 1D basis functions: $\hat{\varphi}_p(x) \hat{\varphi}_q(y)$ for $p \in \mathcal{I}_x = \{0, \dots, N_x\}$ and $q \in \mathcal{I}_y = \{0, \dots, N_y\}$. We can either work with double indices, $\varphi_{p,q}(x, y) = \hat{\varphi}_p(x) \hat{\varphi}_q(y)$, and write

$$u = \sum_{p \in \mathcal{I}_x} \sum_{q \in \mathcal{I}_y} c_{p,q} \varphi_{p,q}(x, y),$$

or we may transform the double index (p, q) to a single index i , using $i = pN_y + q$ or $i = qN_x + p$.

Suppose we choose $\hat{\varphi}_p(x) = x^p$, and try an approximation with $N_x = N_y = 1$:

$$\varphi_{0,0} = 1, \quad \varphi_{1,0} = x, \quad \varphi_{0,1} = y, \quad \varphi_{1,1} = xy.$$

Using a mapping to one index like $i = qN_x + p$, we get

$$\varphi_0 = 1, \quad \varphi_1 = x, \quad \varphi_2 = y, \quad \varphi_3 = xy.$$

Hand calculations. With the specific choice $f(x, y) = (1 + x^2)(1 + 2y^2)$ on $\Omega = [0, L_x] \times [0, L_y]$, we can perform actual calculations:

$$A_{0,0} = (\varphi_0, \varphi_0) = \int_0^{L_y} \int_0^{L_x} \varphi_0(x, y)^2 dx dy = \int_0^{L_y} \int_0^{L_x} dx dy = L_x L_y, \\ A_{1,0} = (\varphi_1, \varphi_0) = \int_0^{L_y} \int_0^{L_x} x dx dy = \frac{1}{2} L_x^2 L_y, \\ A_{0,1} = (\varphi_0, \varphi_1) = \int_0^{L_y} \int_0^{L_x} y dx dy = \frac{1}{2} L_y^2 L_x, \\ A_{0,1} = (\varphi_0, \varphi_1) = \int_0^{L_y} \int_0^{L_x} xy dx dy = \int_0^{L_y} y dy \int_0^{L_x} x dx = \frac{1}{4} L_y^2 L_x^2.$$

The right-hand side vector has the entries

$$\begin{aligned}
b_0 &= (\varphi_0, f) = \int_0^{L_y} \int_0^{L_x} 1 \cdot (1+x^2)(1+2y^2) dx dy \\
&= \int_0^{L_y} (1+2y^2) dy \int_0^{L_x} (1+x^2) dx = (L_y + \frac{2}{3}L_y^3)(L_x + \frac{1}{3}L_x^3) \\
b_1 &= (\varphi_1, f) = \int_0^{L_y} \int_0^{L_x} x(1+x^2)(1+2y^2) dx dy \\
&= \int_0^{L_y} (1+2y^2) dy \int_0^{L_x} x(1+x^2) dx = (L_y + \frac{2}{3}L_y^3)(\frac{1}{2}L_x^2 + \frac{1}{4}L_x^4) \\
b_2 &= (\varphi_2, f) = \int_0^{L_y} \int_0^{L_x} y(1+x^2)(1+2y^2) dx dy \\
&= \int_0^{L_y} y(1+2y^2) dy \int_0^{L_x} (1+x^2) dx = (\frac{1}{2}L_y + \frac{1}{2}L_y^4)(L_x + \frac{1}{3}L_x^3) \\
b_3 &= (\varphi_2, f) = \int_0^{L_y} \int_0^{L_x} xy(1+x^2)(1+2y^2) dx dy \\
&= \int_0^{L_y} y(1+2y^2) dy \int_0^{L_x} x(1+x^2) dx = (\frac{1}{2}L_y + \frac{1}{2}L_y^4)(\frac{1}{2}L_x^2 + \frac{1}{4}L_x^4).
\end{aligned}$$

There is a general pattern in these calculations that we can explore. An arbitrary matrix entry has the formula

$$\begin{aligned}
A_{i,j} &= (\varphi_i, \varphi_j) = \int_0^{L_y} \int_0^{L_x} \varphi_i \varphi_j dx dy \\
&= \int_0^{L_y} \int_0^{L_x} \varphi_{p,q} \varphi_{r,s} dx dy = \int_0^{L_y} \int_0^{L_x} \hat{\varphi}_p(x) \hat{\varphi}_q(y) \hat{\varphi}_r(x) \hat{\varphi}_s(y) dx dy \\
&= \int_0^{L_y} \hat{\varphi}_q(y) \hat{\varphi}_s(y) dy \int_0^{L_x} \hat{\varphi}_p(x) \hat{\varphi}_r(x) dx \\
&= \hat{A}_{p,r}^{(x)} \hat{A}_{q,s}^{(y)},
\end{aligned}$$

where

$$\hat{A}_{p,r}^{(x)} = \int_0^{L_x} \hat{\varphi}_p(x) \hat{\varphi}_r(x) dx, \quad \hat{A}_{q,s}^{(y)} = \int_0^{L_y} \hat{\varphi}_q(y) \hat{\varphi}_s(y) dy,$$

are matrix entries for one-dimensional approximations. Moreover, $i = qN_y + q$ and $j = sN_y + r$.

With $\hat{\varphi}_p(x) = x^p$ we have

$$\hat{A}_{p,r}^{(x)} = \frac{1}{p+r+1} L_x^{p+r+1}, \quad \hat{A}_{q,s}^{(y)} = \frac{1}{q+s+1} L_y^{q+s+1},$$

and

$$A_{i,j} = \hat{A}_{p,r}^{(x)} \hat{A}_{q,s}^{(y)} = \frac{1}{p+r+1} L_x^{p+r+1} \frac{1}{q+s+1} L_y^{q+s+1},$$

for $p, r \in \mathcal{I}_x$ and $q, s \in \mathcal{I}_y$.

Corresponding reasoning for the right-hand side leads to

$$\begin{aligned}
b_i &= (\varphi_i, f) = \int_0^{L_y} \int_0^{L_x} \varphi_i f dx dy \\
&= \int_0^{L_y} \int_0^{L_x} \hat{\varphi}_p(x) \hat{\varphi}_q(y) f dx dy \\
&= \int_0^{L_y} \hat{\varphi}_q(y) (1+2y^2) dy \int_0^{L_x} \hat{\varphi}_p(x) x^p (1+x^2) dx \\
&= \int_0^{L_y} y^q (1+2y^2) dy \int_0^{L_x} x^p (1+x^2) dx \\
&= (\frac{1}{q+1} L_y^{q+1} + \frac{2}{q+3} L_y^{q+3}) (\frac{1}{p+1} L_x^{p+1} + \frac{2}{q+3} L_x^{p+3})
\end{aligned}$$

Choosing $L_x = L_y = 2$, we have

$$A = \begin{bmatrix} 4 & 4 & 4 & 4 \\ 4 & \frac{16}{3} & 4 & \frac{16}{3} \\ 4 & 4 & \frac{16}{3} & \frac{16}{3} \\ 4 & \frac{16}{3} & \frac{16}{3} & \frac{64}{9} \end{bmatrix}, \quad b = \begin{bmatrix} \frac{308}{9} \\ \frac{140}{3} \\ 44 \\ 60 \end{bmatrix}, \quad c = \begin{bmatrix} -\frac{1}{9} \\ \frac{4}{3} \\ -\frac{2}{3} \\ 8 \end{bmatrix}.$$

Figure 30 illustrates the result.

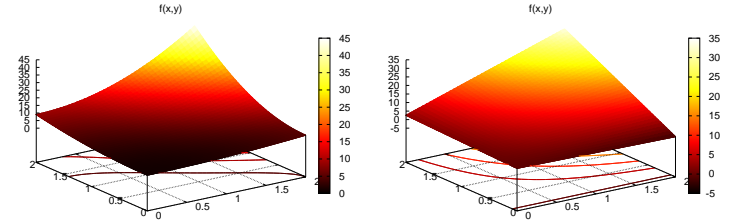


Figure 30: Approximation of a 2D quadratic function (left) by a 2D bilinear function (right) using the Galerkin or least squares method.

8.2 Implementation

The `least_squares` function from Section 2.8 and/or the file `approx1D.py`¹¹ can with very small modifications solve 2D approximation problems. First, let `Omega` now be a list of the intervals in x and y direction. For example, $\Omega = [0, L_x] \times [0, L_y]$ can be represented by `Omega = [[0, L_x], [0, L_y]]`.

Second, the symbolic integration must be extended to 2D:

```
import sympy as sm
integrand = phi[i]*phi[j]
I = sm.integrate(integrand,
    (x, Omega[0][0], Omega[0][1]),
    (y, Omega[1][0], Omega[1][1]))
```

¹¹http://tinyurl.com/jvzzcfn/fem/fe_approx1D.py

provided `integrand` is an expression involving the `sympy` symbols `x` and `y`. The 2D version of numerical integration becomes

```
if isinstance(I, sm.Integral):
    integrand = sm.lambdify([x,y], integrand)
    I = sm.mpmath.quad(integrand,
        [Omega[0][0], Omega[0][1]],
        [Omega[1][0], Omega[1][1]])
```

The right-hand side integrals are modified in a similar way.

Third, we must construct a list of 2D basis functions, e.g.,

```
def taylor(x, y, Nx, Ny):
    return [x**i*y**j for i in range(Nx+1) for j in range(Ny+1)]

def sines(x, y, Nx, Ny):
    return [sm.sin(sm.pi*(i+1)*x)*sm.sin(sm.pi*(j+1)*y)
            for i in range(Nx+1) for j in range(Ny+1)]
```

The complete code appears in `approx2D.py`¹².

The previous hand calculation where a quadratic f was approximated by a bilinear function can be computed symbolically by

```
>>> f = (1+x**2)*(1+2*y**2)
>>> phi = taylor(x, y, 1, 1)
>>> Omega = [[0, 2], [0, 2]]
>>> u = least_squares(f, phi, Omega)
>>> print u
8*x*y - 2*x/3 + 4*y/3 - 1/9
>>> print sm.expand(f)
2*x**2*y**2 + x**2 + 2*y**2 + 1
```

We may continue with adding higher powers to the basis and check that with $N_x \geq 2$ and $N_y \geq 2$ we recover the exact function f :

```
>>> phi = taylor(x, y, 2, 2)
>>> u = least_squares(f, phi, Omega)
>>> print u
2*x**2*y**2 + x**2 + 2*y**2 + 1
>>> print u-f
0
```

9 Finite elements in 2D and 3D

Finite element approximation is particularly powerful in 2D and 3D because the method can handle a geometrically complex domain Ω with ease. The principal idea is, as in 1D, to divide the domain into cells use polynomials for approximating a function over a cell. Two popular cell shapes are triangles and the quadrilaterals. Figures 31, 32, and 33 provide examples. P1 elements means linear functions ($a_0 + a_1x + a_2y$) over triangles, while Q1 elements have bilinear functions ($a_0 + a_1x + a_2y + a_3xy$) over rectangular cells. Higher-order elements can easily be defined.

9.1 Basis functions over triangles in the physical domain

Cells with triangular shape will be in main focus here. With the P1 triangular element, u is a linear function over each cell, with discontinuous derivatives at the cell boundaries, as depicted in Figure 34.

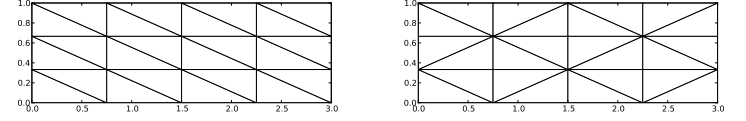


Figure 31: Examples on 2D P1 elements.

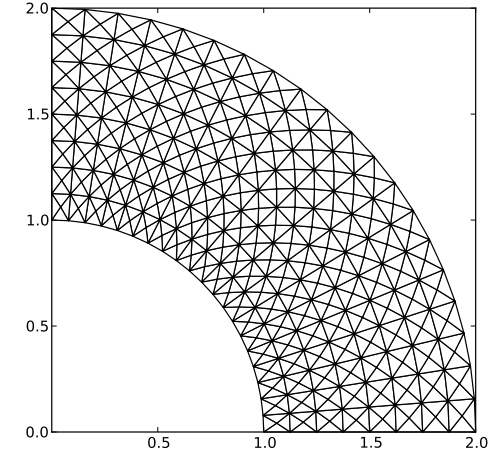


Figure 32: Examples on 2D P1 elements in a deformed geometry.

We give the vertices of the cells global and local numbers as in 1D. The degrees of freedom in the P1 element are the function values at a set of nodes, which are the three vertices. The basis function $\varphi_i(x, y)$ is then 1 at the vertex with global vertex number i and zero at all other vertices. On an element, the three degrees of freedom uniquely determine the linear basis functions in that element, as usual. The global $\varphi_i(x, y)$ function is then a combination of the linear functions (planar surfaces) over all the neighboring cells that have vertex number i in common. Figure 35 tries to illustrate the shape of such a "pyramid"-like function.

Element matrices and vectors. As in 1D, we split the integral over Ω into a sum of integrals over cells. Also as in 1D, φ_i overlaps φ_j (i.e., $\varphi_i\varphi_j \neq 0$) if and only if i and j are vertices in the same cell. Therefore, the integral of $\varphi_i\varphi_j$ over an element is nonzero only when i and j run over the vertex numbers in the element. These nonzero contributions to the coefficient matrix are, as in 1D, collected in an element matrix. The size of the element matrix becomes 3×3 since there are three degrees of freedom that i and j run over. Again, as in 1D, we number the local vertices

¹²http://tinyurl.com/jvzzcfn/fem/fe_approx2D.py

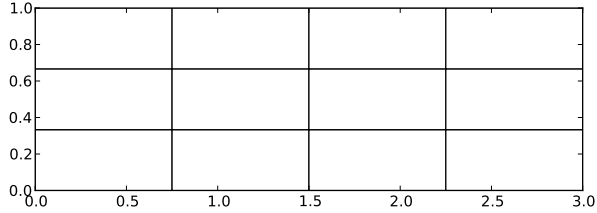


Figure 33: Examples on 2D Q1 elements.

in a cell, starting at 0, and add the entries in the element matrix into the global system matrix, exactly as in 1D. All details and code appear below.

9.2 Basis functions over triangles in the reference cell

As in 1D, we can define the basis functions and the degrees of freedom in a reference cell and then use a mapping from the reference coordinate system to the physical coordinate system. We also have a mapping of local degrees of freedom numbers to global degrees of freedom numbers.

The reference cell in an (X, Y) coordinate system has vertices $(0, 0)$, $(1, 0)$, and $(0, 1)$, corresponding to local vertex numbers 0, 1, and 2, respectively. The P1 element has linear functions $\tilde{\varphi}_r(X, Y)$ as basis functions, $r = 0, 1, 2$. Since a linear function $\tilde{\varphi}_r(X, Y)$ in 2D is on the form $C_{r,0} + C_{r,1}X + C_{r,2}Y$, and hence has three parameters $C_{r,0}$, $C_{r,1}$, and $C_{r,2}$, we need three degrees of freedom. These are in general taken as the function values at a set of nodes. For the P1 element the set of nodes is the three vertices. Figure 36 displays the geometry of the element and the location of the nodes.

Requiring $\tilde{\varphi}_r = 1$ at node number r and $\tilde{\varphi}_r = 0$ at the two other nodes, gives three linear equations to determine $C_{r,0}$, $C_{r,1}$, and $C_{r,2}$. The result is

$$\tilde{\varphi}_0(X, Y) = 1 - X - Y, \quad (108)$$

$$\tilde{\varphi}_1(X, Y) = X, \quad (109)$$

$$\tilde{\varphi}_2(X, Y) = Y \quad (110)$$

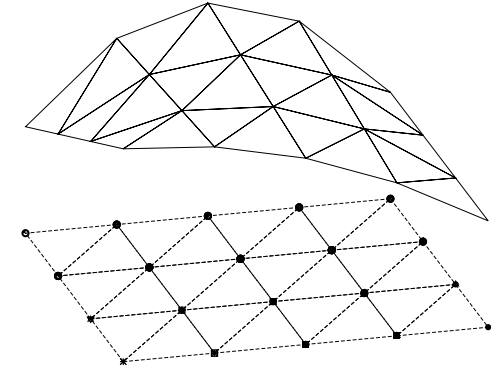


Figure 34: Example on piecewise linear 2D functions defined on triangles.

Higher-order approximations are obtained by increasing the polynomial order, adding additional nodes, and letting the degrees of freedom be function values at the nodes. Figure 37 shows the location of the six nodes in the P2 element.

A polynomial of degree p in X and Y has $n_p = (p+1)(p+2)/2$ terms and hence needs n_p nodes. The values at the nodes constitute n_p degrees of freedom. The location of the nodes for $\tilde{\varphi}_r$ up to degree 6 is displayed in Figure 38.

The generalization to 3D is straightforward: the reference element is a **tetrahedron**¹³ with vertices $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ in a X, Y, Z reference coordinate system. The P1 element has its degrees of freedom as four nodes, which are the four vertices, see Figure 39. The P2 element adds additional nodes along the edges of the cell, yielding a total of 10 nodes and degrees of freedom, see Figure 40.

The interval in 1D, the triangle in 2D, the tetrahedron in 3D, and its generalizations to higher space dimensions are known as *simplex* cells (the geometry) or *simplex* elements (the geometry, basis functions, degrees of freedom, etc.). The plural forms **simplices**¹⁴ and **simplexes** are also a much used shorter terms when referring to this type of cells or elements. The side of a simplex is called a *face*, while the tetrahedron also has *edges*.

Acknowledgment. Figures 36 to 40 are created by Anders Logg and taken from the **FEniCS book**¹⁵: *Automated Solution of Differential Equations by the Finite Element Method*, edited by A. Logg, K.-A. Mardal, and G. N. Wells, published by **Springer**¹⁶, 2012.

¹³<http://en.wikipedia.org/wiki/Tetrahedron>

¹⁴<http://en.wikipedia.org/wiki/Simplex>

¹⁵<https://launchpad.net/fenics-book>

¹⁶<http://goo.gl/lbyVMH>

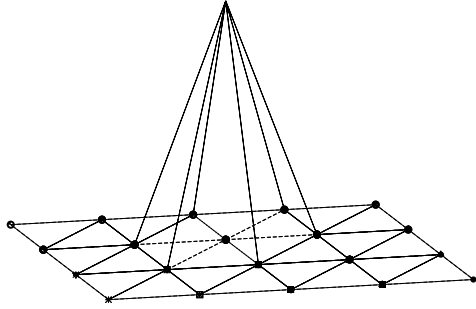


Figure 35: Example on a piecewise linear 2D basis function over a patch of triangles.

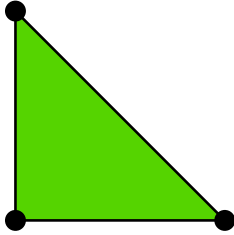


Figure 36: 2D P1 element.

9.3 Affine mapping of the reference cell

Let $\tilde{\varphi}_r^{(1)}$ denote the basis functions associated with the P1 element in 1D, 2D, or 3D, and let $\mathbf{x}_{q(e,r)}$ be the physical coordinates of local vertex number r in cell e . Furthermore, let \mathbf{X} be a point in the reference coordinate system corresponding to the point \mathbf{x} in the physical coordinate system. The affine mapping of any \mathbf{X} onto \mathbf{x} is then defined by

$$\mathbf{x} = \sum_r \tilde{\varphi}_r^{(1)}(\mathbf{X}) \mathbf{x}_{q(e,r)}, \quad (111)$$

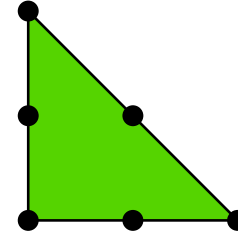


Figure 37: 2D P2 element.

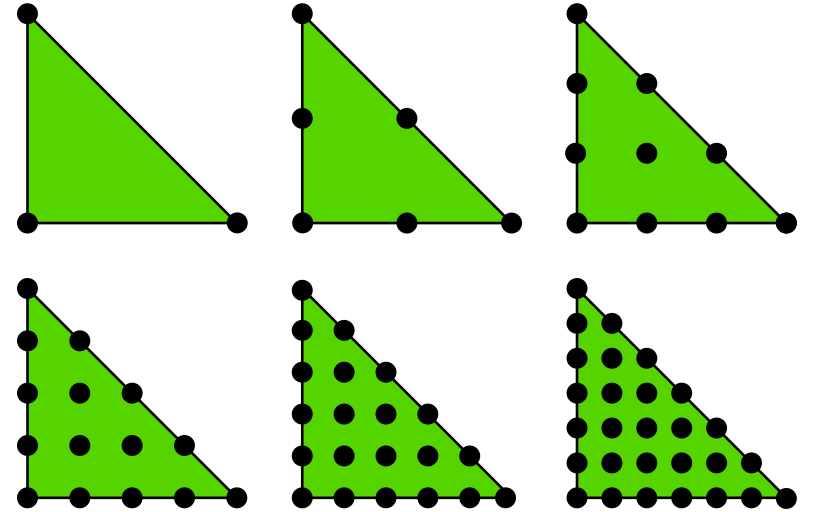


Figure 38: 2D P1, P2, P3, P4, P5, and P6 elements.

where r runs over the local vertex numbers in the cell. The affine mapping maps the straight or planar faces of the reference cell onto straight or planar faces in the physical coordinate system. The mapping can be used for both P1 and higher-order elements.

9.4 Isoparametric mapping of the reference cell

Instead of using the P1 basis functions in the mapping (111), we may use the basis functions of the actual element:

$$\mathbf{x} = \sum_r \tilde{\varphi}_r(\mathbf{X}) \mathbf{x}_{q(e,r)}, \quad (112)$$

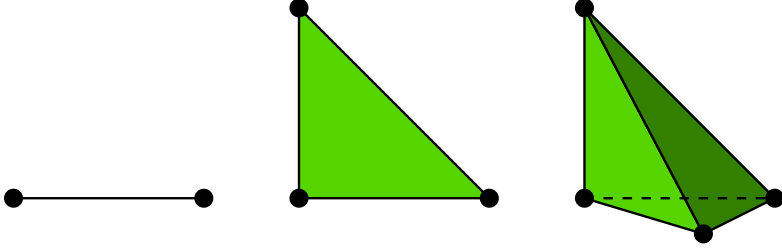


Figure 39: P1 elements in 1D, 2D, and 3D.

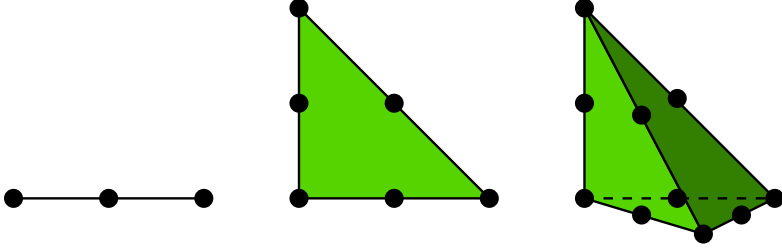


Figure 40: P2 elements in 1D, 2D, and 3D.

where r runs over all nodes, i.e., all points associated with the degrees of freedom. This is called an *isoparametric mapping*. For P1 elements it is identical to the affine mapping (111), but for higher-order elements the mapping of the straight or planar faces of the reference cell will result in a *curved* face in the physical coordinate system. For example, when we use the basis functions of the triangular P2 element in 2D in (112), the straight faces of the reference triangle are mapped onto curved faces of parabolic shape in the physical coordinate system, see Figure 42.

From (111) or (112) it is easy to realize that the vertices are correctly mapped. Consider a vertex with local number s . Then $\tilde{\varphi}_s = 1$ at this vertex and zero at the others. This means that only one term in the sum is nonzero and $\mathbf{x} = \mathbf{x}_{q(e,s)}$, which is the coordinate of this vertex in the global coordinate system.

9.5 Computing integrals

Let $\tilde{\Omega}^r$ denote the reference cell and $\Omega^{(e)}$ the cell in the physical coordinate system. The transformation of the integral from the physical to the reference coordinate system reads

$$\int_{\Omega^{(e)}} \varphi_i(\mathbf{x}) \varphi_j(\mathbf{x}) d\mathbf{x} = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\mathbf{X}) \tilde{\varphi}_j(\mathbf{X}) \det J d\mathbf{X}, \quad (113)$$

$$\int_{\Omega^{(e)}} \varphi_i(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\mathbf{X}) f(\mathbf{x}(\mathbf{X})) \det J d\mathbf{X}, \quad (114)$$

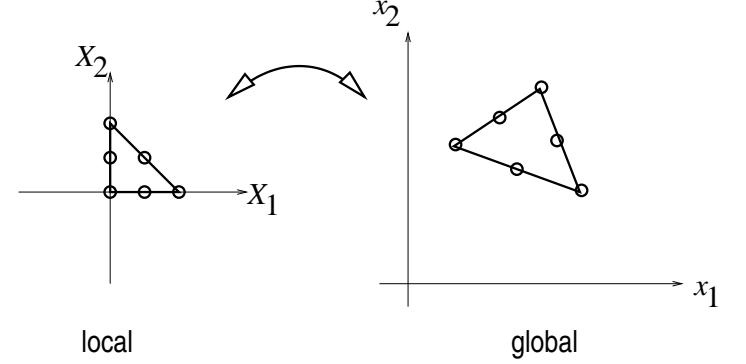


Figure 41: Affine mapping of a P1 element.

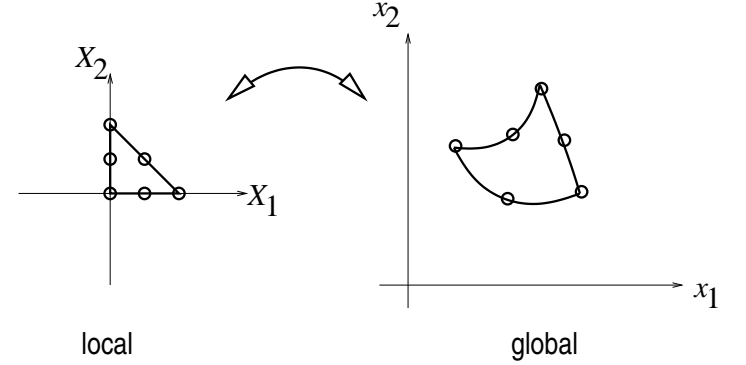


Figure 42: Isoparametric mapping of a P2 element.

where $d\mathbf{x} = dx dy$ in 2D and $d\mathbf{x} = dx dy dz$ in 3D, with a similar definition of $d\mathbf{X}$. The quantity $\det J$ is the determinant of the Jacobian of the mapping $\mathbf{x}(\mathbf{X})$. In 2D,

$$J = \begin{bmatrix} \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} \\ \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y} \end{bmatrix}, \quad \det J = \frac{\partial x}{\partial X} \frac{\partial y}{\partial Y} - \frac{\partial x}{\partial Y} \frac{\partial y}{\partial X}. \quad (115)$$

With the affine mapping (111), $\det J = 2\Delta$, where Δ is the area or volume of the cell in the physical coordinate system.

Remark. Observe that finite elements in 2D and 3D builds on the same *ideas* and *concepts* as in 1D, but there is simply more to compute because the specific mathematical formulas in 2D and 3D are more complicated.

10 Exercises

Exercise 1: Linear algebra refresher I

Look up the topic of *vector space* in your favorite linear algebra book or search for the term at Wikipedia. Prove that vectors in the plane (a, b) form a vector space by showing that all the axioms of a vector space are satisfied. Similarly, prove that all linear functions of the form $ax + b$ constitute a vector space, $a, b \in \mathbb{R}$.

On the contrary, show that all quadratic functions of the form $1 + ax^2 + bx$ do not constitute a vector space. Filename: `linalg1`.

Exercise 2: Linear algebra refresher II

As an extension of Exercise 1, check out the topic of *inner product spaces*. Suggest a possible inner product for the space of all linear functions of the form $ax + b$, $a, b \in \mathbb{R}$. Show that this inner product satisfies the general requirements of an inner product in a vector space. Filename: `linalg2`.

Exercise 3: Approximate a three-dimensional vector in a plane

Given $\mathbf{f} = (1, 1, 1)$ in \mathbb{R}^3 , find the best approximation vector \mathbf{u} in the plane spanned by the unit vectors $(1, 0)$ and $(0, 1)$. Repeat the calculations using the vectors $(2, 1)$ and $(1, 2)$. Filename: `vec111_approx`.

Exercise 4: Approximate the sine function by power functions

Let V be a function space with basis functions x^{2i+1} , $i = 0, 1, \dots, N$. Find the best approximation to $f(x) = \sin(x)$ among all functions in V , using $N = 8$ for a domain that includes more and more half-periods of the sine function: $\Omega = [0, k\pi/2]$, $k = 2, 3, \dots, 12$. How does a Taylor series of $\sin(x)$ around x up to degree 9 behave for the largest domain?

Hint. One can make a loop over k and call the `least_squares` and `comparison_plot` from the `approx1D` module.

Filename: `sin_powers.py`.

Exercise 5: Approximate a steep function by sines

Find the best approximation of $f(x) = \tanh(s(x - \pi))$ on $[0, 2\pi]$ in the space V with basis $\varphi_i(x) = \sin((2i+1)x)$, $i \in I$. Make a movie showing how $u = \sum_{j \in I} c_j \varphi_j(x)$ approximates $f(x)$ as N grows. Choose s such that f is steep ($s = 20$ may be appropriate).

Hint. One may naively call the `least_squares_orth` and `comparison_plot` from the `approx1D` module in a loop and extend the basis with one new element in each pass. This approach implies a lot of recomputations. A more efficient strategy is to let `least_squares_orth` compute with only one basis function at a time and accumulate the corresponding u in the total solution.

Filename: `tanh_sines_approx1.py`.

Exercise 6: Fourier series as a least squares approximation

Given a function $f(x)$ on an interval $[0, L]$, find the formula for the coefficients of the Fourier series of f :

$$f(x) = a_0 + \sum_{j=1}^{\infty} a_j \cos\left(j \frac{\pi x}{L}\right) + \sum_{j=1}^{\infty} b_j \sin\left(j \frac{\pi x}{L}\right).$$

Let an infinite-dimensional vector space V have the basis functions $\cos j \frac{\pi x}{L}$ for $j = 0, 1, \dots, \infty$ and $\sin j \frac{\pi x}{L}$ for $j = 1, \dots, \infty$. Show that the least squares approximation method from Section 2

leads to a linear system whose solution coincides with the standard formulas for the coefficients in a Fourier series of $f(x)$ (see also Section 2.7). You may choose

$$\varphi_{2i} = \cos\left(i \frac{\pi}{L} x\right), \quad \varphi_{2i+1} = \sin\left(i \frac{\pi}{L} x\right),$$

for $i = 0, 1, \dots, N \rightarrow \infty$.

Choose $f(x) = \tanh(s(x - \frac{1}{2}))$ on $\Omega = [0, 1]$, which is a smooth function, but with considerable steepness around $x = 1/2$ as s grows in size. Calculate the coefficients in the Fourier expansion by solving the linear system, arising from the least squares or Galerkin methods, by hand. Plot some truncated versions of the series together with $f(x)$ to show how the series expansion converges for $s = 10$ and $s = 100$. Filename: `Fourier_approx.py`.

Exercise 7: Approximate a steep function by Lagrange polynomials

Use interpolation/collocation with uniformly distributed points and Chebyshev nodes to approximate

$$f(x) = -\tanh(s(x - \frac{1}{2}))$$

by Lagrange polynomials for $s = 10, 100$ and $N = 3, 6, 9, 11$. Make separate plots of the approximation for each combination of s , point type (Chebyshev or uniform), and N . Filename: `tanh_Lagrange.py`.

Exercise 8: Define finite element meshes

Consider a domain $\Omega = [0, 2]$ divided into the three elements $[0, 1]$, $[1, 1.2]$, and $[1.2, 2]$, with two nodes in each element (P1 elements). Set up the list of coordinates and nodes (**nodes**) and the numbers of the nodes that belong to each element (**elements**) in two cases: 1) nodes and elements numbered from left to right, and 2) nodes and elements numbered from right to left.

Thereafter, subdivide the element $[1.2, 2]$ into two new equal-sized elements. Add the new node and the two new elements to the data structures created above, and try to minimize the modifications. Filename: `fe_numberings.py`.

Exercise 9: Construct matrix sparsity patterns

Exercise 8 describes a element mesh with a total of five elements, but with two different element and node orderings. For each of the two orderings, make a 5×5 matrix and fill in the entries that will be nonzero.

Hint. A matrix entry (i, j) is nonzero if i and j are nodes in the same element.

Filename: `fe_sparsity_pattern.pdf`.

Exercise 10: Perform symbolic finite element computations

Find formulas for the coefficient matrix and right-hand side when approximating $f(x) = \sin(x)$ on $\Omega = [0, \pi]$ by two P1 elements of size $\pi/2$. Solve the system and compare $u(\pi/2)$ with the exact value 1.

Filename: `sin_approx_P1.py`.

Exercise 11: Approximate a steep function by P1 and P2 elements

Given

$$f(x) = \tanh(s(x - \frac{1}{2}))$$

use the Galerkin or least squares method with finite elements to find an approximate function $u(x)$. Choose $s = 40$ and try $N_e = 4, 8, 16$ P1 elements and $N_e = 2, 4, 8$ P2 elements. Integrate $f\varphi_i$ numerically. Filename: `tanh_fe_P1P2_approx.py`.

Exercise 12: Approximate a tanh function by P3 and P4 elements

Solve Exercise 11 using $N_e = 1, 2, 4$ P3 and P4 elements. How will a collocation/interpolation method work in this case with the same number of nodes? Filename: `tanh_fe_P3P4_approx.py`.

Exercise 13: Investigate the approximation errors in finite elements

A fundamental question is how accurate the finite element approximation is in terms of the cell length h and the degree d of the basis functions. We can investigate this empirically by choosing an f function, say $f(x) = A \sin(\omega x)$ on $\Omega = [0, 2\pi/\omega]$, and compute the approximation error for a series of h and d values. The theory predicts that the error should behave as h^{d+1} . Use experiments to verify this asymptotic behavior (i.e., for small enough h). Filename: `Asinwt_interpolation_error.py`.

Exercise 14: Approximate a step function by finite elements

Approximate the step function

$$f(x) = \begin{cases} 1 & x < 1/2, \\ 2 & x \geq 1/2 \end{cases}$$

by 2, 4, and 8 P1 and P2 elements. Compare approximations visually.

Hint. This f can also be expressed in terms of the Heaviside function $H(x)$: $f(x) = H(x - 1/2)$. Therefore, f can be defined by

```
f = sm.Heaviside(x - sm.Rational(1,2))
```

making the `approximate` function in the `fe_approx1D.py` module an obvious candidate to solve the problem. However, `sympy` does not handle symbolic integration with this particular integrand, and the `approximate` function faces a problem when converting `f` to a Python function (for plotting) since `Heaviside` is not an available function in `numpy`. It is better to make special-purpose code for this case or perform all calculations by hand.

Filename: `Heaviside_approx_P1P2.py`.

Exercise 15: 2D approximation with orthogonal functions

Assume we have basis functions $\varphi_i(x, y)$ in 2D that are orthogonal such that $(\varphi_i, \varphi_j) = 0$ when $i \neq j$. The function `least_squares` in the file `approx2D.py`¹⁷ will then spend much time on computing off-diagonal terms in the coefficient matrix that we know are zero. To speed up the computations, make a version `least_squares_orth` that utilizes the orthogonality among the basis functions. Apply the function to approximate

$$f(x, y) = x(1-x)y(1-y)e^{-x-y}$$

on $\Omega = [0, 1] \times [0, 1]$ via basis functions

$$\varphi_i(x, y) = \sin(p\pi x) \sin(q\pi y), \quad i = qN_x + p.$$

Hint. Get ideas from the function `least_squares_orth` in Section 2.8 and file `approx1D.py`¹⁸. Filename: `approx2D_lsorth_sin.py`.

¹⁷http://tinyurl.com/jvzzcfn/fem/fe_approx2D.py

¹⁸http://tinyurl.com/jvzzcfn/fem/fe_approx1D.py

Exercise 16: Use the Trapezoidal rule and P1 elements

Consider approximation of some $f(x)$ on an interval Ω using the least squares or Galerkin methods with P1 elements. Derive the element matrix and vector using the Trapezoidal rule (102) for calculating integrals on the reference element. Assemble the contributions, assuming a uniform cell partitioning, and show that the resulting linear system has the form $c_i = f(x_i)$ for $i \in I$. Filename: `fe_trapez.pdf`.

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