Study Guide: Introduction to Finite Element Methods

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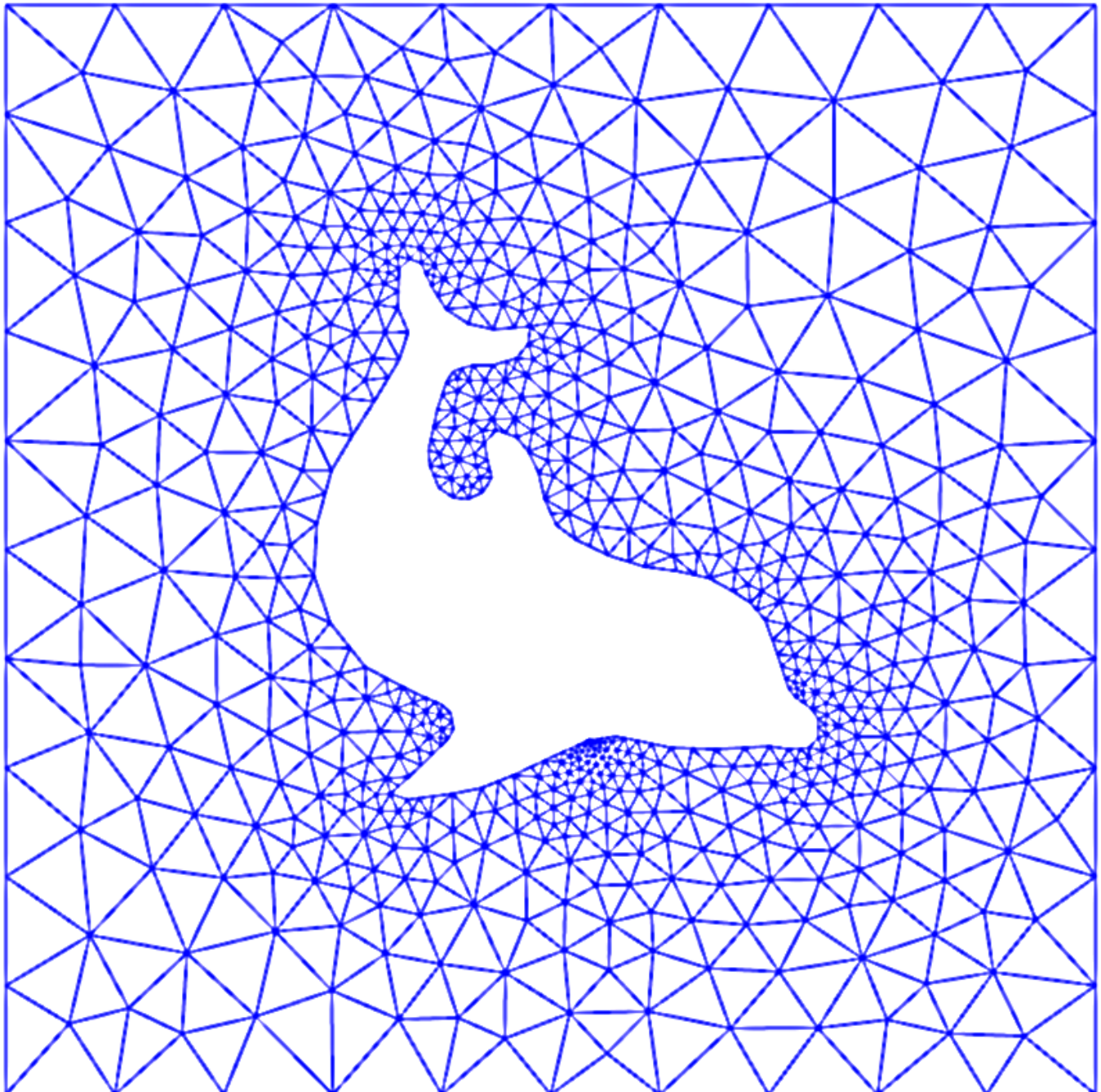
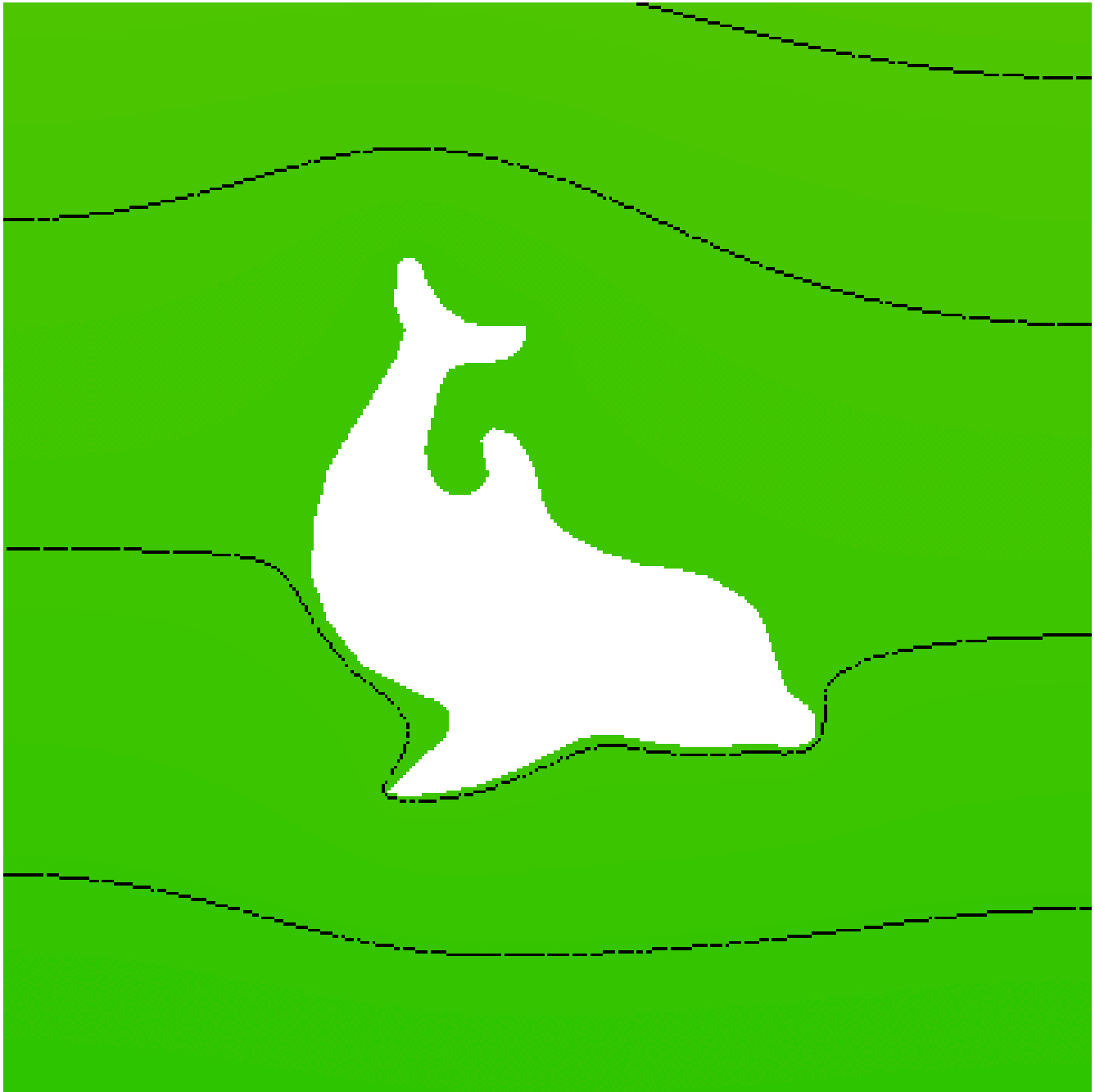
Why finite elements?

- Can with ease solve PDEs in domains with *complex geometry*
- Can with ease provide higher-order approximations
- Has (in simpler stationary problems) a rigorus mathematical analysis framework (not much considered here)

Domain for flow around a dolphin



The flow



Basic ingredients of the finite element method

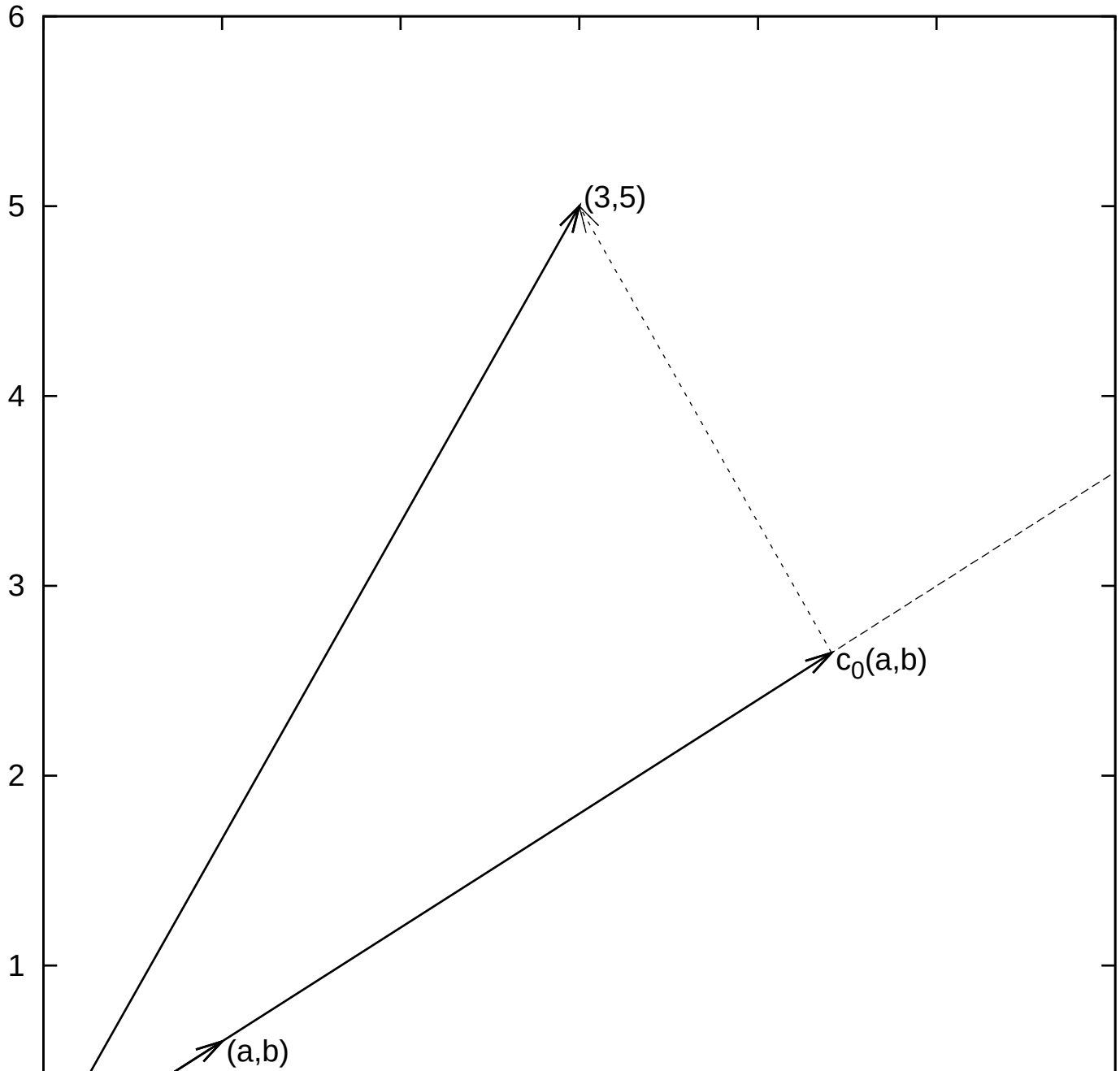
- Transform the PDE problem to a *variational form*
- Define function approximation over *finite elements*
- Use a machinery to derive *linear systems*
- Solve linear systems

Our learning strategy

- Start with approximation of functions, not PDEs
- Introduce finite element *approximations*
- See later how this is applied to PDEs

Reason: the finite element method has many concepts and a jungle of details. This strategy minimizes the mixing of ideas, concepts, and technical details.

Approximation in vector spaces



Approximation set-up

General idea of finding an approximation $u(x)$ to some given $f(x)$:

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

where

- $\psi_i(x)$ are prescribed functions
- c_i, $i = 0, \ldots, N$ are unknown coefficients to be determined

How to determine the coefficients?

We shall address three approaches:

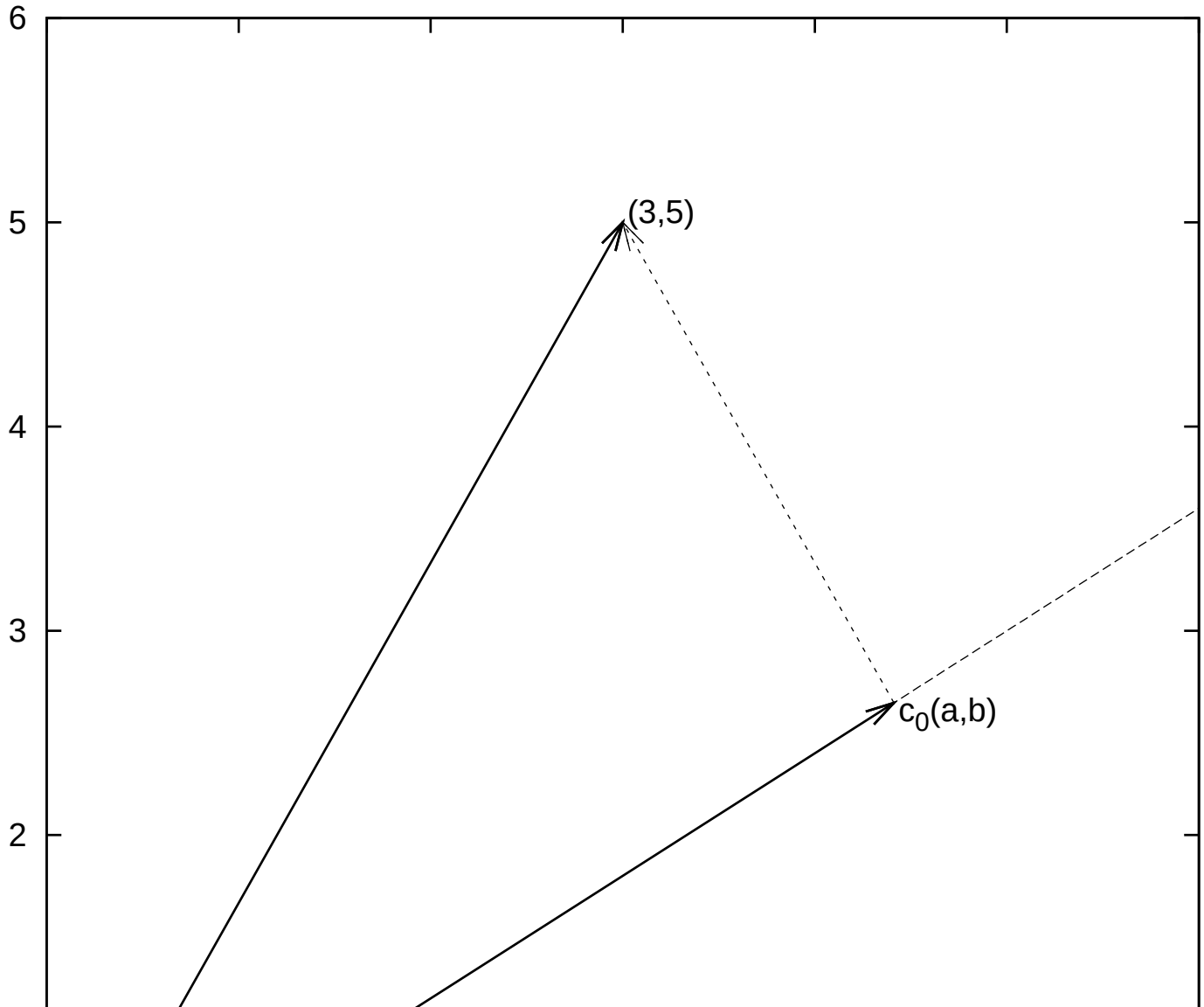
- The least squares method
- The projection (or Galerkin) method
- The interpolation (or collocation) method

Underlying motivation for our notation.

Our mathematical framework for doing this is phrased in a way such that it becomes easy to understand and use the FEniCS software package for finite element computing.

Approximation of planar vectors; problem

Given a vector $\mathbf{f} = (3, 5)$, find an approximation to $\mathbf{f}$ directed along a given line.



Approximation of planar vectors; vector space terminology

$$V = \text{span}\,\{\psi_0\} \tag{2}$$

- ψ_0 is a basis vector in the space V
- Seek $\mathbf{u} = c_0\psi_0 \in V$
- Determine c_0 such that $\mathbf{u}$ is the "best" approximation to $\mathbf{f}$
- Visually, "best" is obvious

Define

- the error $\mathbf{e} = \mathbf{f} - \mathbf{u}$
- the (Eucledian) scalar product of two vectors: $(\mathbf{u}, \mathbf{v})$
- the norm of $\mathbf{e}$: $||\mathbf{e}|| = \sqrt{(\mathbf{e}, \mathbf{e})}$

The least squares method; principle

- Idea: find c_0 such that $||\mathbf{e}||$ is minimized
- Actually, we always minimize $E = ||\mathbf{e}||^2$

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

The least squares method; calculations

$$E(c_0) = (\mathbf{e}, \mathbf{e}) = (\mathbf{f}, \mathbf{f}) - 2c_0(\mathbf{f}, \psi_0) + c_0^2(\psi_0, \psi_0) \tag{3}$$

$$\frac{\partial E}{\partial c_0} = -2(\mathbf{f}, \psi_0) + 2c_0(\psi_0, \psi_0) = 0 \tag{4}$$

$$c_0 = \frac{(\mathbf{f}, \psi_0)}{(\psi_0, \psi_0)} \tag{5}$$

$$c_0 = \frac{3a + 5b}{a^2 + b^2} \tag{6}$$

Observation for later: the vanishing derivative (4) can be alternatively written as

$$(\mathbf{e}, \psi_0) = 0 \tag{7}$$

The projection (or Galerkin) method

- Backgrund: minimizing $||\mathbf{e}||^2$ implies that $\mathbf{e}$ is orthogonal to *any* vector $\mathbf{v}$ in the space V (visually clear, but can easily be computed too)
- Alternative idea: demand $(\mathbf{e}, \mathbf{v}) = 0, \quad \forall \mathbf{v} \in V$
- Equivalent statement: $(\mathbf{e}, \psi_0) = 0$ (see notes for why)
- Insert $\mathbf{e} = \mathbf{f} - c_0\psi_0$ and solve for c_0
- Same equation for c_0 and hence same solution as in the least squares method

Approximation of general vectors

Given a vector $\mathbf{f}$, find an approximation $\mathbf{u} \in V$:

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

- We have a set of linearly independent basis vectors $\psi_0, \ldots, \psi_N$
- Any $\mathbf{u} \in V$ can then be written as $\mathbf{u} = \sum_{j=0}^{N} c_j \psi_j$

The least squares method

Idea: find $c_0, \ldots, c_N$ such that $E = ||\mathbf{e}||^2$ is minimized, $\mathbf{e} = \mathbf{f} - \mathbf{u}$.

$$E(c_0, \ldots, c_N) = (\mathbf{e}, \mathbf{e}) = (\mathbf{f} - \sum_j c_j \psi_j, \mathbf{f} - \sum_j c_j \psi_j)$$

$$= (\mathbf{f}, \mathbf{f}) - 2\sum_{j=0}^{N} c_j(\mathbf{f}, \psi_j) + \sum_{p=0}^{N}\sum_{q=0}^{N} c_p c_q (\psi_p, \psi_q)$$

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

After some work we end up with a *linear system*

$$\sum_{j=0}^{N} A_{i,j} c_j = b_i, \quad i = 0, \ldots, N \tag{8}$$

$$A_{i,j} = (\psi_i, \psi_j) \tag{9}$$

$$b_i = (\psi_i, \mathbf{f}) \tag{10}$$

The projection (or Galerkin) method

Can be shown that minimizing $||\mathbf{e}||$ implies that $\mathbf{e}$ is orthogonal to all $\mathbf{v} \in V$:

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

which implies that $\mathbf{e}$ most be orthogonal to each basis vector:

$$(\mathbf{e}, \psi_i) = 0, \quad i = 0, \ldots, N \tag{11}$$

This orthogonality condition is the principle of the projection (or Galerkin) method. Leads to the same linear system as in the least squares method.

Approximation of functions

Let V be a *function space* spanned by a set of *basis functions* $\psi_0, \ldots, \psi_N$,

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

Find $u \in V$ as a linear combination of the basis functions:

$$u = \sum_{j \in I} c_j \psi_j, \quad I = \{0, 1, \ldots, N\} \tag{12}$$

The least squares method

- Extend the ideas from the vector case: minimize the (square) norm of the error.
- What norm? $(f, g) = \int_\Omega f(x)g(x)\,dx$

$$E = (e, e) = (f - u, f - u) = (f(x) - \sum_{j \in I} c_j \psi_j(x), f(x) - \sum_{j \in I} c_j \psi_j(x)) \tag{13}$$

$$E(c_0, \ldots, c_N) = (f, f) - 2\sum_{j \in I} c_j (f, \psi_i) + \sum_{p \in I} \sum_{q \in I} c_p c_q (\psi_p, \psi_q) \tag{14}$$

$$\frac{\partial E}{\partial c_i} = 0, \quad i =\in I$$

After computations *identical to the vector case*, we get a linear system

$$\sum_{j \in I}^{N} A_{i,j} c_j = b_i, \quad i \in I \tag{15}$$

The projection (or Galerkin) method

As before, minimizing (e, e) is equivalent to the projection (or Galerkin) method

$$(e, v) = 0, \quad \forall v \in V \tag{18}$$

which means, as before,

$$(e, \psi_i) = 0, \quad i \in I \tag{19}$$

With the same algebra as in the multi-dimensional vector case, we get the same linear system as arose from the least squares method.

Example: linear approximation; problem

Problem.

Approximate a parabola $f(x) = 10(x-1)^2 - 1$ by a straight line.

$$V = \operatorname{span}\{1, x\}$$

That is, $\psi_0(x) = 1$, $\psi_1(x) = x$, and $N = 1$. We seek

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

Example: linear approximation; solution

$$A_{0,0} = (\psi_0, \psi_0) = \int_1^2 1 \cdot 1 \, dx = 1 \tag{20}$$

$$A_{0,1} = (\psi_0, \psi_1) = \int_1^2 1 \cdot x \, dx = 3/2 \tag{21}$$

$$A_{1,0} = A_{0,1} = 3/2 \tag{22}$$

$$A_{1,1} = (\psi_1, \psi_1) = \int_1^2 x \cdot x \, dx = 7/3 \tag{23}$$

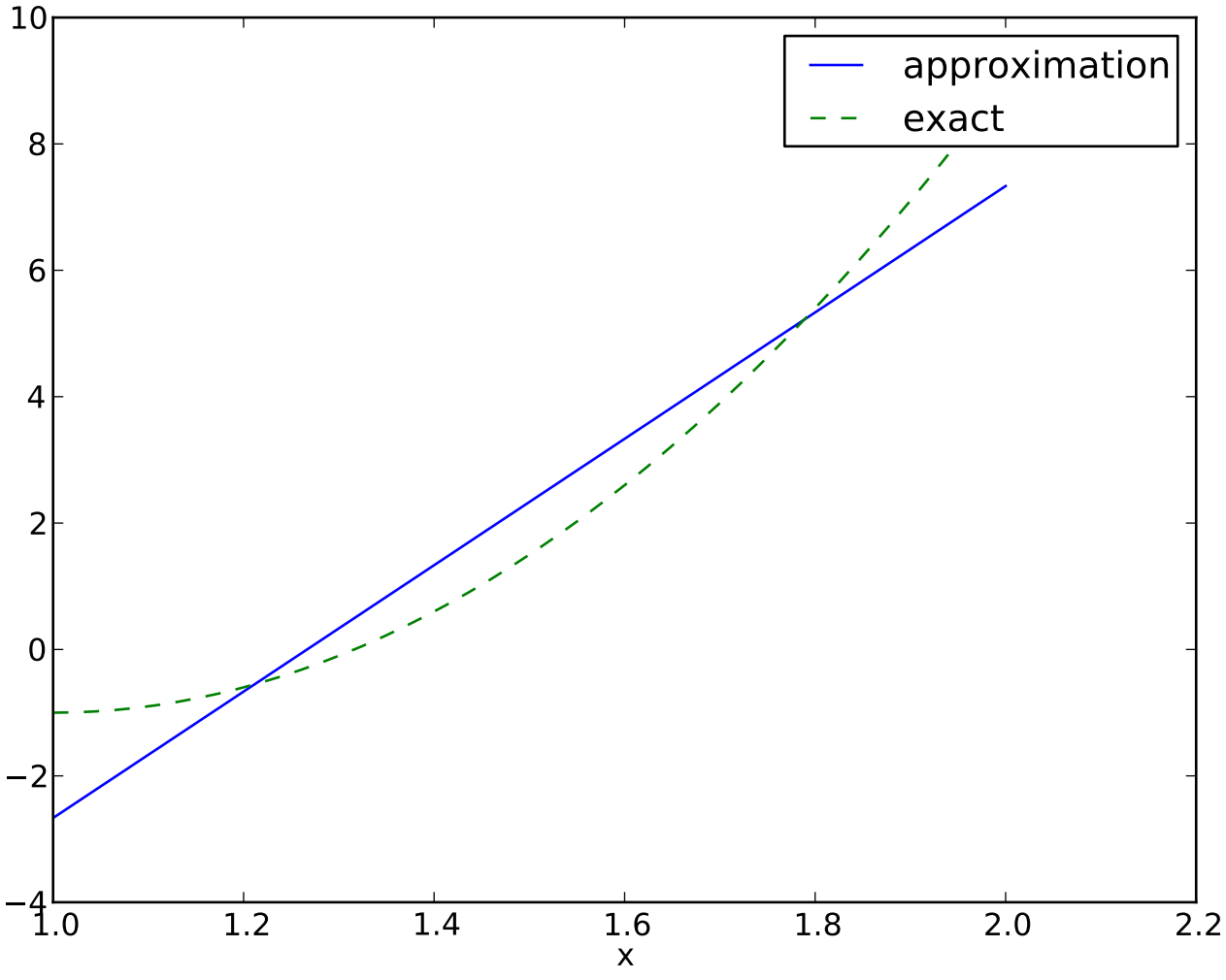
$$b_1 = (f, \psi_0) = \int_1^2 (10(x-1)^2 - 1) \cdot 1 \, dx = 7/3 \tag{24}$$

$$b_2 = (f, \psi_1) = \int_1^2 (10(x-1)^2 - 1) \cdot x \, dx = 13/3 \tag{25}$$

Solution of 2x2 linear system:

$$c_0 = -38/3, \quad c_1 = 10, \quad u(x) = 10x - \frac{38}{3} \tag{26}$$

Example: linear approximation; plot



Implementation of the least squares method; ideas

Consider 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 $\{\psi_i\}_{i \in I}$,
- `Omega` is a 2-tuple/list holding the domain Ω

Carry out the integrations, solve the linear system, and return $u(x) = \sum_j c_j \psi_j(x)$

Implementation of the least squares method; code

```
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: symmetric coefficient matrix so we can halve the integrations.

Implementation of the least squares method; plotting

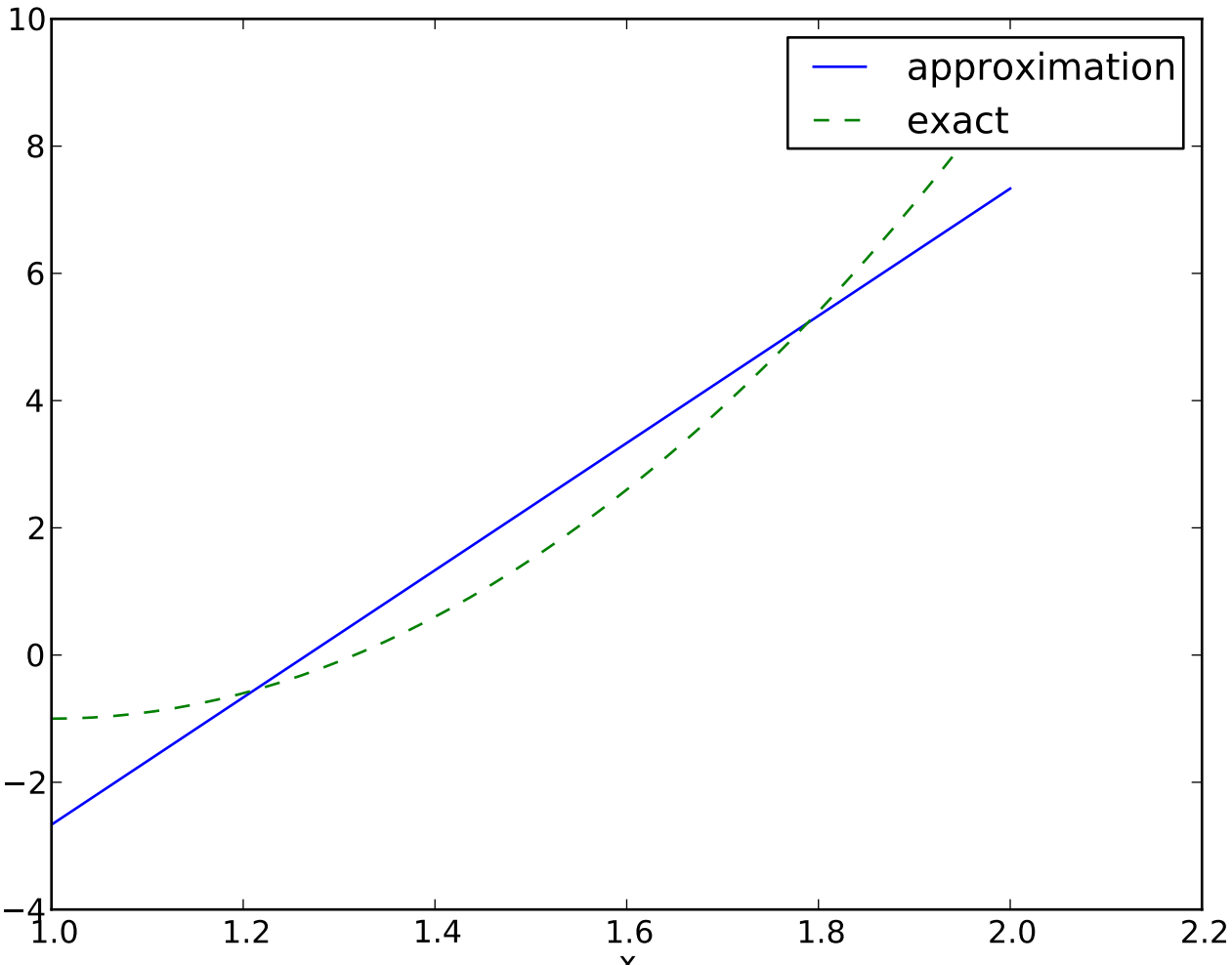
Compare f and u visually:

```
def comparison_plot(f, u, Omega, filename='tmp.pdf'):
    x = sm.Symbol('x')
    # Turn f and u to ordinary Python functions
    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)
```

All code in module `approx1D.py`

Implementation of the least squares method; application

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



Perfect approximation; parabola approximating parabola

- What if we add $\psi_2 = x^2$ to the space V?
- That is, approximating a parabola by any parabola?
- (Hopefully we get the exact parabola!)

```
>>> 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
```

Perfect approximation; the general result

- What if we use $\psi_i(x) = x^i$ for $i = 0, \ldots, N = 40$?
- The output from `least_squares` is $c_i = 0$ for $i > 2$

General result.

If $f \in V$, least squares and projection/Galerkin give $u = f$.

Perfect approximation; proof of the general result

If $f \in V$, $f = \sum_{j \in I} d_j \psi_j$, for some $\{d_i\}_{i \in I}$. Then

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

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 $i \in I$ and u is identical to f.

Finite-precision/numerical computations

The previous computations were symbolic. What if we solve the linear system numerically with standard arrays?

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*

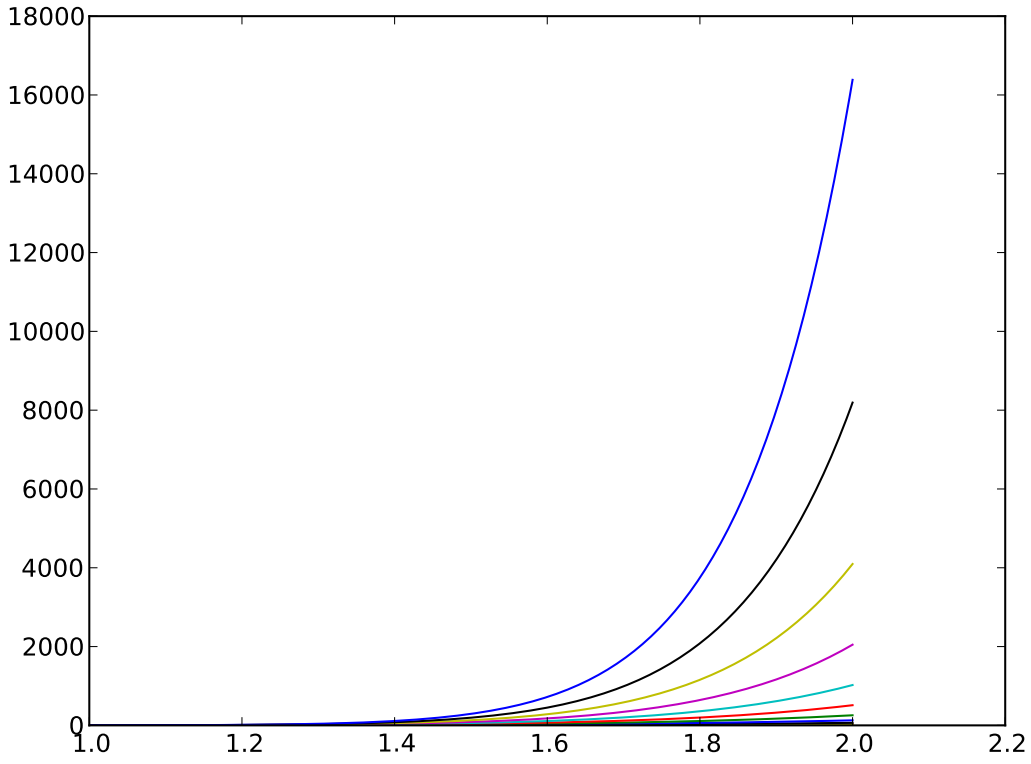
- Column 2: `sympy.mpmath.fp.matrix` and `sympy.mpmath.fp.lu_solve`

Ill-conditioning (1)

Observations:

- Significant round-off errors in the numerical computations (!)
- But if we plot the approximations they look good (!)

Problem: The basis functions x^i become almost linearly dependent for large N.



Ill-conditioning (2)

- Almost linearly dependent basis functions give almost singular matrices
- Such matrices are said to be *ill conditioned*, and Gaussian elimination is severely affected by round-off errors
- The basis $1, x, x^2, x^3, x^4, \ldots$ is a bad basis
- Polynomials are fine as basis, but the more orthogonal they are, $(\psi_i, \psi_j) \approx 0$, the better

Fourier series approximation; problem and code

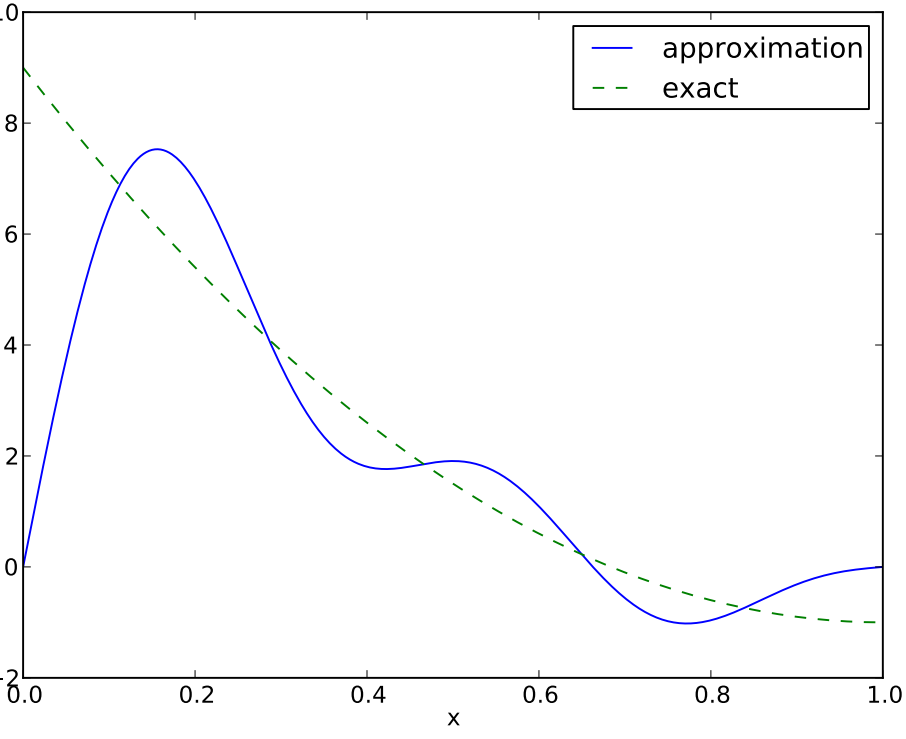
Consider

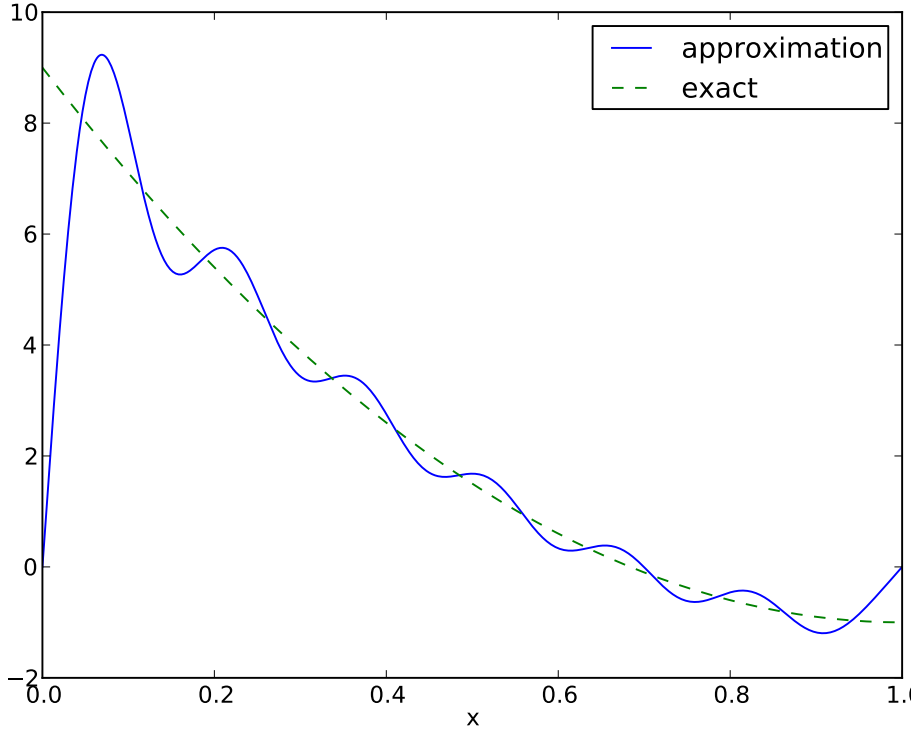
$$V = \text{span}\left\{\sin \pi x, \sin 2\pi x, \ldots, \sin(N+1)\pi x\right\}$$

```
N = 3
from sympy import sin, pi
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)
```

Fourier series approximation; plot

$N = 3$ vs $N = 11$:





Fourier series approximation; improvements

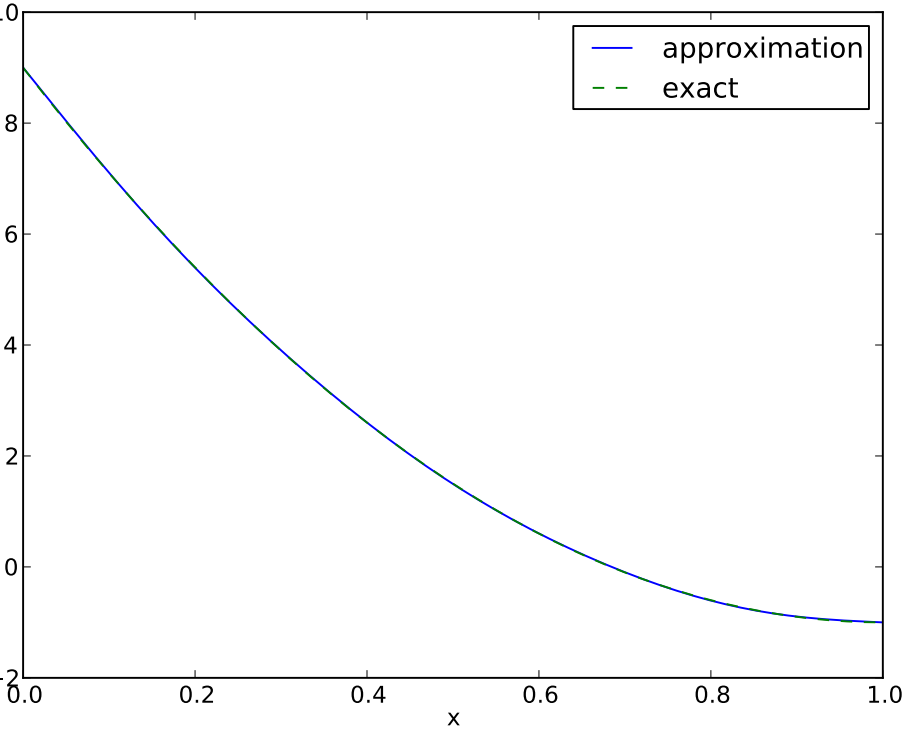
- Considerably improvement by $N = 11$
- But always discrepancy of $f(0) - u(0) = 9$ at $x = 0$, because all the $\psi_i(0) = 0$ and hence $u(0) = 0$
- Possible remedy: add a term that leads to correct boundary values

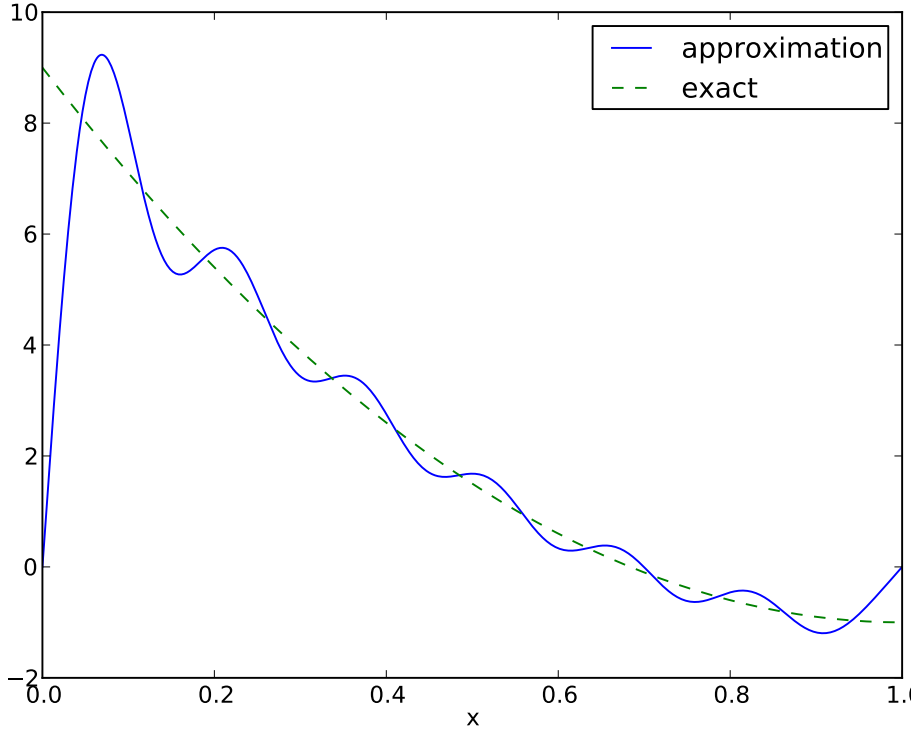
$$u(x) = f(0)(1 - x) + xf(1) + \sum_{j \in I} c_j \psi_j(x) \tag{27}$$

The extra term ensures $u(0) = f(0)$ and $u(1) = f(1)$ and is a strikingly good help to get a good approximation!

Fourier series approximation; final results

$N = 3$ vs $N = 11$:





Orthogonal basis functions

This choice of sine functions as basis functions is popular because

- the basis functions are orthogonal: $(\psi_i, \psi_j) = 0$
- implying that $A_{i,j}$ is a diagonal matrix
- implying that we can solve for $c_i = 2\int_0^1 f(x)\sin((i+1)\pi x)dx$

In general for an orthogonal basis, $A_{i,j}$ is diagonal and we can easily solve for c_i:

$$c_i = \frac{b_i}{A_{i,i}} = \frac{(f, \psi_i)}{(\psi_i, \psi_i)}$$

The collocation or interpolation method; ideas and math

Here is another idea for approximating $f(x)$ by $u(x) = \sum_j c_j \psi_j$:

- Force $u(x_i) = f(x_i)$ at some selected *collocation* points $\{x_i\}_{i \in I}$
- Then u interpolates f
- The method is known as *interpolation* or *collocation*

$$u(x_i) = \sum_{j \in I} c_j \psi_j(x_i) = f(x_i) \quad i \in I, N \tag{28}$$

This is a linear system with no need for integration:

$$\sum_{j \in I} A_{i,j} c_j = b_i, \quad i \in I \tag{29}$$

$$A_{i,j} = \psi_j(x_i) \tag{30}$$

$$b_i = f(x_i) \tag{31}$$

No symmetric matrix: $\psi_j(x_i) \neq \psi_i(x_j)$ in general

The collocation or interpolation method; implementation

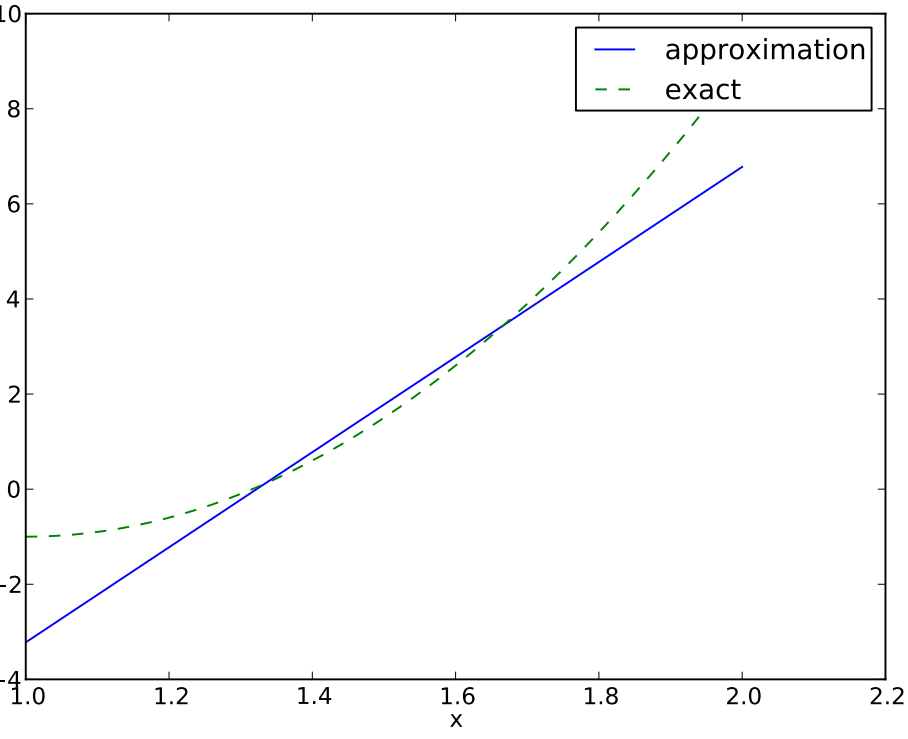
`points` holds the interpolation/collocation points

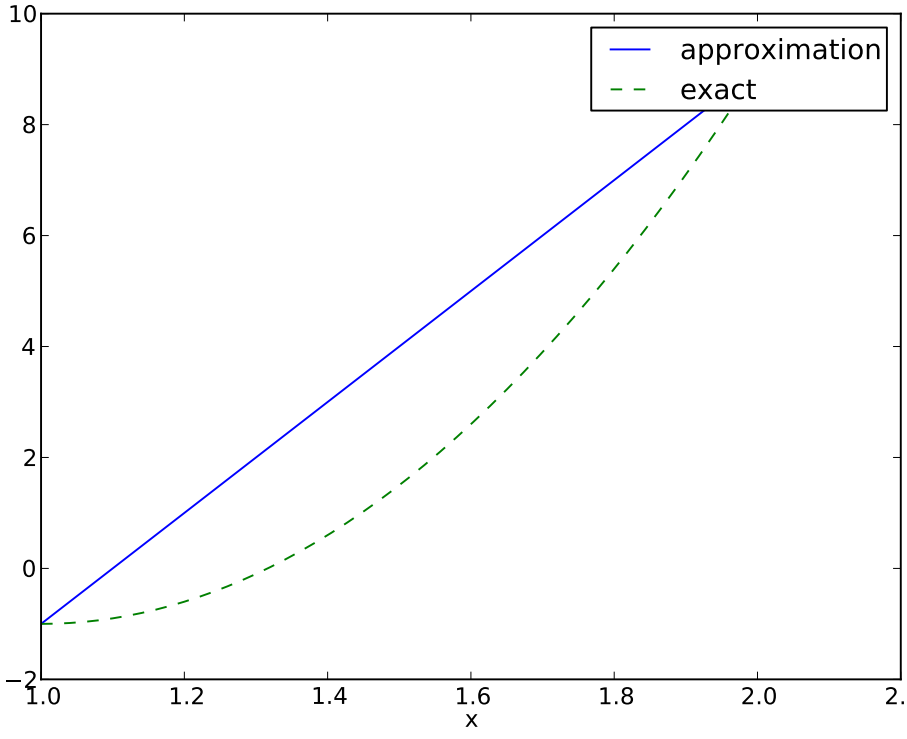
```
def interpolation(f, psi, points):
    N = len(psi) - 1
    A = sm.zeros((N+1, N+1))
    b = sm.zeros((N+1, 1))
    x = sm.Symbol('x')
    # Turn psi and f into Python functions
    psi = [sm.lambdify([x], psi[i]) for i in range(N+1)]
    f = sm.lambdify([x], f)
    for i in range(N+1):
        for 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 collocation or interpolation method; approximating a parabola by linear functions

- Potential difficulty: how to choose x_i?
- The results are sensitive to the points!

$(4/3, 5/3)$ vs $(1, 2)$:





Lagrange polynomials; motivation and ideas

Motivation:

- The interpolation/collocation method avoids integration
- With a diagonal matrix $A_{i,j} = \psi_j(x_i)$ we can solve the linear system by hand

The *Lagrange interpolating polynomials* ψ_j have the property that

$$\psi_i(x_j) = \delta_{ij}, \quad \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Hence, $c_i = f(x_i)$ and

$$u(x) = \sum_{j \in I} f(x_i)\psi_i(x) \tag{32}$$

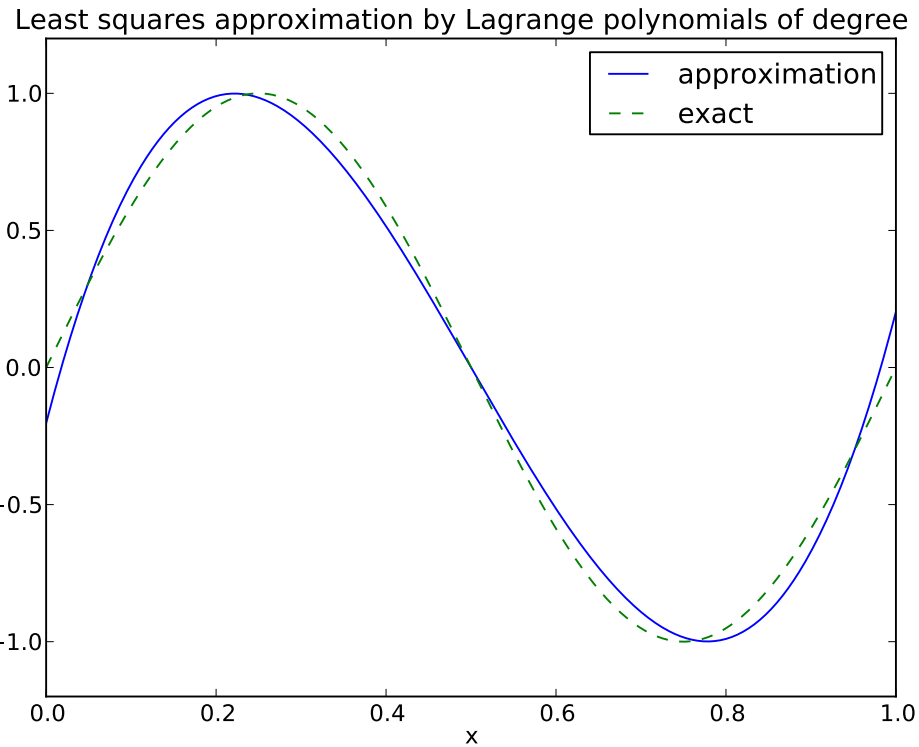
- Lagrange polynomials and interpolation/collocation look convenient
- Lagrange polynomials are very much used in the finite element method

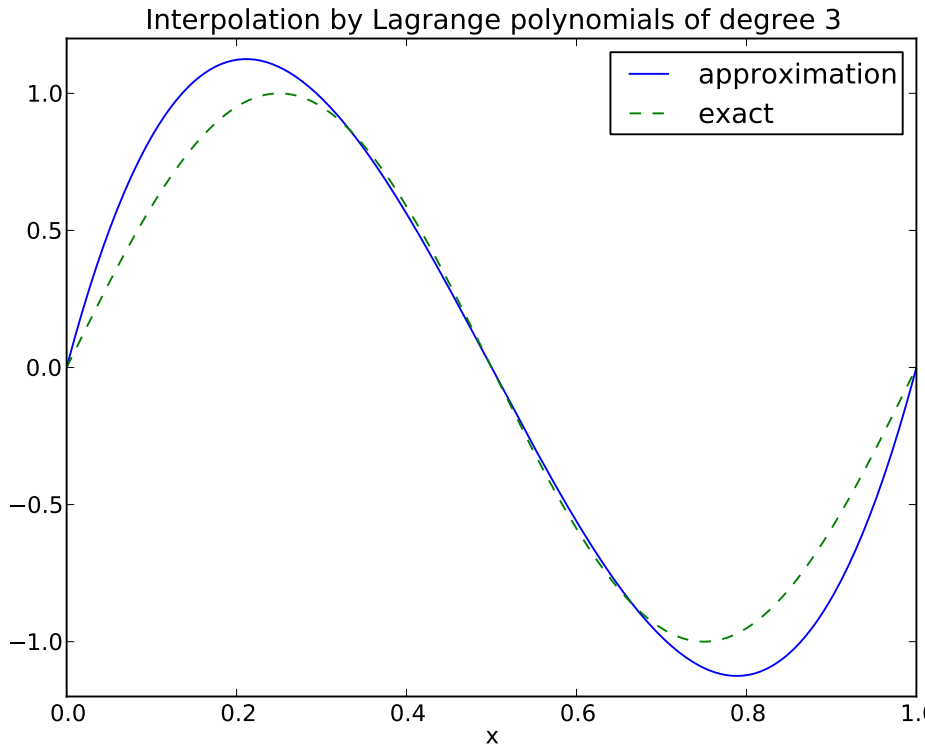
Lagrange polynomials; formula and code

$$\psi_i(x) = \prod_{j=0, j\neq i}^{N} \frac{x - x_j}{x_i - x_j} = \frac{x - x_0}{x_i - x_0} \cdots \frac{x - x_{i-1}}{x_i - x_{i-1}} \frac{x - x_{i+1}}{x_i - x_{i+1}} \cdots \frac{x - x_N}{x_i - x_N} \tag{33}$$

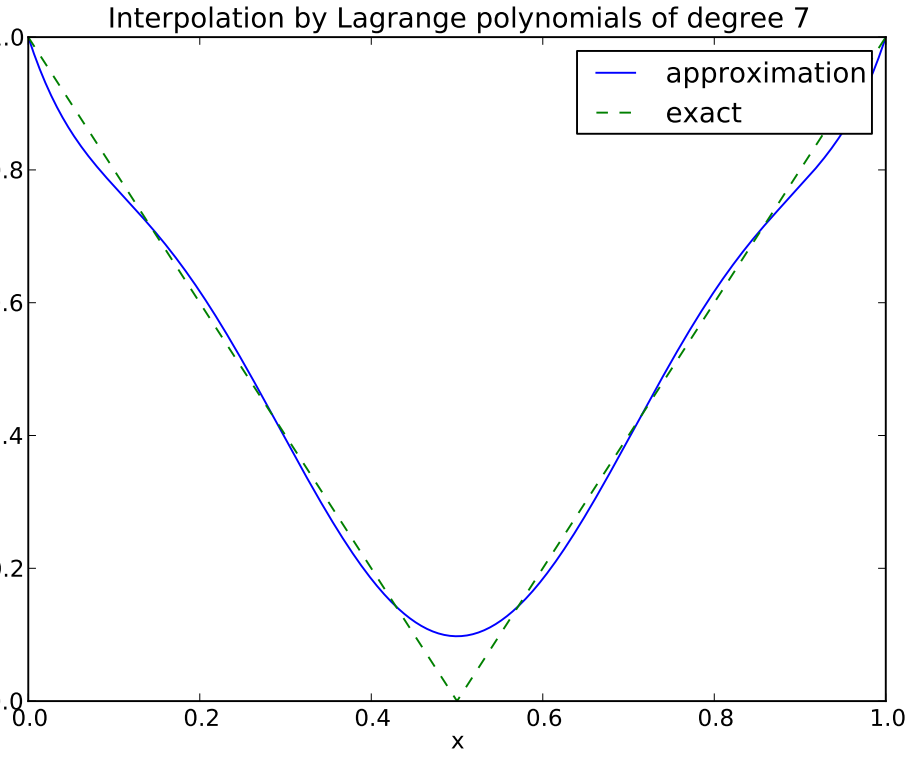
```
def Lagrange_polynomial(x, i, points):
    p = 1
    for k in range(len(points)):
        if k != i:
            p *= (x - points[k])/(points[i] - points[k])
    return p
```

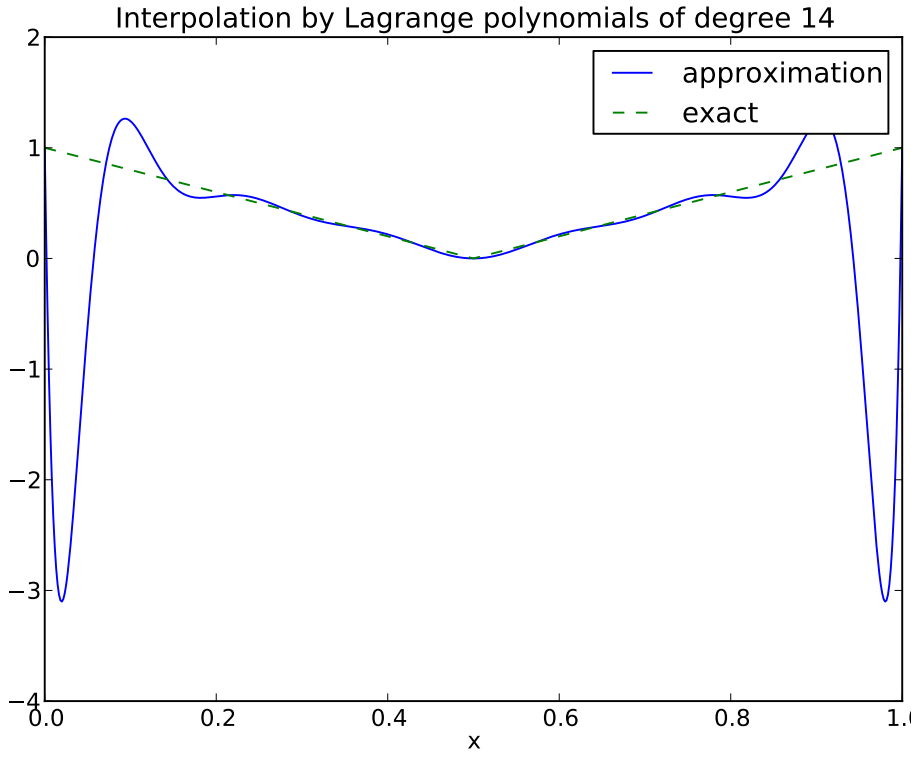
Lagrange polynomials; successful example





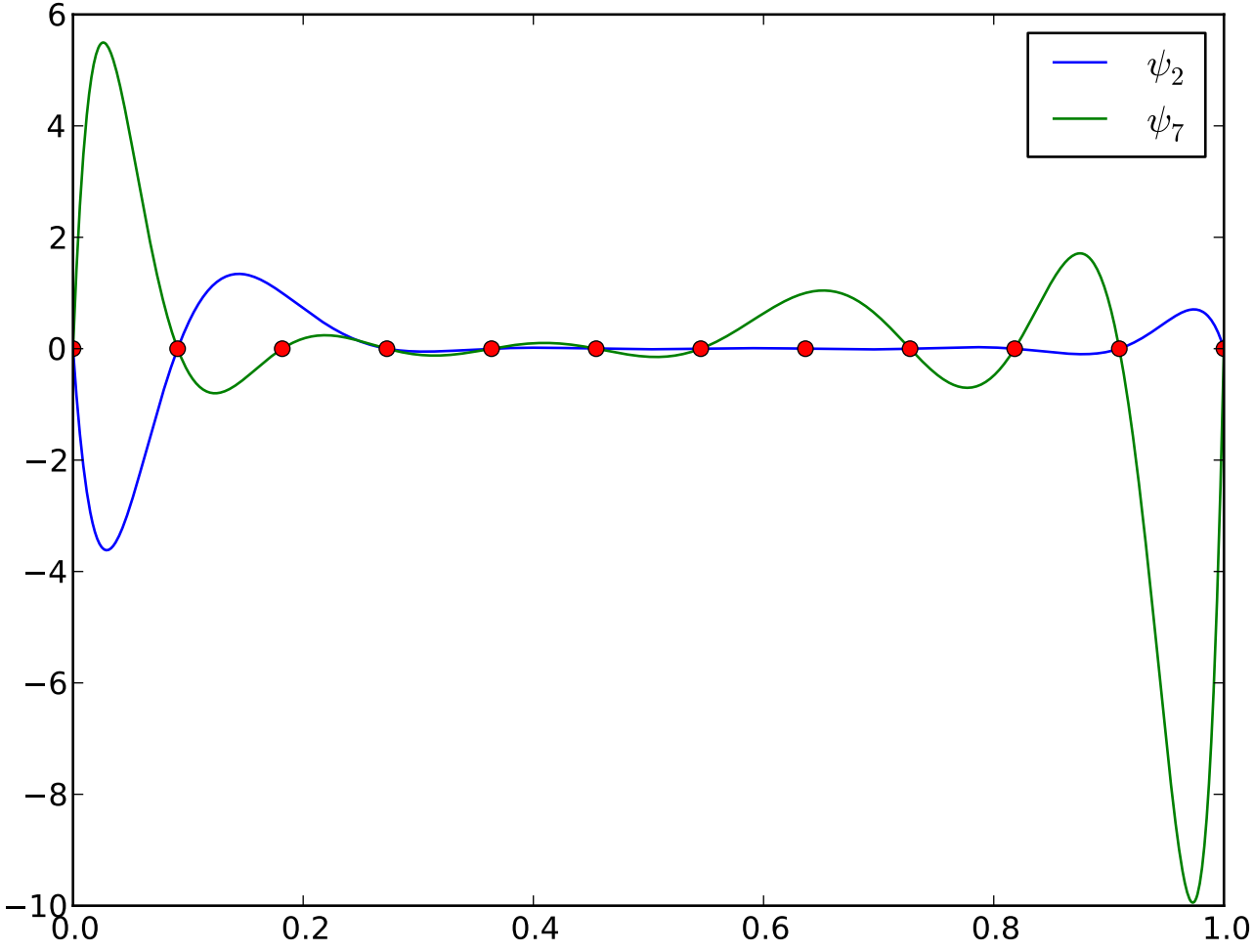
Lagrange polynomials; a less successful example





Lagrange polynomials; oscillatory behavior

12 points, degree 11, plot of two of the Lagrange polynomials - note that they are zero at all points except one.



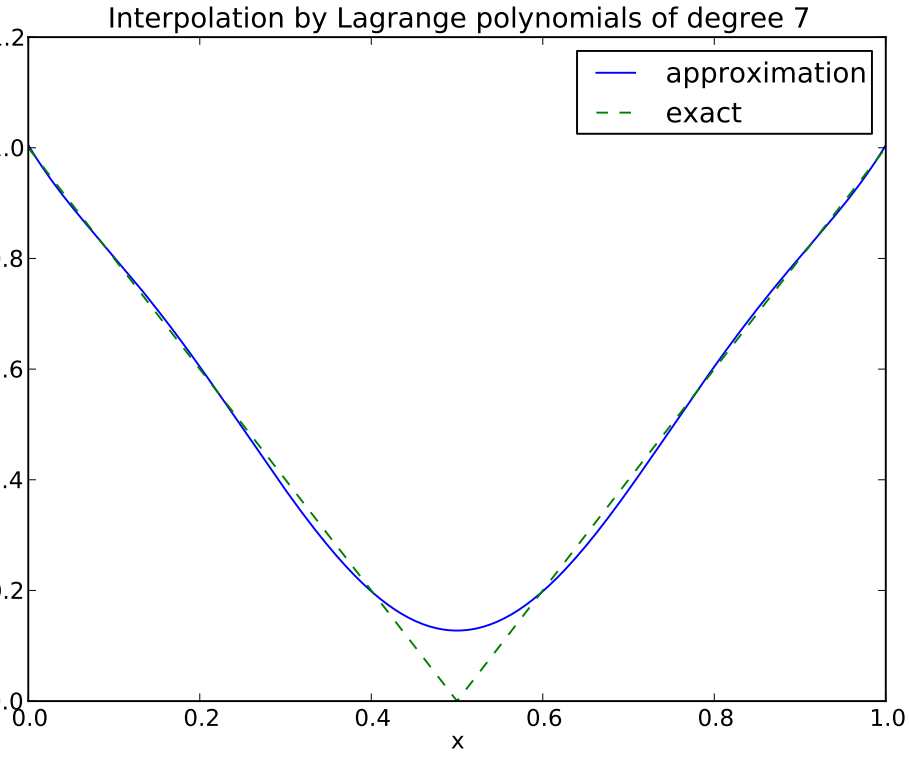
Lagrange polynomials; remedy for strong oscillations

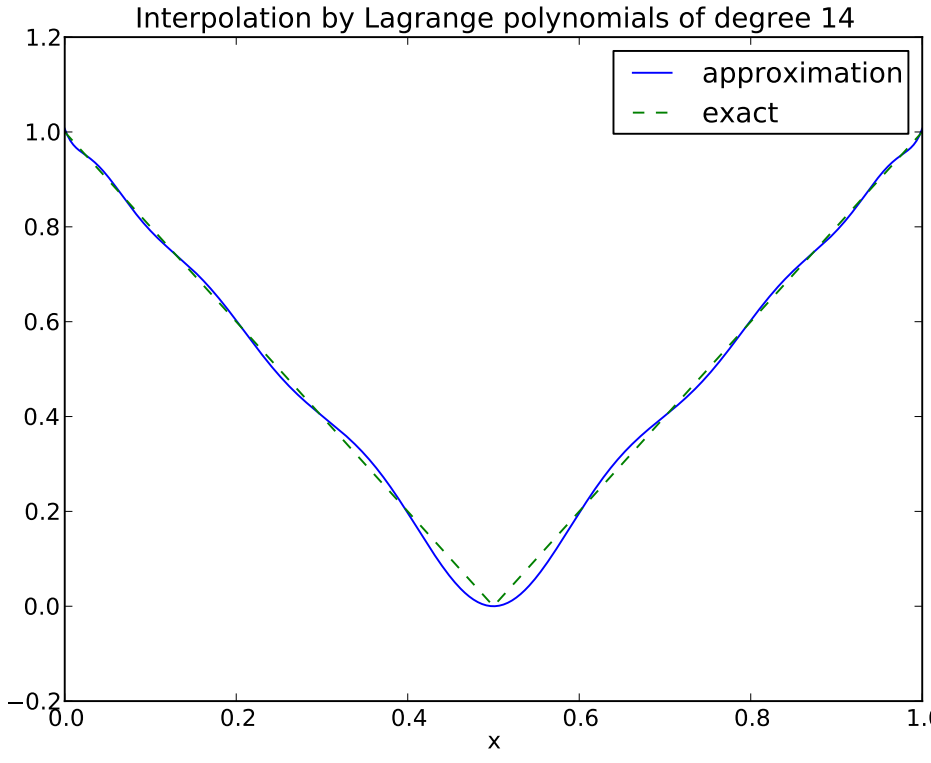
The oscillations can be reduced by a more clever choice of interpolation points, called the *Chebyshev nodes*:

$$x_i = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\cos\left(\frac{2i+1}{2(N+1)}pi\right), \quad i = 0\ldots, N \quad (34)$$

on an interval $[a, b]$.

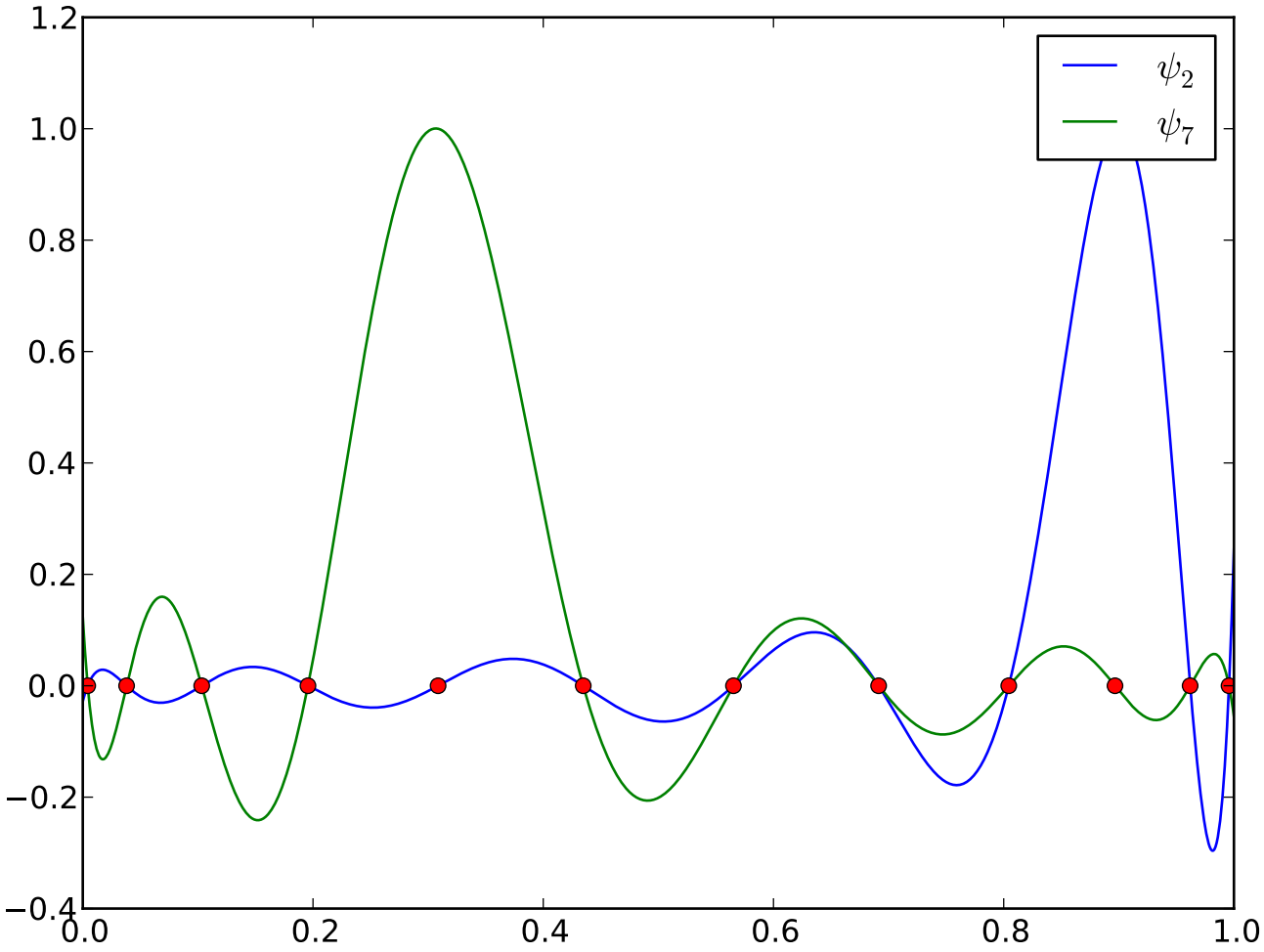
Lagrange polynomials; recalculation with Chebyshev nodes





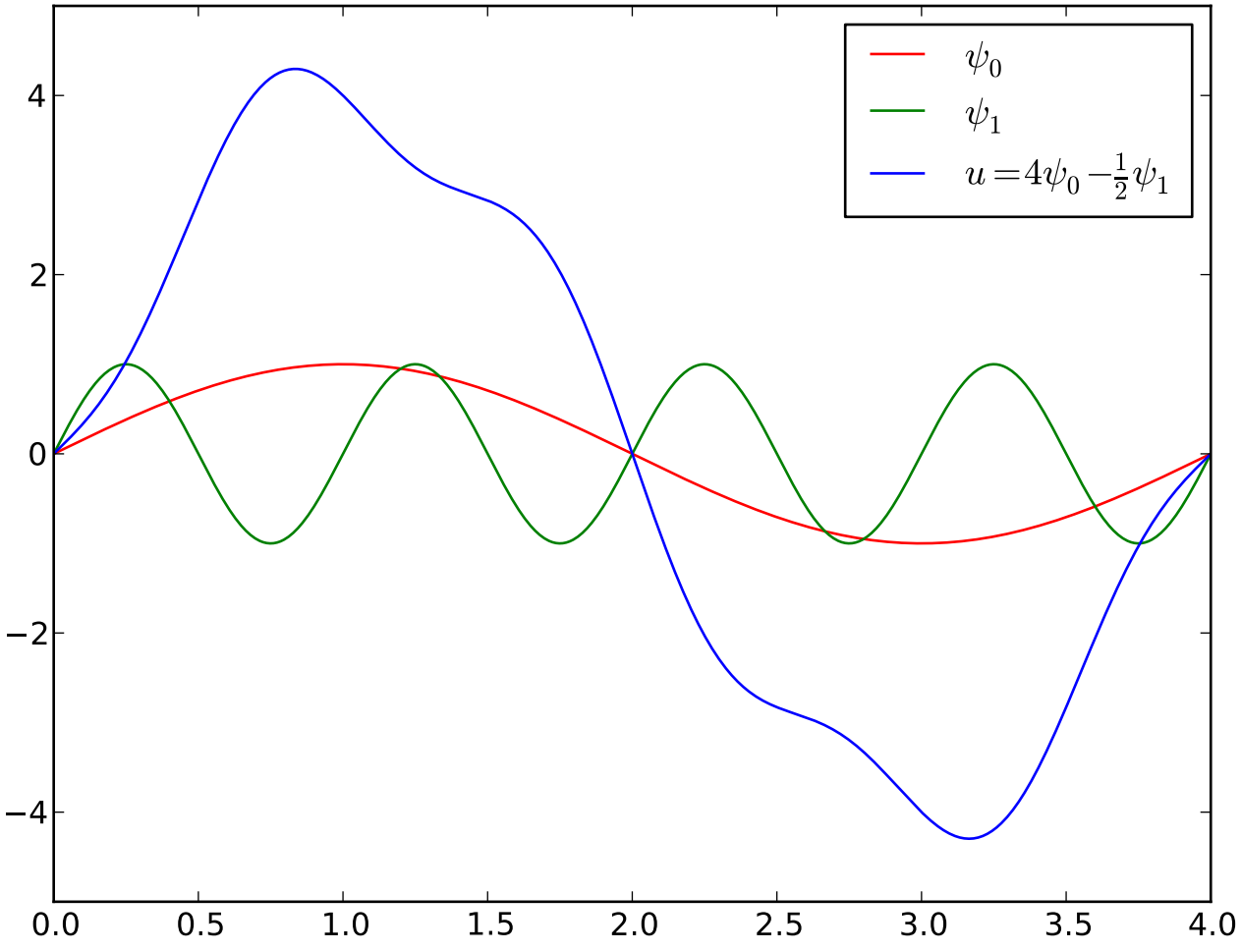
Lagrange polynomials; less oscillations with Chebyshev nodes

12 points, degree 11, plot of two of the Lagrange polynomials - note that they are zero at all points except one.



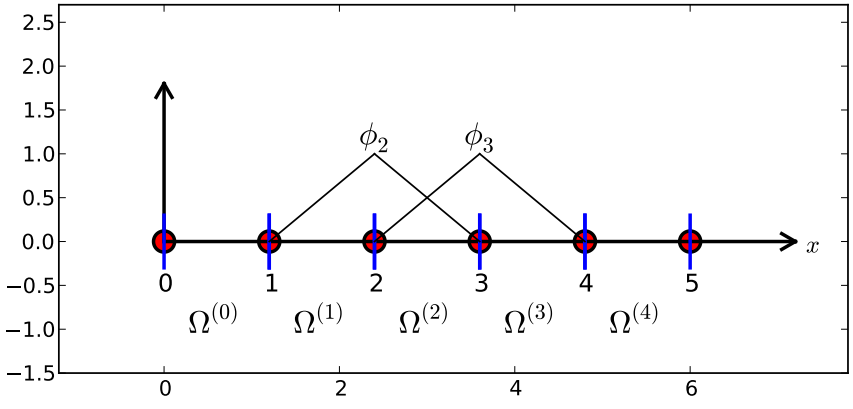
Finite element basis functions

The basis functions have so far been global: $\psi_i(x) \neq 0$ almost everywhere

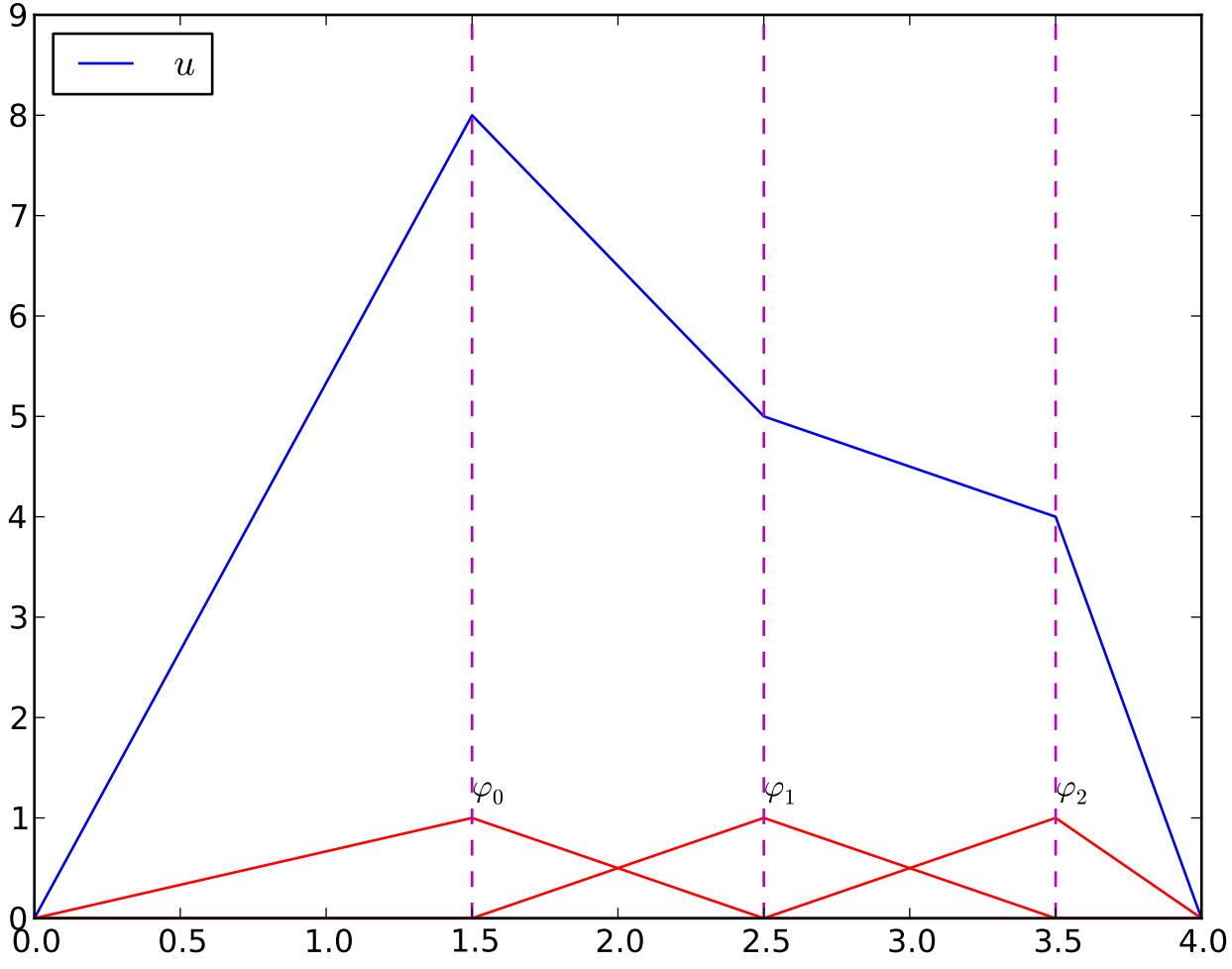


In the finite element method we use basis functions with local support

- *Local support*: $\psi_i(x) \neq 0$ for x in a small subdomain of Ω
- Typically hat-shaped
- $u(x)$ based on these ψ_i is a piecewise polynomial defined over many (small) subdomains
- We introduce φ_i as the name of these finite element hat functions (and for now choose $\psi_i = \varphi_i$)



The linear combination of hat functions is a piecewise linear function



Elements and nodes

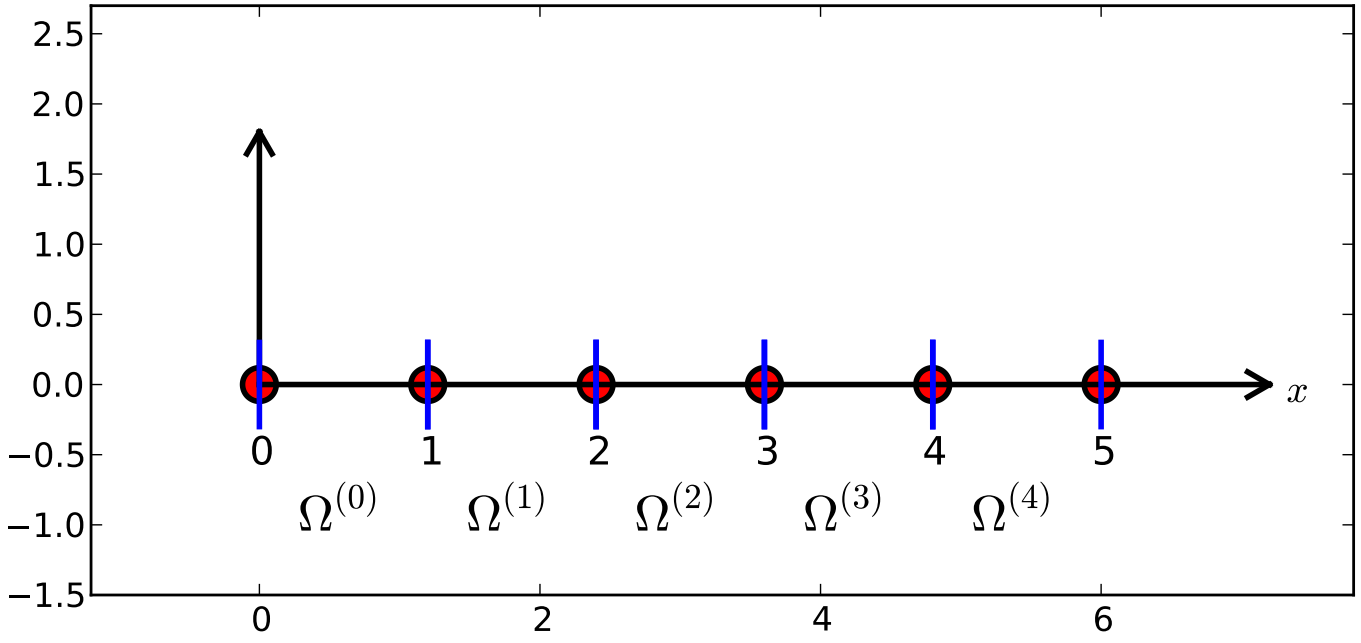
Split Ω into non-overlapping subdomains called *elements*:

$$\Omega = \Omega^{(0)} \cup \cdots \cup \Omega^{(N_e)} \tag{35}$$

On each element, introduce points called *nodes*: $x_0, \ldots, x_{N_n}$

- The finite element basis functions are named $\varphi_i(x)$
- $\varphi_i = 1$ at node i and 0 at all other nodes
- φ_i is a Lagrange polynomial on each element
- For nodes at the boundary between two elements, φ_i is made up of a Lagrange polynomial over each element

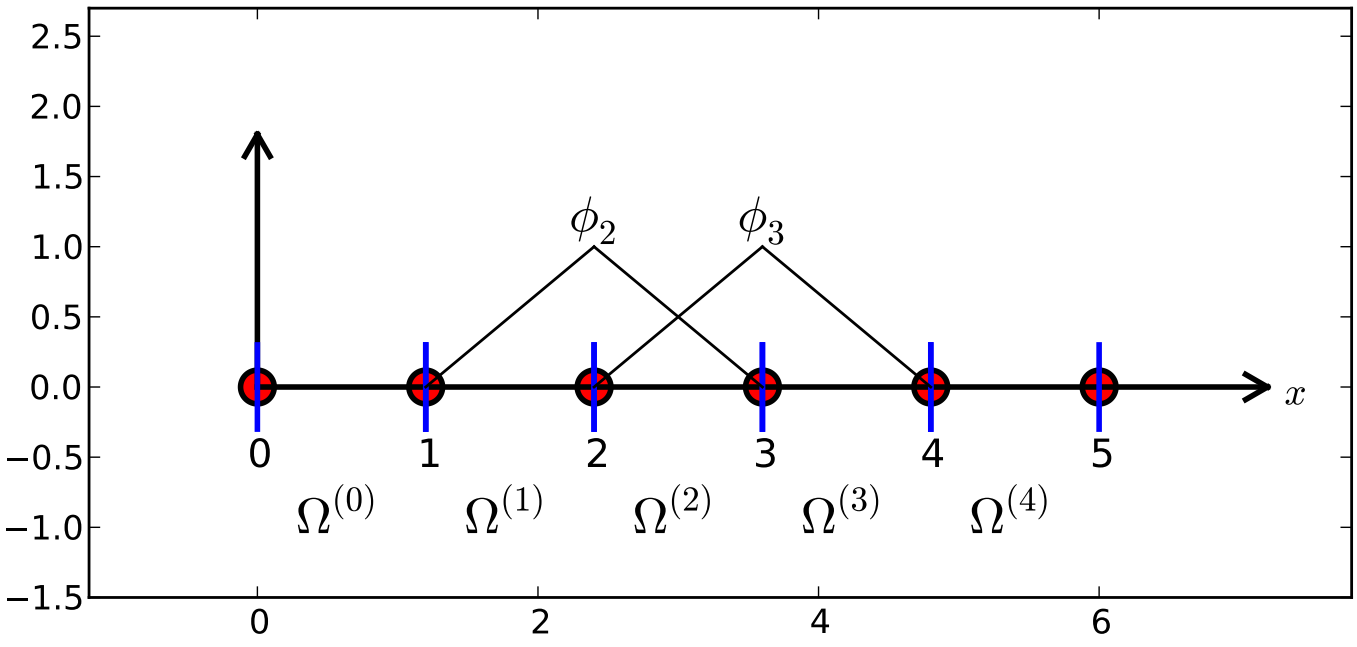
Example on elements with two nodes (P1 elements)



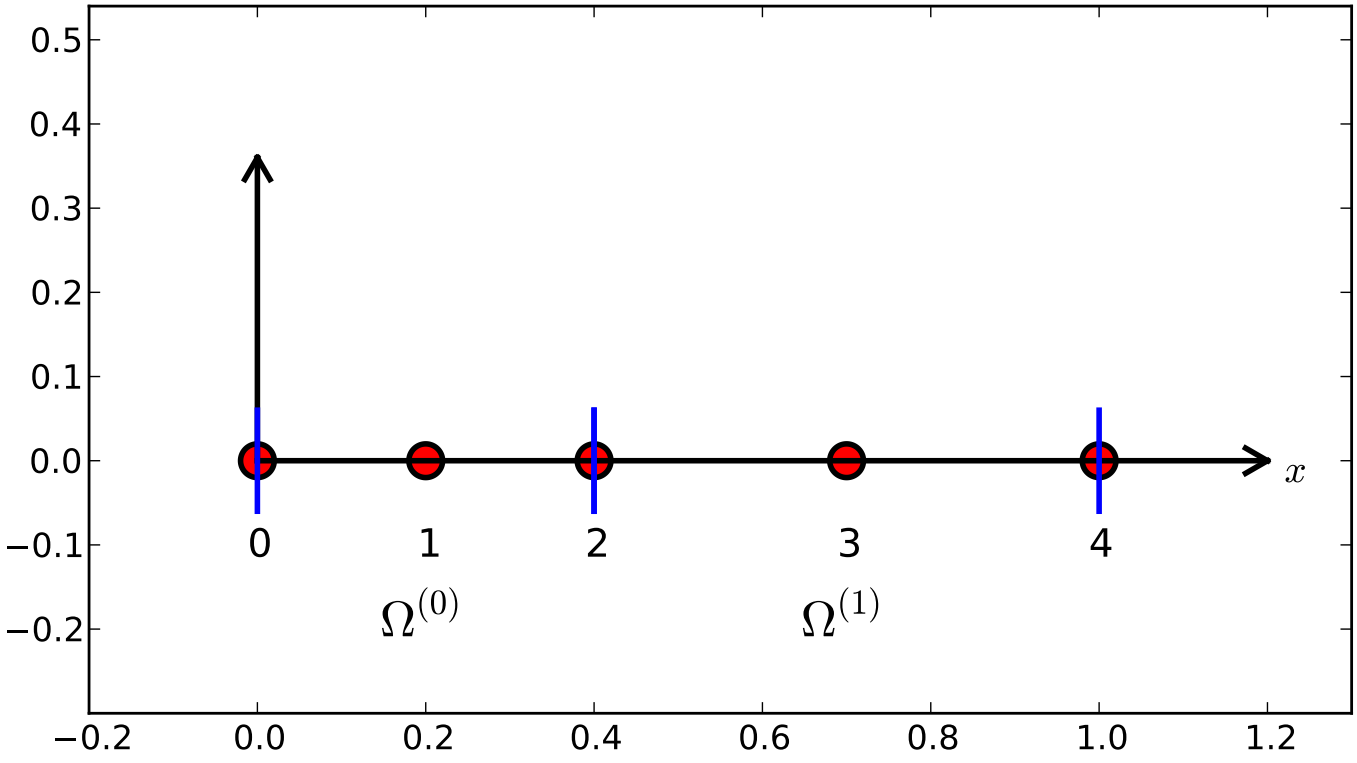
Data structure: `nodes` holds coordinates or nodes, `elements` holds the node numbers in each element

```
nodes = [0, 1.2, 2.4, 3.6, 4.8, 5]
elements = [[0, 1], [1, 2], [2, 3], [3, 4], [4, 5]]
```

Illustration of two basis functions on the mesh

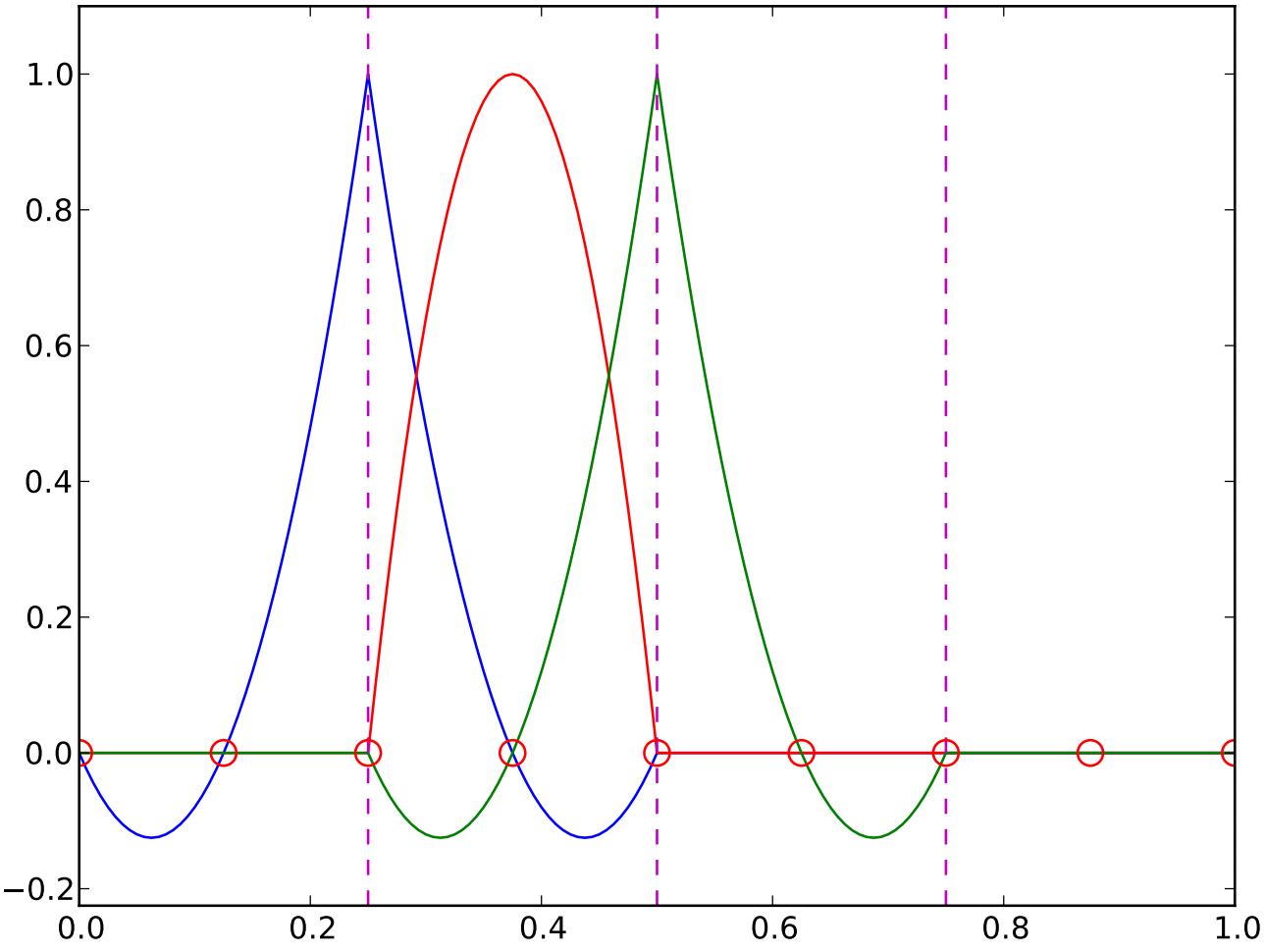


Example on elements with three nodes (P2 elements)

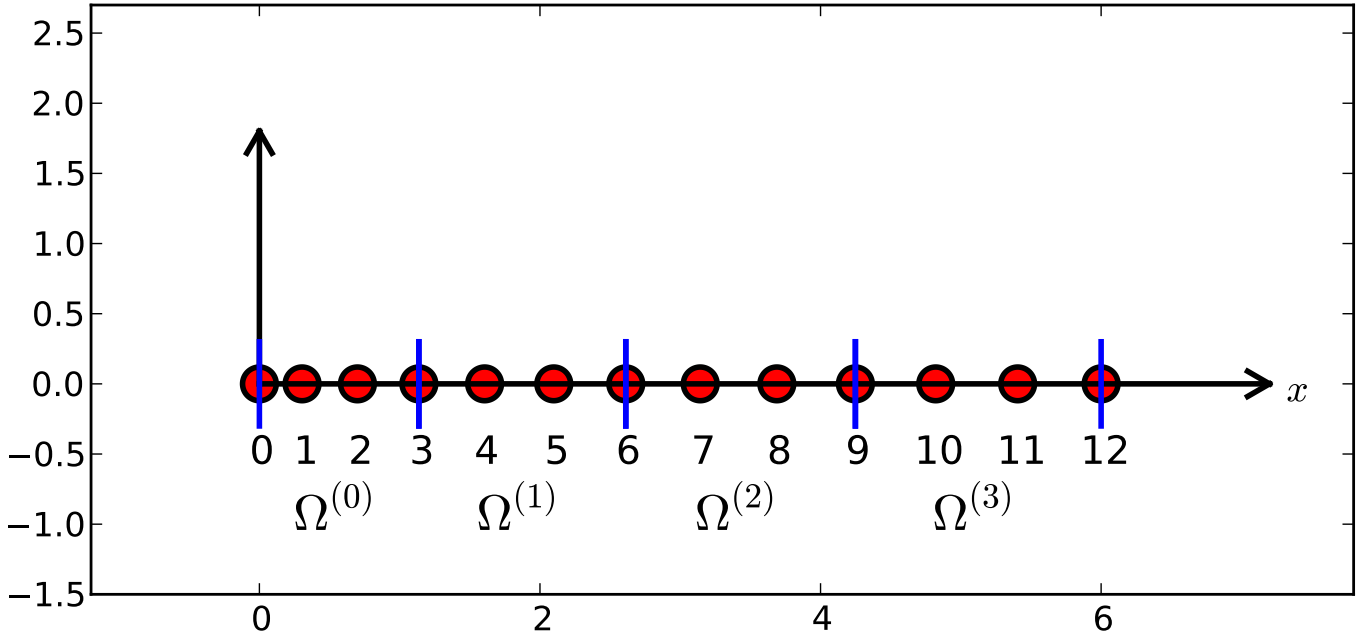



```
nodes = [0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1.0]
elements = [[0, 1, 2], [2, 3, 4], [4, 5, 6], [6, 7, 8]]
```

Some corresponding basis functions (P2 elements)

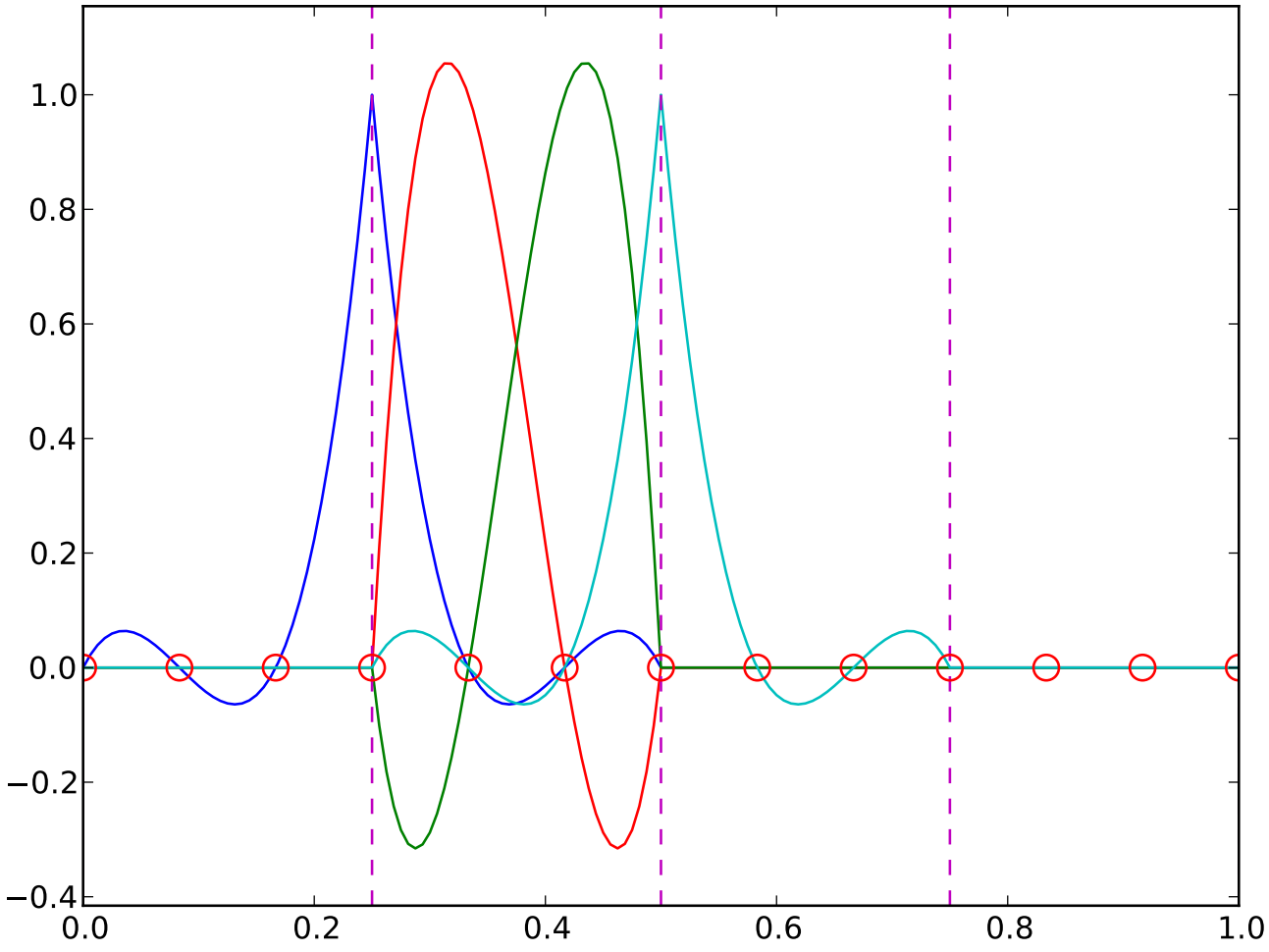


Examples on elements with four nodes per element (P3 elements)

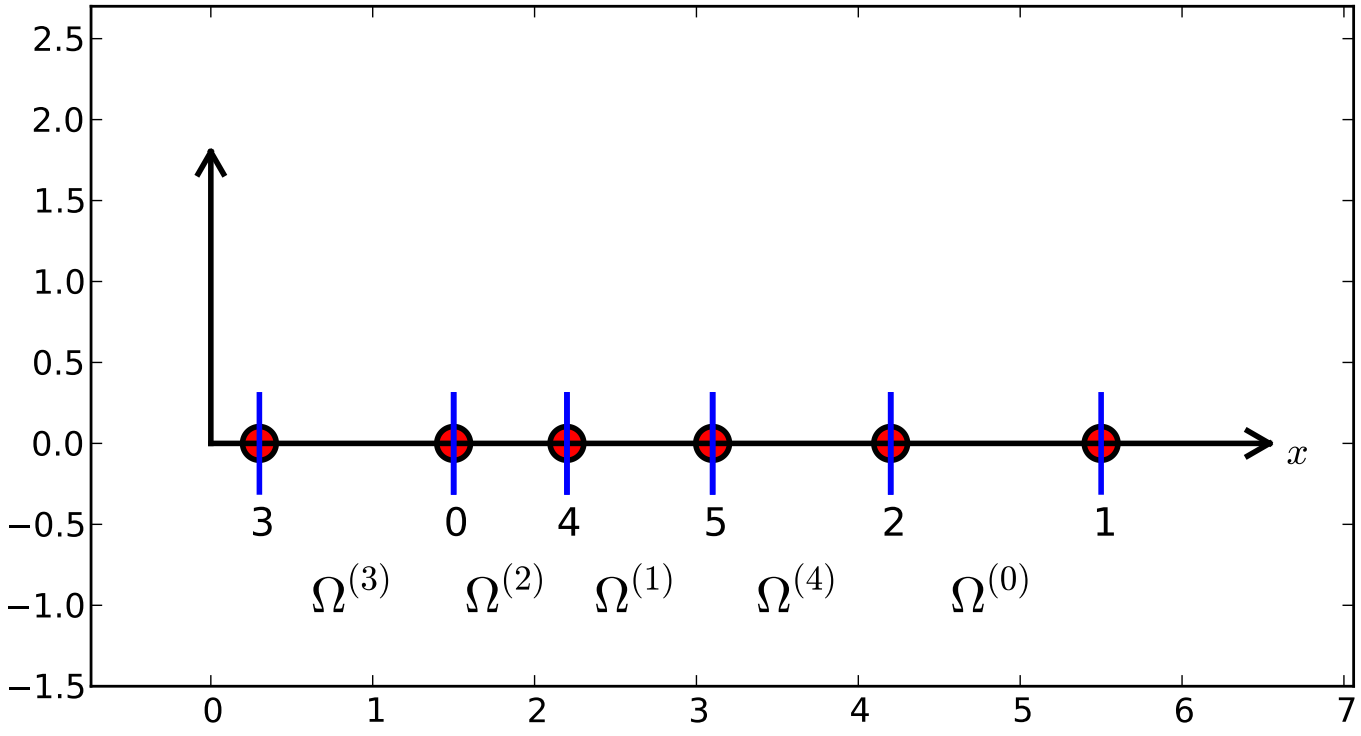



```
d = 3  # d+1 nodes per element
num_elements = 4
num_nodes = num_elements*d + 1
nodes = [i*0.5 for i in range(num_nodes)]
elements = [[i*d+j for j in range(d+1)] for i in range(num_elements
```

Some corresponding basis functions (P3 elements)



The numbering does not need to be regular from left to right




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

Interpretation of the coefficients c_i

Important property: c_i is the value of u at node i, x_i:

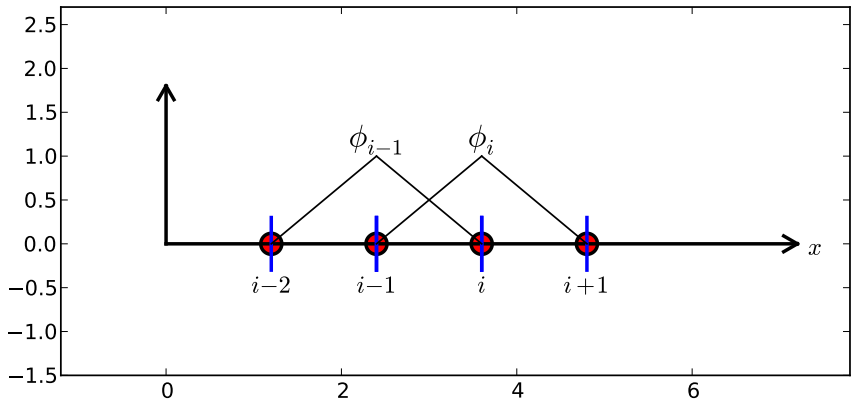
$$u(x_i) = \sum_{j \in I} c_j \varphi_j(x_i) = c_i \varphi_i(x_i) = c_i \tag{36}$$

because $\varphi_j(x_i) = 0$ if $i \neq j$

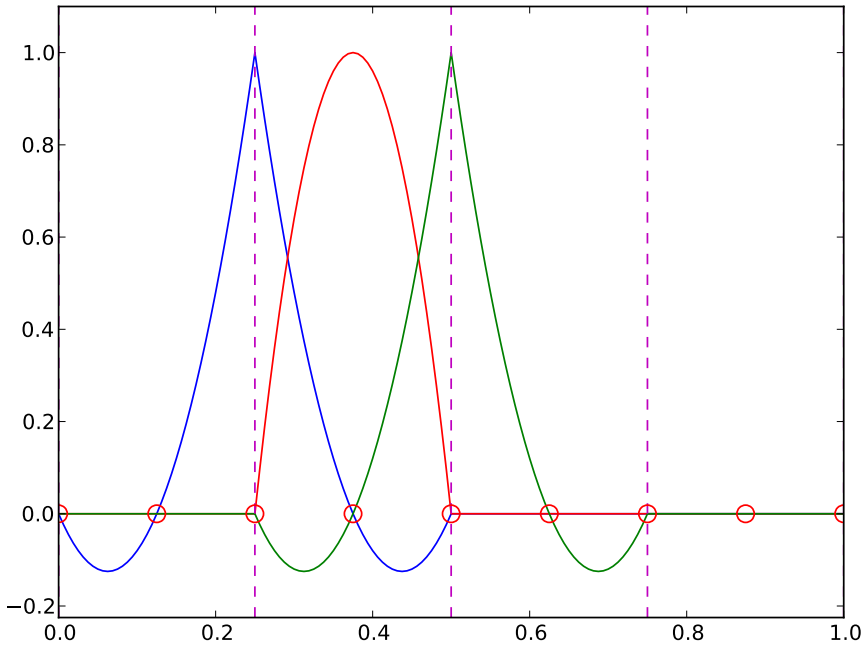
Properties of the basis functions

- $\varphi_i(x) \neq 0$ 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 $A_{i,j} = \int \varphi_i \varphi_j \, \mathrm{d}x$, *most of the elements in the coefficient matrix will be zero*

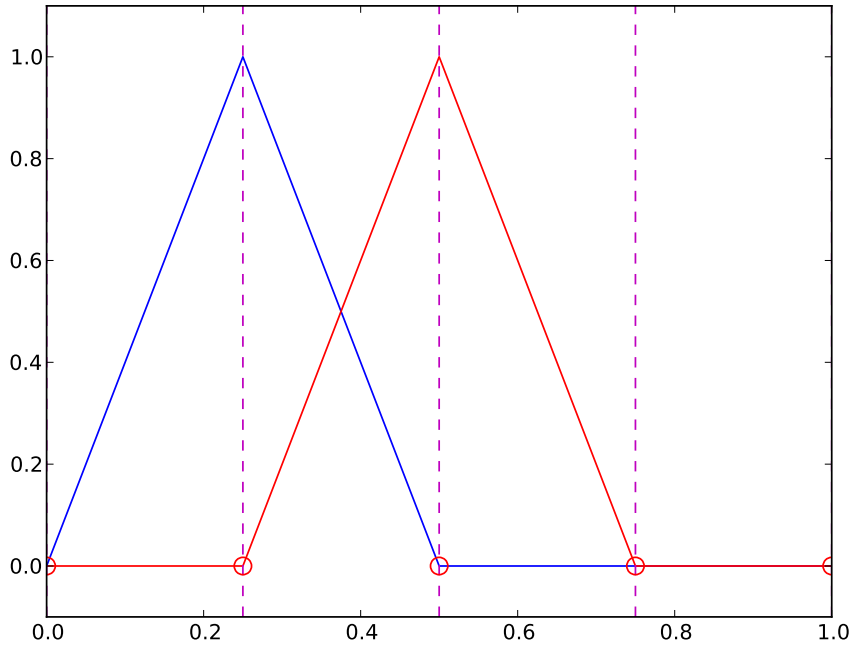


How to construct quadratic φ_i (P2 elements)



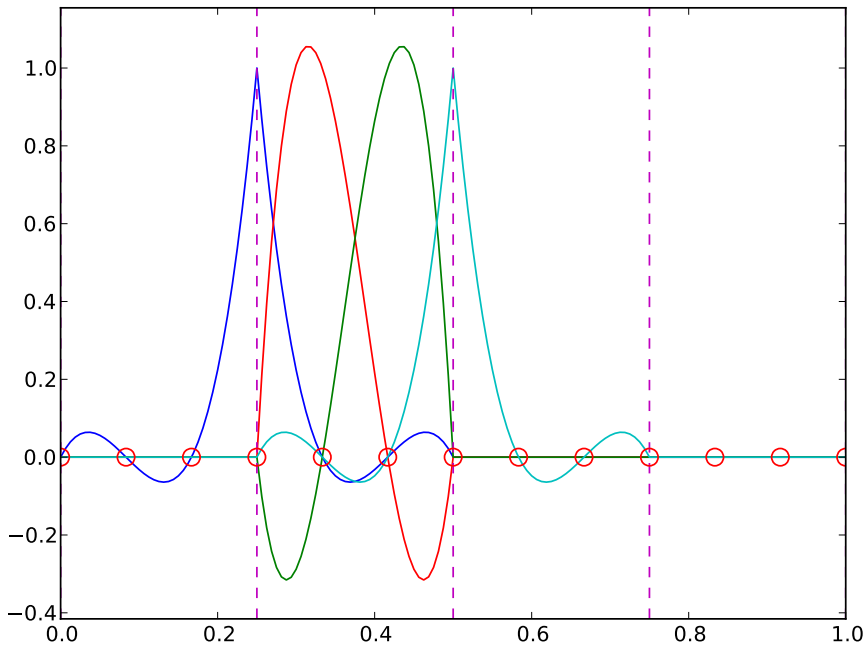
1. Associate Lagrange polynomials with the nodes in an element
2. When the polynomial is 1 on the element boundary, combine it with the polynomial in the neighboring element

Example on linear φ_i (P1 elements)



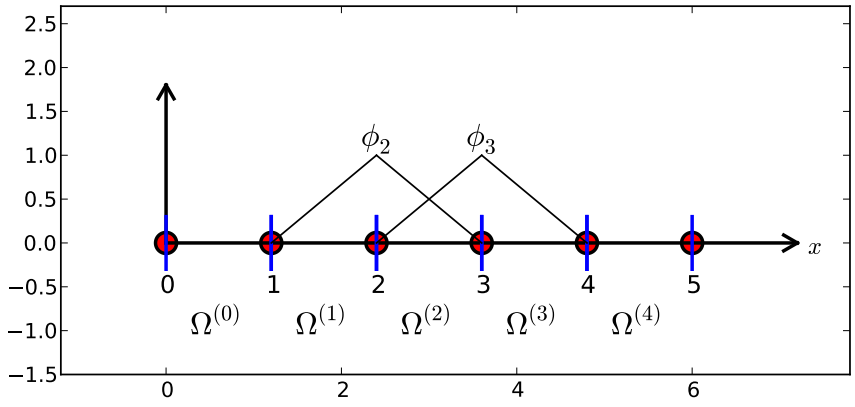
$$\varphi_i(x) = \begin{cases} 0, & x < x_{i-1} \\ (x - x_{i-1})/h & x_{i-1} \le x < x_i \\ 1 - (x - x_i)/h, & x_i \le x < x_{i+1} \\ 0, & x \ge x_{i+1} \end{cases} \tag{37}$$

Example on cubic φ_i (P3 elements)



Calculating the linear system for c_i

Computing a specific matrix entry (1)

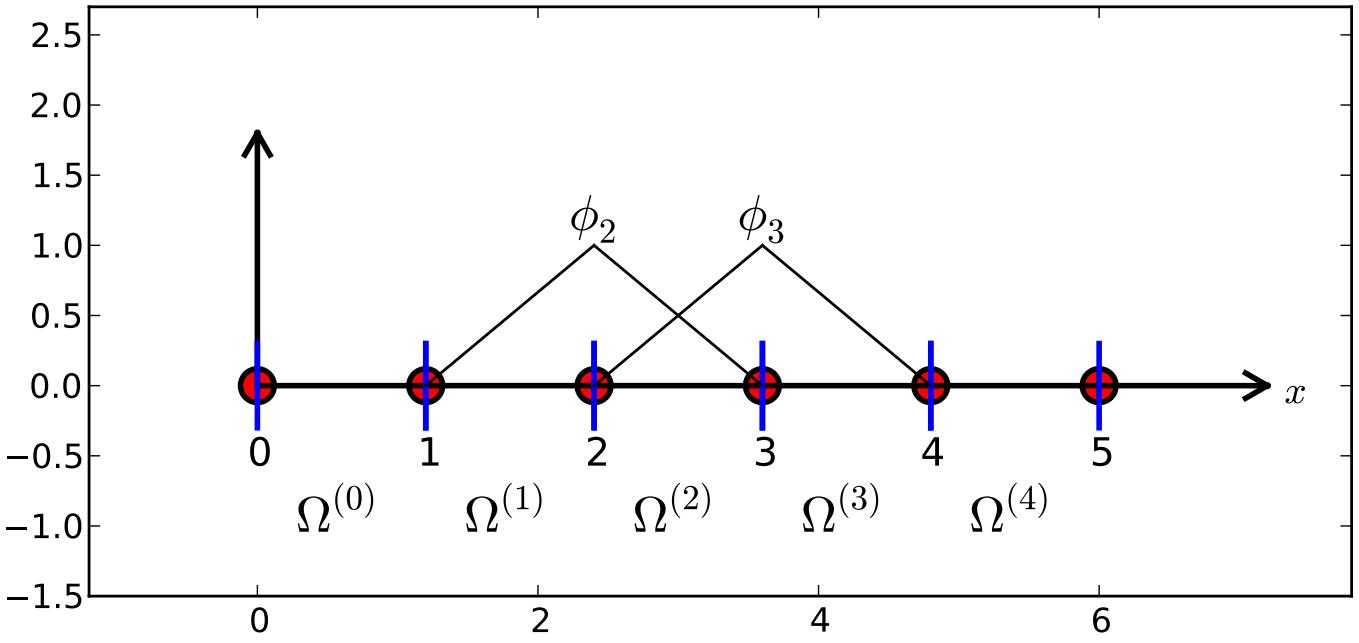


$A_{2,3} = \int_\Omega \varphi_2 \varphi_3 dx$: $\varphi_2 \varphi_3 \neq 0$ only over element 2. There,

$$\varphi_3(x) = (x - x_2)/h, \quad \varphi_2(x) = 1 - (x - x_2)/h$$

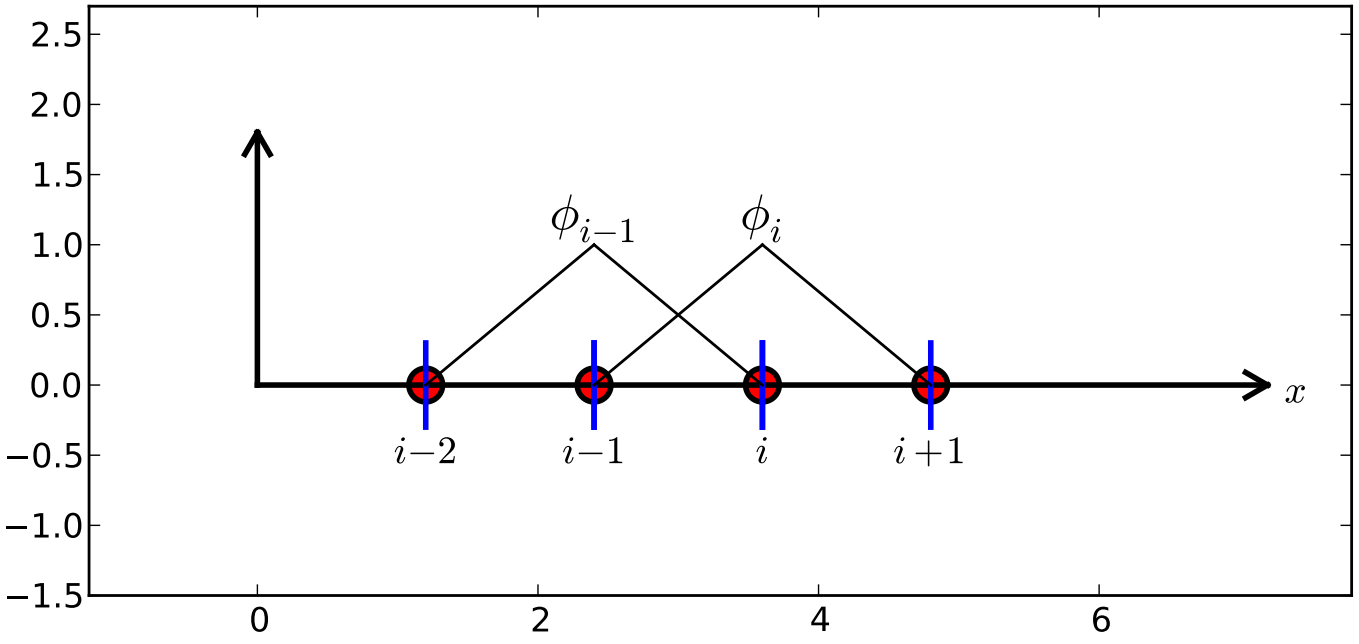
$$A_{2,3} = \int_\Omega \varphi_2 \varphi_3 \, \mathrm{d}x = \int_{x_2}^{x_3} \left(1 - \frac{x - x_2}{h}\right) \frac{x - x_2}{h} \, \mathrm{d}x = \frac{h}{6}$$

Computing a specific matrix entry (2)



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

Calculating a general row in the matrix; figure



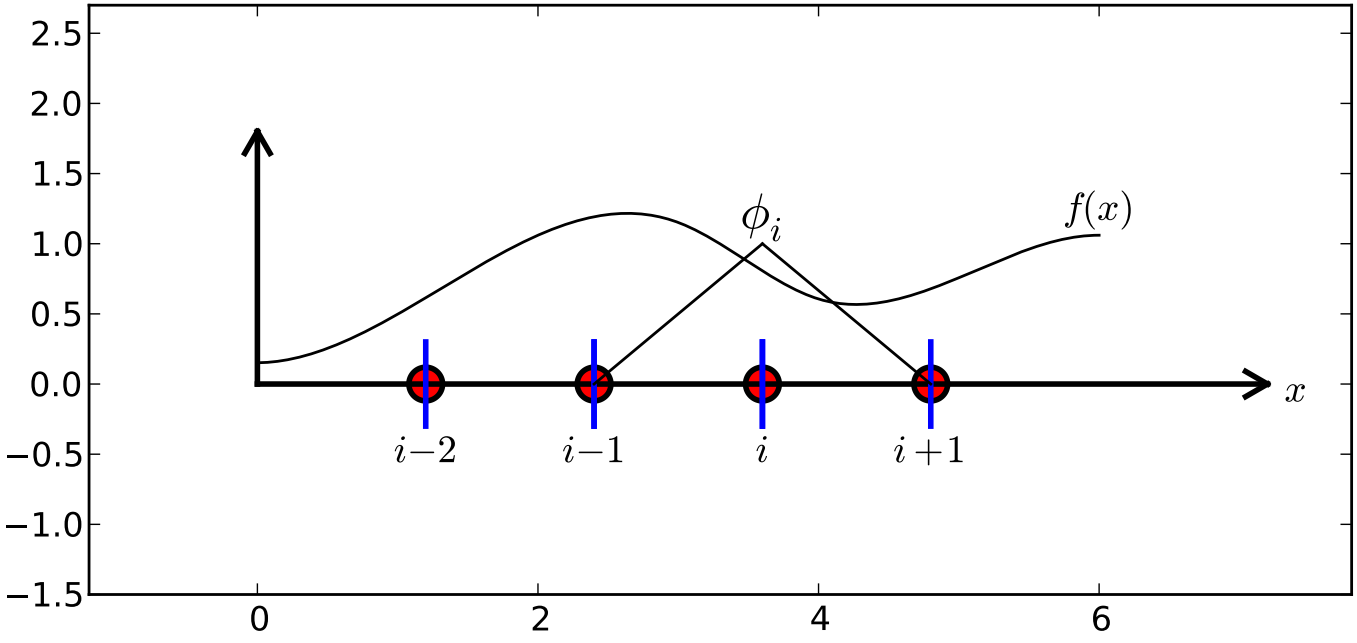
$$A_{i,i-1} = \int_\Omega \varphi_i \varphi_{i-1} \, \mathrm{d}x = ?$$

Calculating a general row in the matrix; details

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

- $A_{i,i+1} = A_{i,i-1}$ due to symmetry
- $A_{i,i} = h/3$ (same calculation as for $A_{2,2}$)
- $A_{0,0} = A_{N,N} = h/3$ (only one element)

Calculation of the right-hand side



$$b_i = \int_\Omega \varphi_i(x) f(x)\,\mathrm{d}x = \int_{x_{i-1}}^{x_i} \frac{x - x_{i-1}}{h} f(x)\,\mathrm{d}x + \int_{x_i}^{x_{i+1}} \left(1 - \frac{x - x_i}{h}\right) f(x) \tag{38}$$

Need a specific $f(x)$ to do more...

Specific example with two elements; linear system and solution

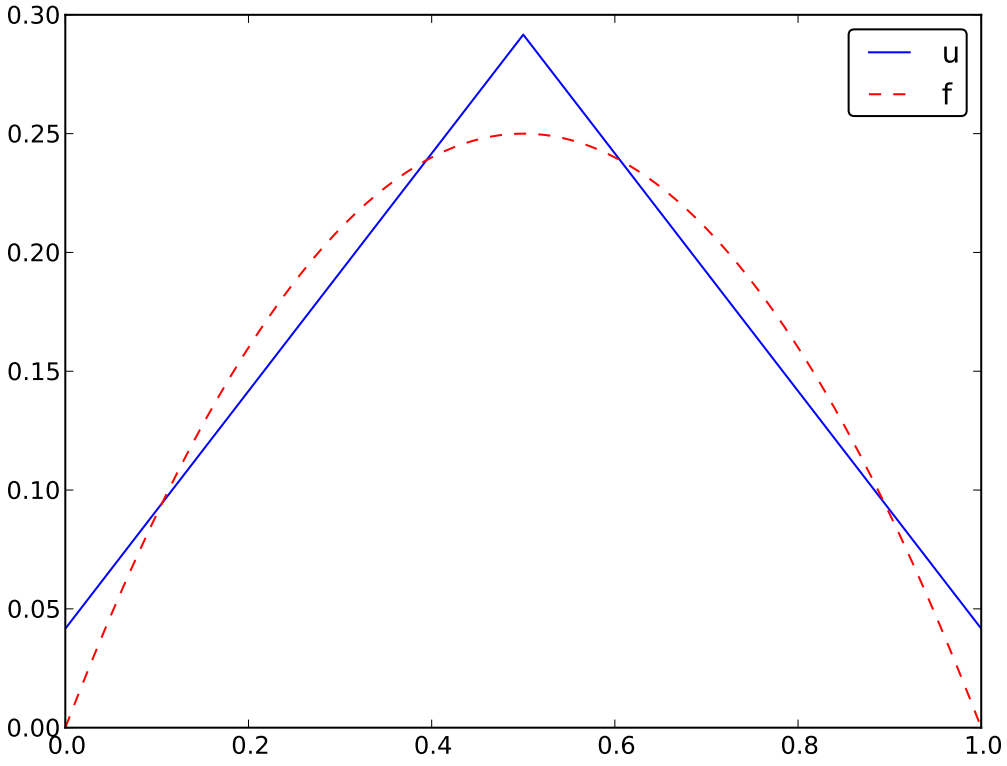
- $f(x) = x(1-x)$ on $\Omega = [0,1]$
- Two equal-sized elements $[0, 0.5]$ and $[0.5, 1]$

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

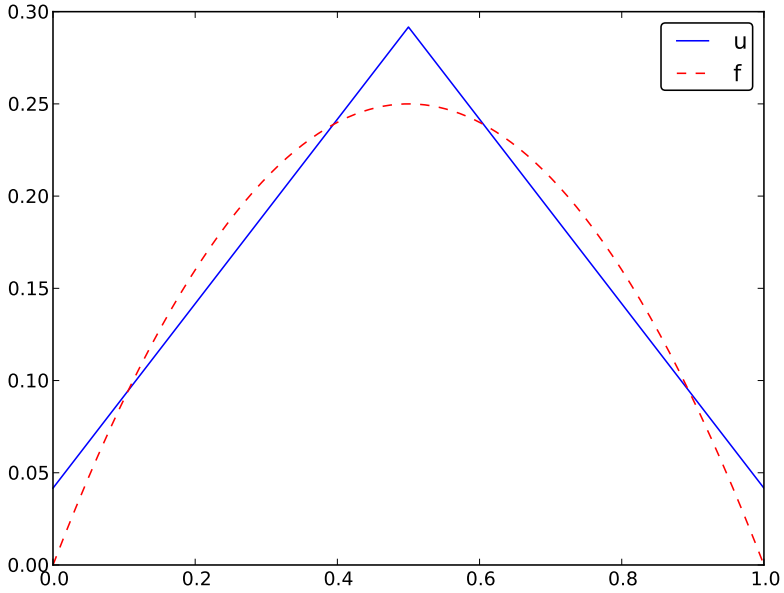
$$c_0 = \frac{h^2}{6}, \quad c_1 = h - \frac{5}{6}h^2, \quad c_2 = 2h - \frac{23}{6}h^2$$

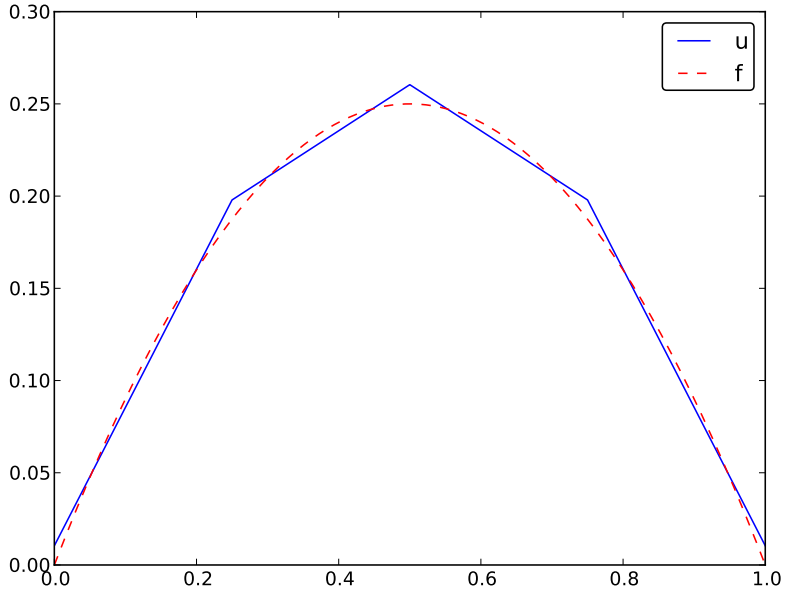
Specific example with two elements; plot

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



Specific example: what about four elements?





Assembly of elementwise computations

Split the integrals into elementwise integrals

$$A_{i,j} = \int_\Omega \varphi_i \varphi_j dx = \sum_e \int_{\Omega^{(e)}} \varphi_i \varphi_j dx, \quad A_{i,j}^{(e)} = \int_{\Omega^{(e)}} \varphi_i \varphi_j dx \quad (39)$$

Important:

- $A_{i,j}^{(e)} \neq 0$ if and only if i and j are nodes in element e (otherwise no overlap between the basis functions)
- all the nonzero elements in $A_{i,j}^{(e)}$ are collected in an *element matrix*

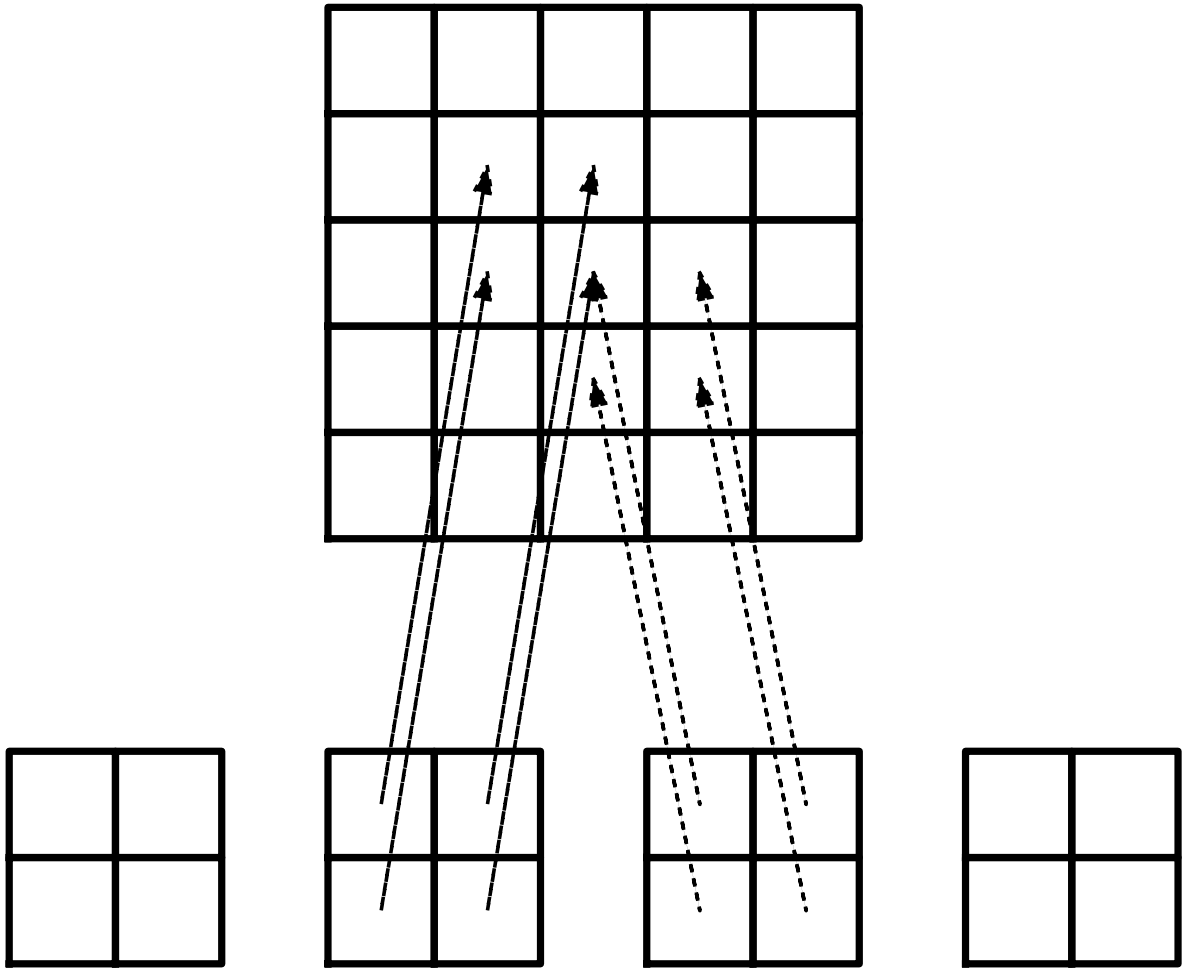
The element matrix

$$\tilde{A}^{(e)} = \{\tilde{A}^{(e)}_{r,s}\}, \quad \tilde{A}^{(e)}_{r,s} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}\varphi_{q(e,s)}dx, \quad r,s \in I_d = \{0,\ldots,d\}$$

- r, s run over *local node numbers* in an element; i, j run over *global node numbers*
- $i = q(e, r)$: mapping of local node number r in element e to the global node number i (math equivalent to `i=elements[e][r]`)
- Add $\tilde{A}^{(e)}_{r,s}$ into the global $A_{i,j}$ (*assembly*)

$$A_{q(e,r),q(e,s)} := A_{q(e,r),q(e,s)} + \tilde{A}^{(e)}_{r,s}, \quad r,s \in I_d \tag{40}$$

Illustration of the matrix assembly: regularly numbered P1 elements



Animation

Illustration of the matrix assembly: regularly numbered P3 elements

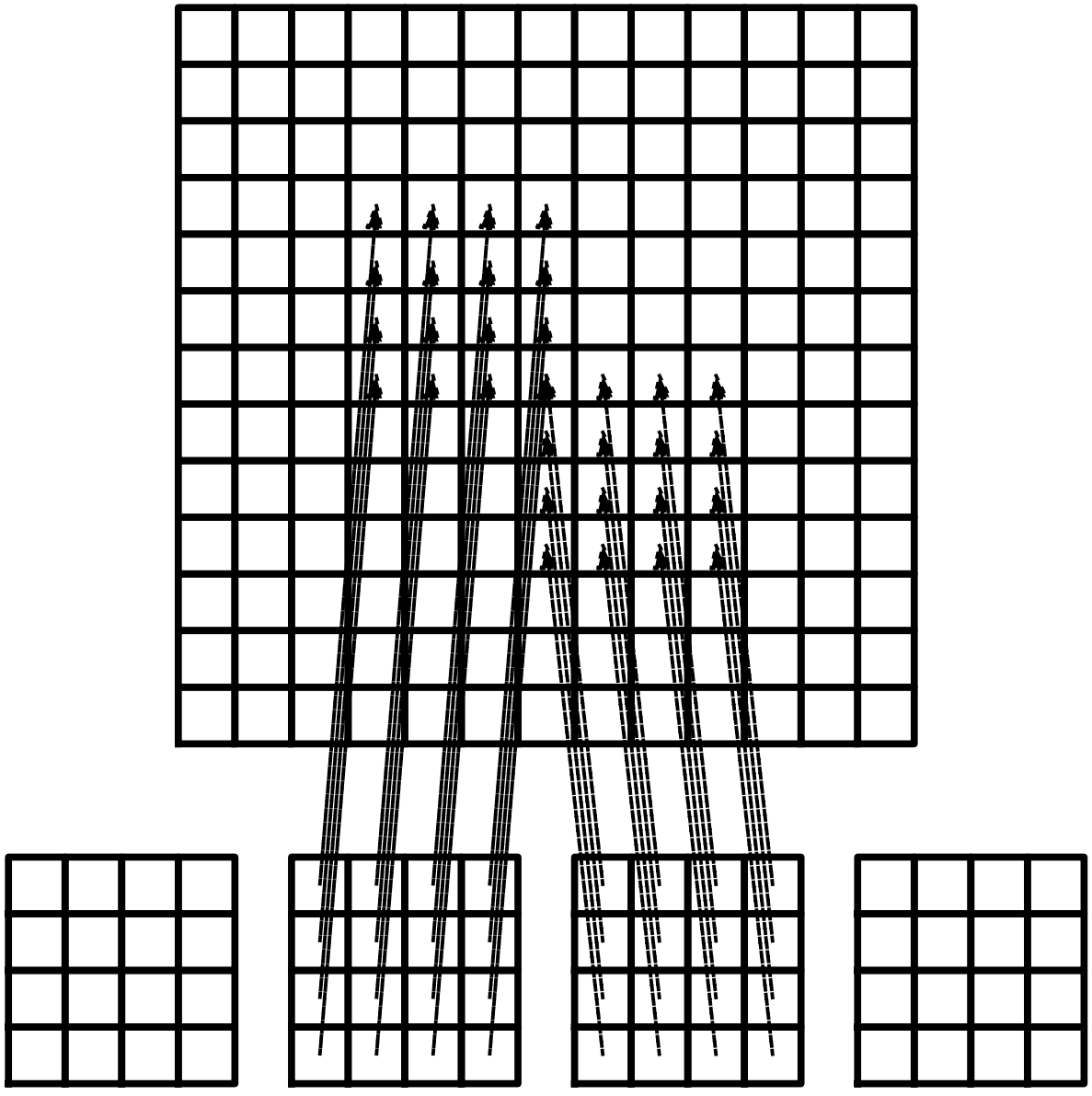
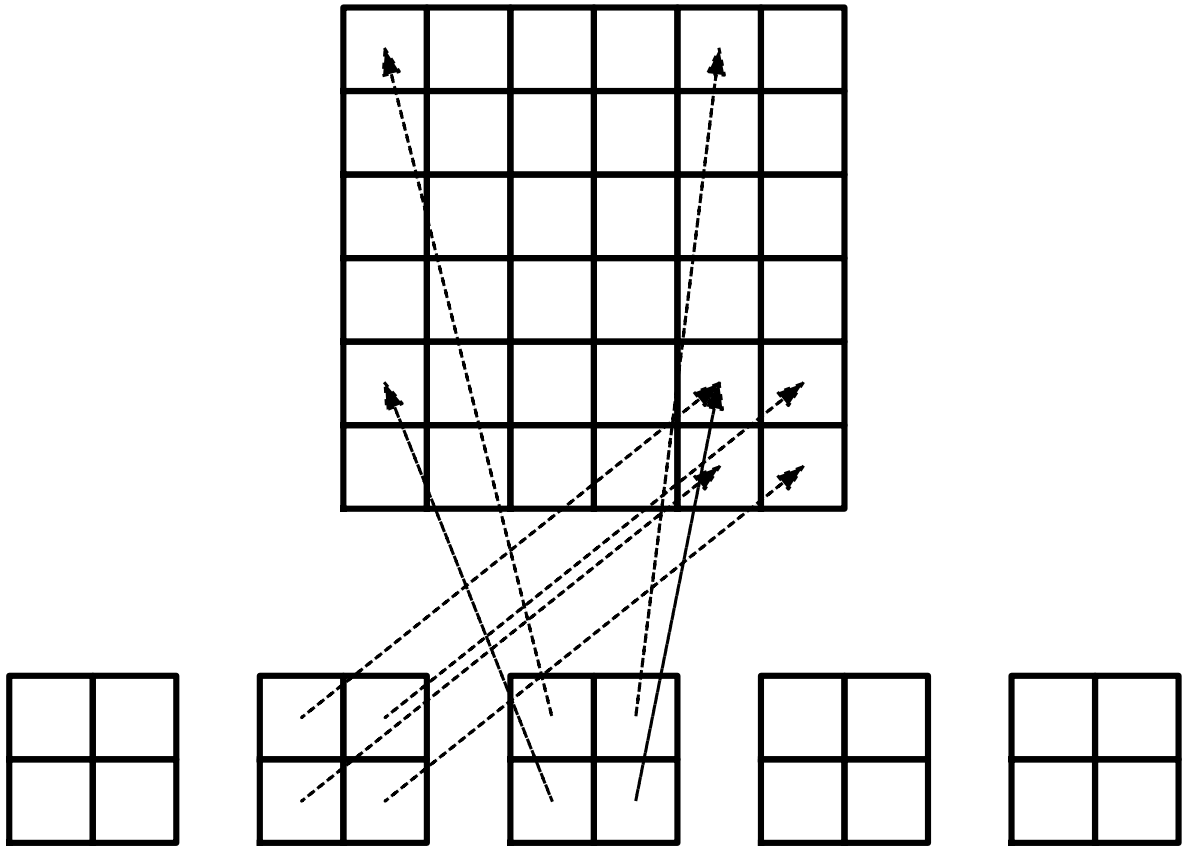


Illustration of the matrix assembly: irregularly numbered P1 elements



Animation

Assembly of the right-hand side

$$b_i = \int_\Omega f(x)\varphi_i(x)dx = \sum_e \int_{\Omega^{(e)}} f(x)\varphi_i(x)dx, \quad b_i^{(e)} = \int_{\Omega^{(e)}} f(x)\varphi_i(x)dx \tag{41}$$

Important:

- $b_i^{(e)} \neq 0$ if and only if global node i is a node in element e (otherwise $\varphi_i = 0$)
- The $d+1$ nonzero $b_i^{(e)}$ can be collected in an *element vector* $\tilde{b}_r^{(e)} = \{\tilde{b}_r^{(e)}\}$, $r \in I_d$

Assembly:

$$b_{q(e,r)} := b_{q(e,r)} + \tilde{b}_r^{(e)}, \quad r, s \in I_d \tag{42}$$

Mapping to a reference element

Instead of computing

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

we now map $[x_L, x_R]$ to a standardized reference element domain $[-1, 1]$ with local coordinate X

Affine mapping

$$x = \frac{1}{2}(x_L + x_R) + \frac{1}{2}(x_R - x_L)X \tag{43}$$

or rewritten as

$$x = x_m + \frac{1}{2}hX, \qquad x_m = (x_L + x_R)/2 \tag{44}$$

Integral transformation

Reference element integration: just change integration variable from x to X. Introduce local basis function

$$\tilde{\varphi}_r(X) = \varphi_{q(e,r)}(x(X)) \tag{45}$$

$$\tilde{A}^{(e)}_{r,s} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}(x)\varphi_{q(e,s)}(x)dx = \int_{-1}^{1} \tilde{\varphi}_r(X)\tilde{\varphi}_s(X) \underbrace{\frac{dx}{dX}}_{\det J = h/2} dX = \int_{-1}^{1} \tilde{\varphi}_r \tag{46}$$

$$\tilde{b}^{(e)}_r = \int_{\Omega^{(e)}} f(x)\varphi_{q(e,r)}(x)dx = \int_{-1}^{1} f(x(X))\tilde{\varphi}_r(X) \det J \, dX \tag{47}$$

Advantages of the reference element

- Always the same domain for integration: $[-1, 1]$
- We only need formulas for $\tilde{\varphi}_r(X)$ over one element (no piecewise polynomial definition)
- $\tilde{\varphi}_r(X)$ is the same for all elements: no dependence on element length and location, which is "factored out" in the mapping and $\det J$

Standardized basis functions for P1 elements

$$\tilde{\varphi}_0(X) = \frac{1}{2}(1 - X) \tag{48}$$

$$\tilde{\varphi}_1(X) = \frac{1}{2}(1 + X) \tag{49}$$

Standardized basis functions for P2 elements

P2 elements:

$$\tilde{\varphi}_0(X) = \frac{1}{2}(X-1)X \tag{50}$$

$$\tilde{\varphi}_1(X) = 1 - X^2 \tag{51}$$

$$\tilde{\varphi}_2(X) = \frac{1}{2}(X+1)X \tag{52}$$

Easy to generalize to arbitrary order!

Integration over a reference element; element matrix

P1 elements and $f(x) = x(1-x)$.

$$\tilde{A}^{(e)}_{0,0} = \int_{-1}^{1} \tilde{\varphi}_0(X)\tilde{\varphi}_0(X)\frac{h}{2}dX$$
$$= \int_{-1}^{1} \frac{1}{2}(1-X)\frac{1}{2}(1-X)\frac{h}{2}dX = \frac{h}{8}\int_{-1}^{1}(1-X)^2 dX = \frac{h}{3} \tag{53}$$

$$\tilde{A}^{(e)}_{1,0} = \int_{-1}^{1} \tilde{\varphi}_1(X)\tilde{\varphi}_0(X)\frac{h}{2}dX$$
$$= \int_{-1}^{1} \frac{1}{2}(1+X)\frac{1}{2}(1-X)\frac{h}{2}dX = \frac{h}{8}\int_{-1}^{1}(1-X^2) dX = \frac{h}{6} \tag{54}$$

$$\tilde{A}^{(e)}_{0,1} = \tilde{A}^{(e)}_{1,0} \tag{55}$$

$$\tilde{A}^{(e)}_{1,1} = \int_{-1}^{1} \tilde{\varphi}_1(X)\tilde{\varphi}_1(X)\frac{h}{2}dX$$
$$= \int_{-1}^{1} \frac{1}{2}(1+X)\frac{1}{2}(1+X)\frac{h}{2}dX = \frac{h}{8}\int_{-1}^{1}(1+X)^2 dX = \frac{h}{3}$$

Integration over a reference element; element vector

$$\tilde{b}_0^{(e)} = \int_{-1}^{1} f(x(X))\tilde{\varphi}_0(X)\frac{h}{2}dX$$
$$= \int_{-1}^{1} (x_m + \frac{1}{2}hX)(1 - (x_m + \frac{1}{2}hX))\frac{1}{2}(1 - X)\frac{h}{2}dX$$
$$= -\frac{1}{24}h^3 + \frac{1}{6}h^2 x_m - \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m \quad (57)$$
$$\tilde{b}_1^{(e)} = \int_{-1}^{1} f(x(X))\tilde{\varphi}_1(X)\frac{h}{2}dX$$
$$= \int_{-1}^{1} (x_m + \frac{1}{2}hX)(1 - (x_m + \frac{1}{2}hX))\frac{1}{2}(1 + X)\frac{h}{2}dX$$
$$= -\frac{1}{24}h^3 - \frac{1}{6}h^2 x_m + \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m \quad (58)$$

x_m: element midpoint.

Tedious calculations! Let's use symbolic software

```
>>> 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
```

Can printe out in LaTeX too (convenient for copying into reports):

```
>>> 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}
```

Implementation

- Coming functions appear in `fe_approx1D.py`
- Functions can operate in symbolic or numeric mode
- The code documents all steps in finite element calculations!

Compute finite element basis functions in the reference element

Let $\tilde{\varphi}_r(X)$ be 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

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

Compute 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
```

Example on symbolic vs numeric element matrix

```
>>> 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]
```

Compute the element vector

```
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
```

Note `f.subs('x', x)`: replace `x` by $x(X)$ such that `f` contains `X`

Fallback on numerical integration if symbolic integration fails

- Element matrix: only polynomials and `sympy` always succeeds
- Element vector: $\int f\tilde{\varphi}\,\mathrm{d}x$ can fail (`sympy` then returns an `Integral` object instead of a number)

```
def element_vector(f, phi, Omega_e, symbolic=True):
        ...
        I = sm.integrate(f*phi[r]*detJ, (X, -1, 1))  # try...
        if 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
        ...
```

Linear system assembly and solution

```
def assemble(nodes, elements, phi, f, symbolic=True):
    N_n, N_e = len(nodes), len(elements)
    zeros = sm.zeros if symbolic else np.zeros
    A = zeros((N_n, N_n))
    b = zeros((N_n, 1))
    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
```

Linear system solution

```
if symbolic:
    c = A.LUsolve(b)            # sympy arrays, symbolic Gaussian el
else:
    c = np.linalg.solve(A, b)   # numpy arrays, numerical solve
```

Note: the symbolic computation of `A` and `b` and the symbolic solution can be very tedious.

Example on computing symbolic approximations

```
>>> 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)]
```

Example on computing numerical approximations

```
>>> 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, 0.083333333333333,                   0]
[0.083333333333333,  0.333333333333333, 0.083333333333333]
[                 0, 0.083333333333333,  0.166666666666667]
>>> b
[          0.03125]
[0.104166666666667]
[          0.03125]
>>> c = A.LUsolve(b)
>>> c
[0.041666666666666]
[ 0.291666666666667]
[0.041666666666666]
```

The structure of the coefficient matrix

```
>>> 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,   0]
[h/6, 2*h/3,   h/6,     0,     0,     0,     0,     0,   0]
[  0,   h/6, 2*h/3,   h/6,     0,     0,     0,     0,   0]
[  0,     0,   h/6, 2*h/3,   h/6,     0,     0,     0,   0]
[  0,     0,     0,   h/6, 2*h/3,   h/6,     0,     0,   0]
[  0,     0,     0,     0,   h/6, 2*h/3,   h/6,     0,   0]
[  0,     0,     0,     0,     0,   h/6, 2*h/3,   h/6,   0]
[  0,     0,     0,     0,     0,     0,   h/6, 2*h/3, h/6]
[  0,     0,     0,     0,     0,     0,     0,   h/6, h/3]
```

Note: do this by hand to understand what is going on!

General result: the coefficient matrix is sparse

- Sparse = most of the entries are zeros
- Below: P1 elements

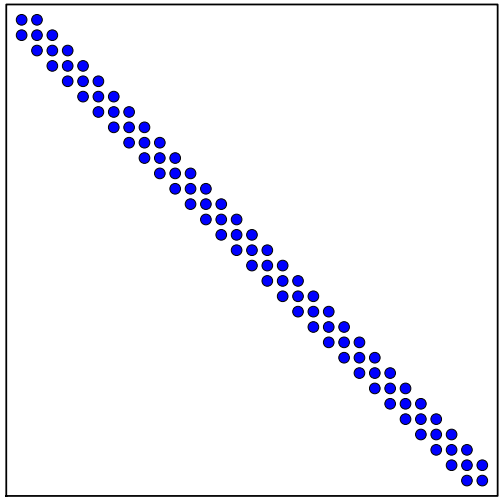
$$A = \frac{h}{6}\begin{pmatrix} 2 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 1 & 4 & 1 & \ddots & & & & & \vdots \\ 0 & 1 & 4 & 1 & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & 1 & 4 & 1 & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & 1 & 4 & 1 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 1 & 2 \end{pmatrix} \tag{59}$$

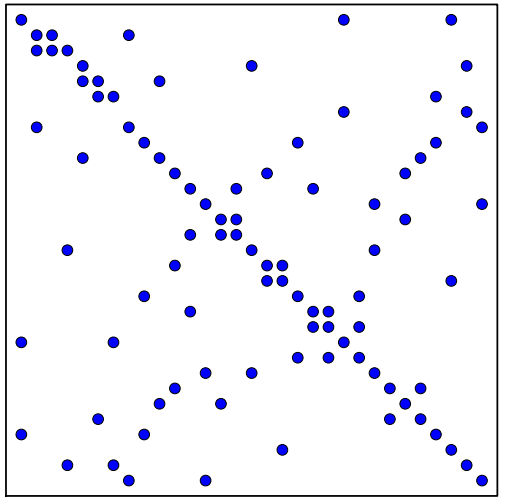
Exemplifying the sparsity for P2 elements

$$A = \frac{h}{30}\begin{pmatrix} 4 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 16 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & 8 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 16 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & 4 \end{pmatrix} \tag{60}$$

Matrix sparsity pattern for regular/random numbering of P1 elements

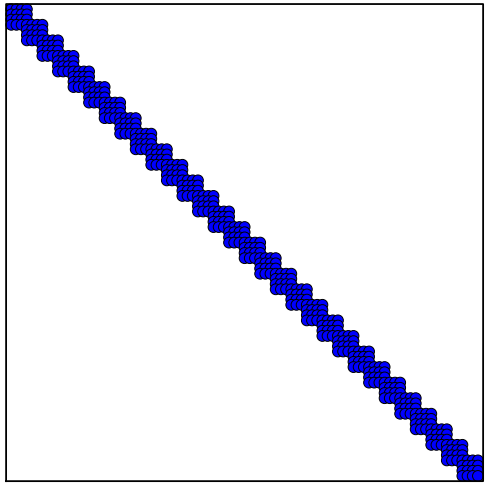
- Left: number nodes and elements from left to right
- Right: number nodes and elements arbitrarily

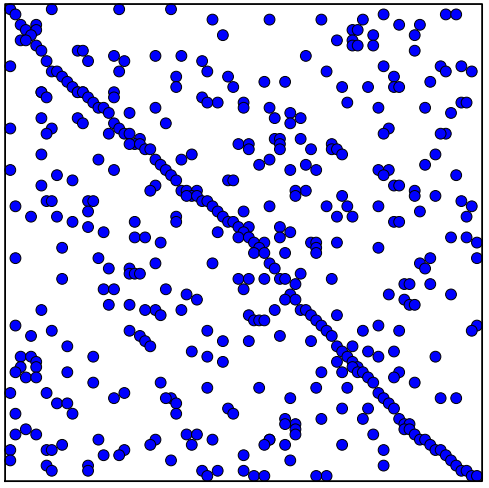




Matrix sparsity pattern for regular/random numbering of P3 elements

- Left: number nodes and elements from left to right
- Right: number nodes and elements arbitrarily





Sparse matrix storage and solution

The minimum storage requirements for the coefficient matrix $A_{i,j}$:

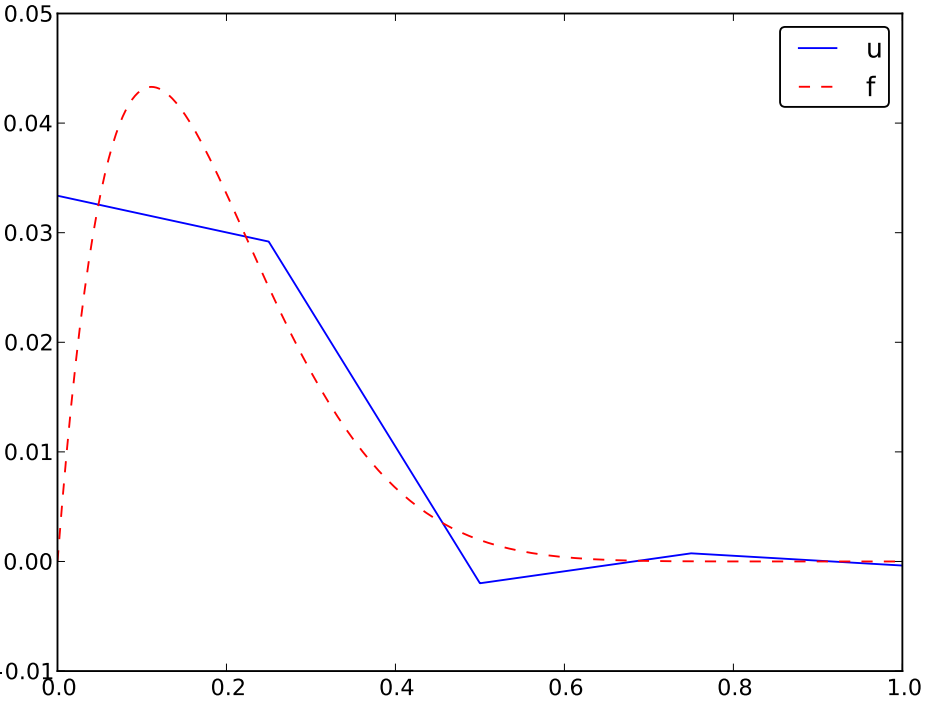
- P1 elements: only 3 nonzero entires per row
- P2 elements: only 5 nonzero entires per row
- P3 elements: only 7 nonzero entires per row
- It is important to utilize sparse storage and sparse solvers
- In Python: `scipy.sparse` package

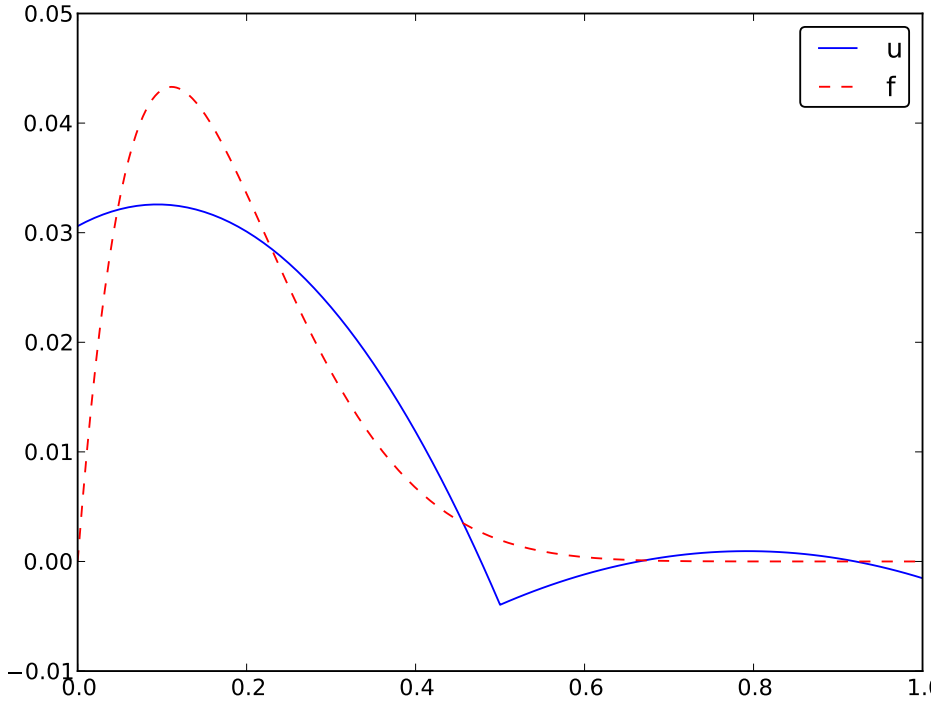
Approximate $f \sim x^9$ by various elements; code

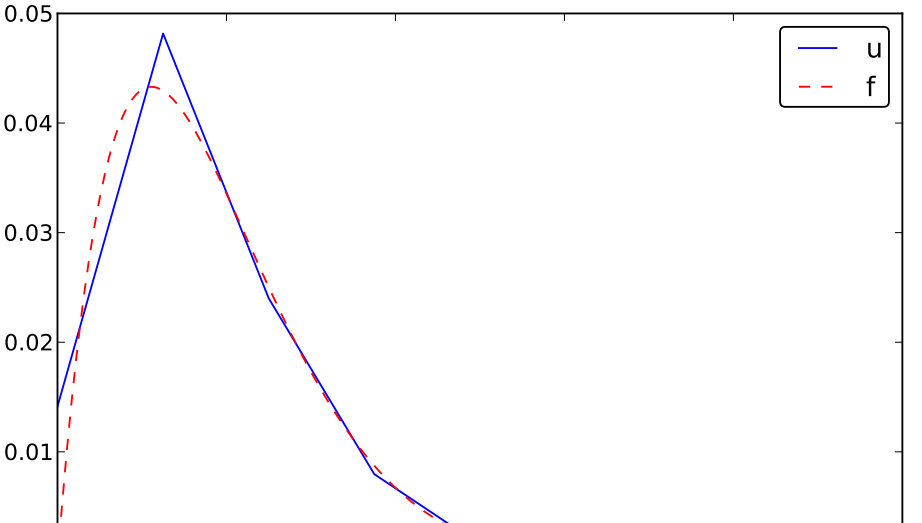
Compute a mesh with N_e elements, basis functions of degree d, and approximate a given symbolic expression $f(x)$ by a finite element expansion $u(x) = \sum_j c_j \varphi_j(x)$:

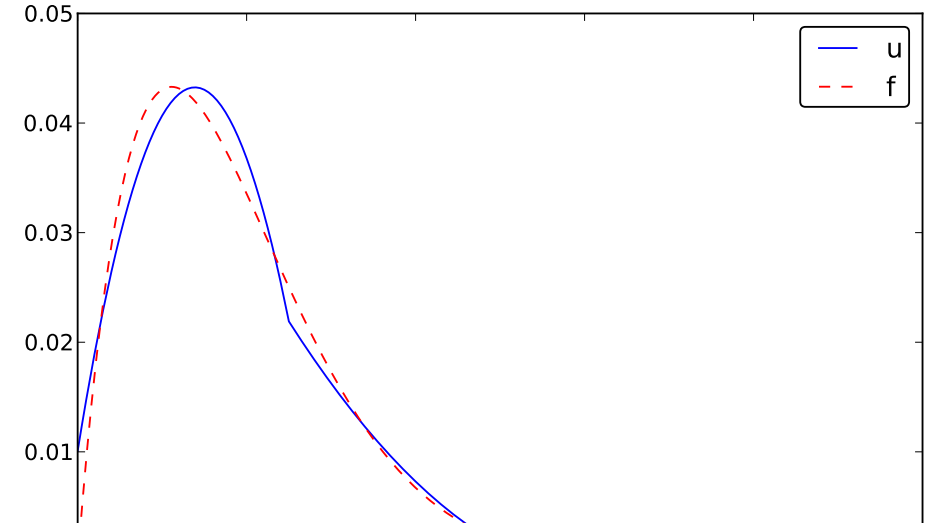
```
import sympy as sm
from fe_approx1D import approximate
x = sm.Symbol('x')

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)
```

Approximate $f \sim x^9$ by various elements; plot









Comparison of finite element and finite difference approximation

- Finite difference approximation of a function $f(x)$: simply choose $u_i = f(x_i)$ (interpolation)
- Galerkin/projection and least squares method: must derive and solve a linear system
- What is *really* the difference in u?

Interpolation/collocation with finite elements

Let $\{x_i\}_{i\in I}$ be the nodes in the mesh. Collocation means

$$u(x_i) = f(x_i), \quad i \in I, \tag{61}$$

which translates to

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

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

$$c_i = f(x_i) \tag{62}$$

Same result as the standard finite difference approach, finite elements define u also between the x_i points

How does finite elements compare with finite differences?

- Scope: work with P1 elements
- Use projection/Galerkin or least squares (equivalent)
- Interpret the resulting linear system as finite difference equations

The P1 finite element machinery results in a linear system where equation no i is

$$\frac{h}{6}(u_{i-1} + 4u_i + u_{i+1}) = (f, \varphi_i) \tag{63}$$

Note:

- We have used u_i for c_i to simplify notation with finite differences
- The finite difference counterpart is just $u_i = f_i$

Expressing the left-hand side in finite difference operator notation

Rewrite the left-hand side of finite element equation no i:

$$h(u_i - \frac{1}{6}(-u_{i-1} + 2u_i - u_{i+1})) = [h(u - \frac{h^2}{6} D_x D_x u)]_i \qquad (64)$$

This is the standard finite difference approximation of

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

Treating the right-hand side; Trapezoidal rule

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

Cannot do much unless we specialize f or use *numerical integration*.
Trapezoidal rule using the nodes:

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

$\varphi_i(x_j) = \delta_{ij}$, so this formula collapses to one term:

$$(f,\varphi_i) \approx hf(x_i), \quad i = 1,\ldots,N-1\,. \tag{65}$$

Same result as in collocation (interpolation) and the finite difference method!

Treating the right-hand side; Simpson's rule

$$\int_\Omega g(x)dx \approx \frac{h}{6}\left(g(x_0) + 2\sum_{j=1}^{N-1} g(x_j) + 4\sum_{j=0}^{N-1} g(x_{j+\frac{1}{2}}) + f(x_{2N})\right),$$

Our case: $g = f\varphi_i$. The sums collapse because $\varphi_i = 0$ at most of the points.

$$(f, \varphi_i) \approx \frac{h}{3}(f_{i-\frac{1}{2}} + f_i + f_{i+\frac{1}{2}}) \tag{66}$$

Conclusions:

- While the finite difference method just samples f at x_i, the finite element method applies an average of f around x_i
- On the left-hand side we have a term $\sim hu''$, and u'' also contribute to smoothing
- There is some inherent smoothing in the finite element method

Finite element approximation vs finite differences

With Trapezoidal integration of (f, φ_i), the finite element metod essentially solve

$$u + \frac{h^2}{6} u'' = f, \quad u'(0) = u'(L) = 0, \tag{67}$$

by the finite difference method

$$[u + \frac{h^2}{6} D_x D_x u = f]_i \tag{68}$$

With Simpson integration of (f, φ_i) we essentially solve

$$[u + \frac{h^2}{6} D_x D_x u = \bar{f}]_i, \tag{69}$$

where

$$\bar{f}_i = \frac{1}{3}(f_{i-1/2} + f_i + f_{i+1/2})$$

Note: as $h \to 0$, $hu'' \to 0$ and $\bar{f}_i \to f_i$.

Making finite elements behave as finite differences

- Can we adjust the finite element method so that we do not get the extra hu'' smoothing term and averaging of f?
- This is important in time-dependent problems to incorporate good properties of finite differences into finite elements

Result:

- Compute all integrals by the Trapezoidal method and P1 elements
- Specifically, the coefficient matrix becomes diagonal ("lumped") - no linear system (!)
- Loss of accuracy? The Trapezoidal rule has error $\mathcal{O}(h^2)$, the same as the approximation error in P1 elements

Limitations of the nodes and element concepts

So far,

- *Nodes*: points for defining φ_i and compute u values
- *Elements*: subdomain (containing a few nodes)
- This is a common notion of nodes and elements

One problem:

- Our algorithms need nodes at the element boundaries
- This is often not desirable, so we need to throw the `nodes` and `elements` arrays away and find a more generalized element concept

A generalized element concept

- We introduce *cell* for the subdomain that we up to now called element
- A cell has *vertices* (interval end points)
- *Nodes* are, almost as before, points where we want to compute unknown functions
- *Degrees of freedom* is what the c_j represent (usually function values at nodes)

The concept of a finite element

1. a *reference cell* in a local reference coordinate system
2. a set of *basis functions* $\tilde{\varphi}_i$ defined on the cell
3. a set of *degrees of freedom* (e.g., function values) 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
4. a mapping between local and global degree of freedom numbers (*dof map*)
5. a geometric *mapping* of the reference cell onto to cell in the physical domain: $[-1, 1] \quad \Rightarrow \quad [x_L, x_R]$

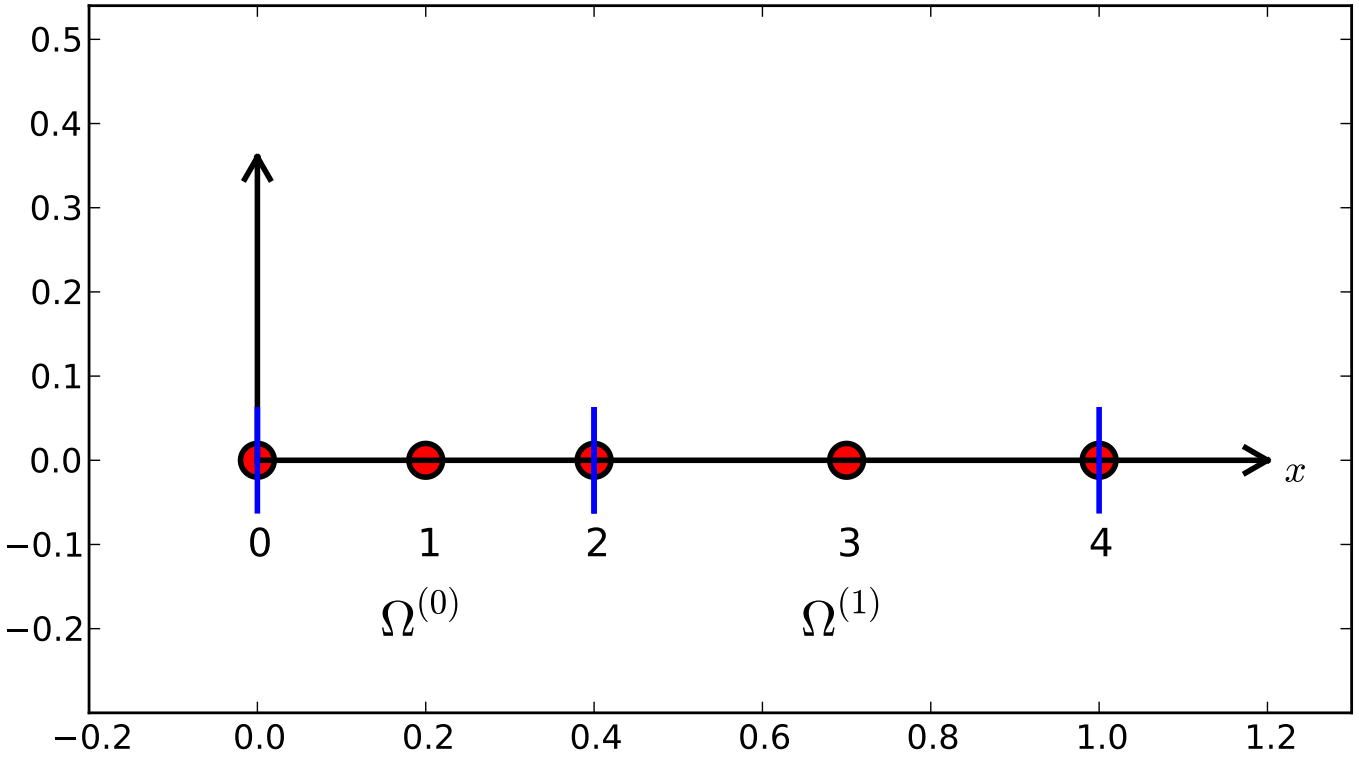
Implementation; basic data structures

- Cell vertex coordinates: `vertices` equals `nodes` for P1 elements
- Element vertices: `cell[e][r]` holds global vertex number of local vertex no `r` in element `e` (same as `elements` for P1 elements)
- `dof_map[e,r]` maps local dof `r` in element `e` to global dof number (same as `elements` for Pd elements)

The assembly process applies `dof_map` (no more `elements` list!):

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

Implementation; example with P2 elements




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

Implementation; example with P0 elements

Example: Same mesh, but u is piecewise constant in each cell (P0 element). Same `vertices` and `cells`, but

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

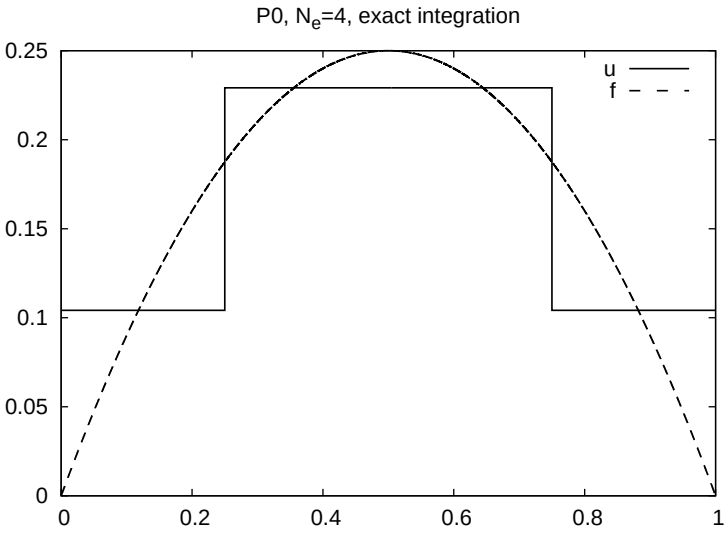
May think of nodes in the middle of each element.

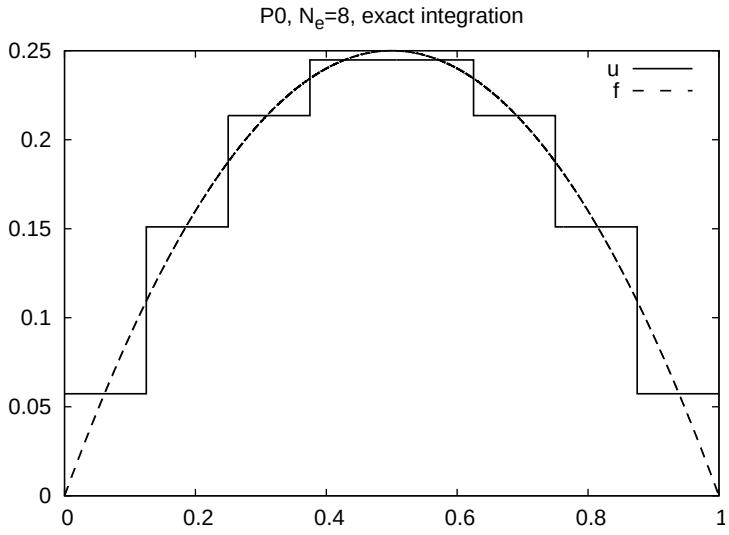
We will hereafter work with `cells`, `vertices`, and `dof_map`.

Example on doing the algorithmic steps

```
# Use modified fe_approx1D module
from fe_approx1D_numint import *

x = sm.Symbol('x')
f = x*(1 - x)

N_e = 10
# Create mesh
vertices, cells, dof_map = mesh_uniform(N_e, d=3, Omega=[0,1])

# Create basis functions on the mesh
phi = [basis(len(dof_map[e])-1) for e in range(N_e)]

# Create linear system and solve it
A, b = assemble(vertices, cells, dof_map, phi, f)
c = np.linalg.solve(A, b)

# Make very fine mesh and sample u(x) on this mesh for plotting
x_u, u = u_glob(c, vertices, cells, dof_map,
                resolution_per_element=51)
plot(x_u, u)
```

Approximating a parabola by P0 elements





The `approximate` function automates the steps in the previous slide:

```
from fe_approx1D_numint import *
x=sm.Symbol("x")
for N_e in 4, 8:
    approximate(x*(1-x), d=0, N_e=N_e, Omega=[0,1])
```

Computing the error of the approximation; principles

$$L^2 \text{ error:} \qquad ||e||_{L^2} = \left(\int_\Omega e^2 dx \right)^{1/2}$$

Accurate approximation of the integral:

- Sample $u(x)$ at many points in each element
- `u_glob` does this and returns `x` and `u`
- Use the Trapezoidal rule based on the samples

Computing the error of the approximation; details

Note.

We need a version of the Trapezoidal rule valid for non-uniformly spaced points:

$$\int_\Omega g(x)dx \approx \sum_{j=0}^{n-1} \frac{1}{2}(g(x_j) + g(x_{j+1}))(x_{j+1} - x_j)$$

```
# Given c, compute x and u values on a very fine mesh
x, u = u_glob(c, vertices, cells, dof_map,
              resolution_per_element=101)
# Compute the error on the very fine mesh
e = f(x) - u
e2 = e**2
# Vectorized Trapezoidal rule
E = np.sqrt(0.5*np.sum((e2[:-1] + e2[1:])*(x[1:] - x[:-1])))
```

How does the error depend on h and d?

Theory and experiments show that the least squares or projection/Galerkin method in combination with Pd elements of equal length h has an error

$$||e||_{L^2} = Ch^{d+1} \tag{70}$$

where C depends on f, but not on h or d.

Cubic Hermite polynomials; definition

- Can we construct $\varphi_i(x)$ with continuous derivatives? Yes!

Consider a reference cell $[-1, 1]$. We introduce two nodes, $X = -1$ and $X = 1$. The degrees of freedom are

- 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 $X = 1$

Derivatives as unknowns ensure the same $\varphi_i'(x)$ value at nodes and thereby continuous derivatives.

Cubic Hermite polynomials; derivation

4 constraints on $\tilde{\varphi}_r$ (1 for dof r, 0 for all others):

- $\tilde{\varphi}_0(X_{(0)}) = 1$, $\tilde{\varphi}_0(X_{(1)}) = 0$, $\tilde{\varphi}_0'(X_{(0)}) = 0$, $\tilde{\varphi}_0'(X_{(1)}) = 0$
- $\tilde{\varphi}_1'(X_{(0)}) = 1$, $\tilde{\varphi}_1'(X_{(1)}) = 0$, $\tilde{\varphi}_1(X_{(0)}) = 0$, $\tilde{\varphi}_1(X_{(1)}) = 0$
- $\tilde{\varphi}_2(X_{(1)}) = 1$, $\tilde{\varphi}_2(X_{(0)}) = 0$, $\tilde{\varphi}_2'(X_{(0)}) = 0$, $\tilde{\varphi}_2'(X_{(1)}) = 0$
- $\tilde{\varphi}_3'(X_{(1)}) = 1$, $\tilde{\varphi}_3'(X_{(0)}) = 0$, $\tilde{\varphi}_3(X_{(0)}) = 0$, $\tilde{\varphi}_3(X_{(1)}) = 0$

This gives 4 linear, coupled equations *for each* $\tilde{\varphi}_r$ to determine the 4 coefficients in the cubic polynomial. Result:

$$\tilde{\varphi}_0(X) = 1 - \frac{3}{4}(X+1)^2 + \frac{1}{4}(X+1)^3 \tag{71}$$

$$\tilde{\varphi}_1(X) = -(X+1)(1 - \frac{1}{2}(X+1))^2 \tag{72}$$

$$\tilde{\varphi}_2(X) = \frac{3}{4}(X+1)^2 - \frac{1}{2}(X+1)^3 \tag{73}$$

$$\tilde{\varphi}_3(X) = -\frac{1}{2}(X+1)(\frac{1}{2}(X+1)^2 - (X+1)) \tag{74}$$

$$\tag{75}$$

Numerical integration

- $\int_\Omega f\varphi_i dx$ must in general be computed by numerical integration
- Numerical integration is often used for the matrix too

Common form:

$$\int_{-1}^{1} g(X)dX \approx \sum_{j=0}^{M} w_j \bar{X}_j, \tag{76}$$

where

- $\bar{X}_j$ are *integration points*
- w_j are *integration weights*
- Different rules correspond to different choices of points and weights

The Midpoint rule

Simplest possibility: the Midpoint rule,

$$\int_{-1}^{1} g(X)dX \approx 2g(0), \quad \bar{X}_0 = 0, \; w_0 = 2, \tag{77}$$

Exact for linear integrands

Newton-Cotes rules

- Idea: use a fixed, uniformly distributed set of points
- The points often coincides with nodes
- Very useful for making $\varphi_i \varphi_j = 0$ and get diagonal ("mass") matrices ("lumping").

The Trapezoidal rule:

$$\int_{-1}^{1} g(X)dX \approx g(-1) + g(1), \quad \bar{X}_0 = -1,\ \bar{X}_1 = 1,\ w_0 = w_1 = 1, \tag{78}$$

Simpson's rule:

$$\int_{-1}^{1} g(X)dX \approx \frac{1}{3}\left(g(-1) + 4g(0) + g(1)\right), \tag{79}$$

where

$$\bar{X}_0 = -1,\ \bar{X}_1 = 0,\ \bar{X}_2 = 1,\ w_0 = w_2 = \frac{1}{3},\ w_1 = \frac{4}{3} \tag{80}$$

Gauss-Legendre rules with optimized points

- Optimize the location of points to get higher accuracy
- Gauss-Legendre rules (quadrature) adjust points and weights to integrate polynomials exactly

$$M = 1: \quad \bar{X}_0 = -\frac{1}{\sqrt{3}},\ \bar{X}_1 = \frac{1}{\sqrt{3}},\ w_0 = w_1 = 1 \tag{81}$$

$$M = 2: \quad \bar{X}_0 = -\sqrt{\frac{3}{5}},\ \bar{X}_0 = 0,\ \bar{X}_2 = \sqrt{\frac{3}{5}},\ w_0 = w_2 = \frac{5}{9},\ w_1 = \frac{8}{9} \tag{82}$$

- $M = 1$: integrates 3rd degree polynomials exactly
- $M = 2$: integrates 5th degree polynomials exactly
- In general, M-point rule integrates a polynomial of degree $2M + 1$ exactly.

See `numint.py` for a large collection of Gauss-Legendre rules.

Approximation of functions in 2D

Extensibility of 1D ideas.

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 $f(x, y, z)$. Key formulas stay the same.

Inner product in 2D:

$$(f, g) = \int_\Omega f(x, y) g(x, y) dxdy \tag{83}$$

Least squares and project/Galerkin lead to a linear system

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

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

$$b_i = (f, \psi_i)$$

Challenge: How to construct 2D basis functions $\psi_i(x, y)$?

2D basis functions as tensor products of 1D functions

Use a 1D basis for x variation and a similar for y variation:

$$V_x = \text{span}\{\hat{\psi}_0(x), \ldots, \hat{\psi}_{N_x}(x)\} \tag{84}$$

$$V_y = \text{span}\{\hat{\psi}_0(y), \ldots, \hat{\psi}_{N_y}(y)\} \tag{85}$$

The 2D vector space can be defined as a *tensor product* $V = V_x \otimes V_y$ with basis functions

$$\psi_{p,q}(x, y) = \hat{\psi}_p(x)\hat{\psi}_q(y) \quad p \in I_x, q \in I_y \, .$$

Tensor products

Given two vectors $a = (a_0, \ldots, a_M)$ and $b = (b_0, \ldots, b_N)$, their *outer tensor product*, also called the *dyadic product*, is $p = a \otimes b$, defined through

$$p_{i,j} = a_i b_j, \quad i = 0, \ldots, M, \; j = 0, \ldots, N\,.$$

Note: p has two indices (as matrix or two-dimensional array)
2D basis as tensor product of 1D spaces:

$$\psi_{p,q}(x, y) = \hat{\psi}_p(x)\hat{\psi}_q(y), \quad p \in I_x, q \in I_y$$

Double or single index?

The 2D basis can employ a double index and double sum:

$$u = \sum_{p \in I_x} \sum_{q \in I_y} c_{p,q} \psi_{p,q}(x, y)$$

Or just a single index:

$$u = \sum_{j \in I} c_j \psi_i(x, y)$$

with

$$\psi_i(x, y) = \hat{\psi}_p(x) \hat{\psi}_q(y), \quad i = pN_y + q \text{ or } i = qN_x + p$$

Example on 2D (bilinear) basis functions; formulas

In 1D we use the basis

$$\{1, x\}$$

2D tensor product (all combinations):

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

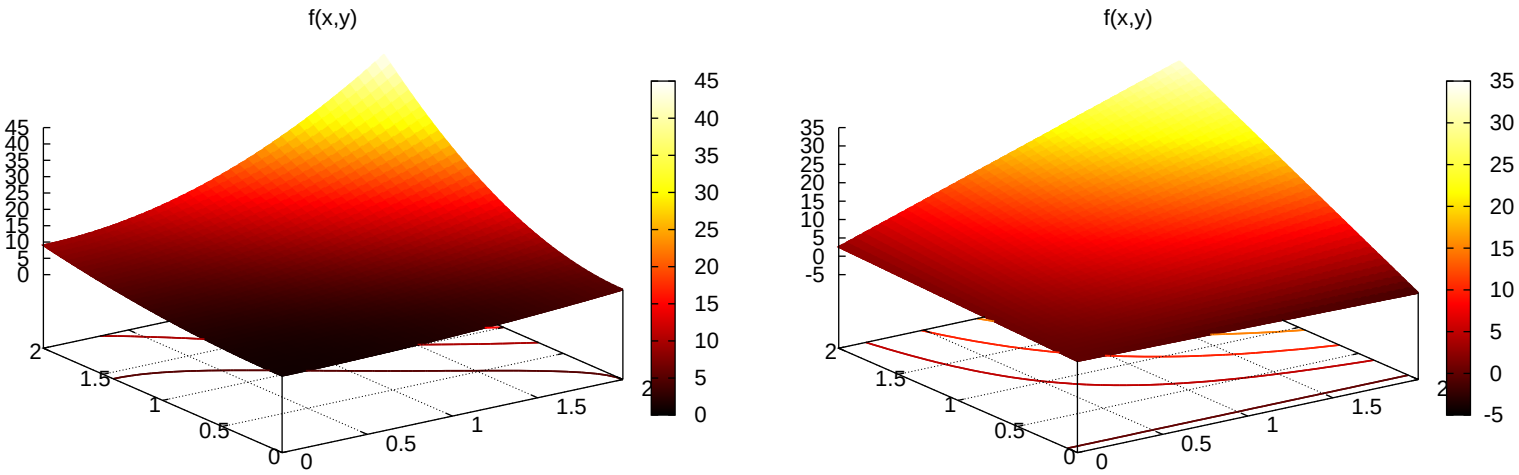
or with a single index:

$$\psi_0 = 1, \quad \psi_1 = x, \quad \psi_2 = y, \quad \psi_3 = xy$$

See notes for details of a hand-calculation.

Example on 2D (bilinear) basis functions; plot

Quadratic $f(x, y) = (1 + x^2)(1 + 2y^2)$ (left), bilinear u (right):



Implementation; principal changes to the 1D code

Very small modification of `approx1D.py`:

- `Omega = [[0, L_x], [0, L_y]]`
- Symbolic integration in 2D
- Construction of 2D (tensor product) basis functions

Implementation; 2D integration

```
import sympy as sm

integrand = psi[i]*psi[j]
I = sm.integrate(integrand,
                 (x, Omega[0][0], Omega[0][1]),
                 (y, Omega[1][0], Omega[1][1]))

# Fall back on numerical integration if symbolic integration
# was unsuccessful
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]])
```

Implementation; 2D basis functions

Tensor product of 1D "Taylor-style" polynomials x^i:

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

Tensor product of 1D sine functions $\sin((i+1)\pi x)$:

```
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)]
```

Complete code in `approx2D.py`

Implementation; application

$$f(x,y) = (1+x^2) * (1+2y^2)$$

```
>>> from approx2D import *
>>> f = (1+x**2)*(1+2*y**2)
>>> psi = taylor(x, y, 1, 1)
>>> Omega = [[0, 2], [0, 2]]
>>> u = least_squares(f, psi, 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
```

Implementation; trying a perfect expansion

Add higher powers to the basis such that $f \in V$:

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

Expected: $u = f$ when $f \in V$

Generalization to 3D

Key idea:

$$V = V_x \otimes V_y \otimes V_z$$

Repeated outer tensor product of multiple vectors.

$$\begin{aligned} a^{(q)} &= (a_0^{(q)}, \ldots, a_{N_q}^{(q)}, \quad q = 0, \ldots, m \\ p &= a^{(0)} \otimes \cdots \otimes a^{(m)} \\ p_{i_0, i_1, \ldots, i_m} &= a_{i_1}^{(0)} a_{i_1}^{(1)} \cdots a_{i_m}^{(m)} \end{aligned}$$

$$\begin{aligned} \psi_{p,q,r}(x, y, z) &= \hat{\psi}_p(x)\hat{\psi}_q(y)\hat{\psi}_r(z) \\ u(x, y, z) &= \sum_{p \in I_x} \sum_{q \in I_y} \sum_{r \in I_z} c_{p,q,r} \psi_{p,q,r}(x, y, z) \end{aligned}$$

Finite elements in 2D and 3D

The two great advantages of the finite element method:

- Can handle complex-shaped domains in 2D and 3D
- Can easily provide higher-order polynomials in the approximation

Finite elements in 1D: mostly for learning, insight, debugging

Examples on cell types

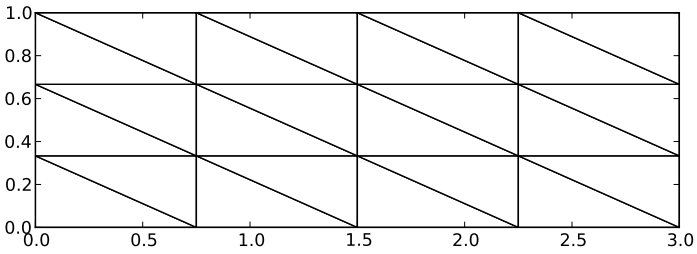
2D:

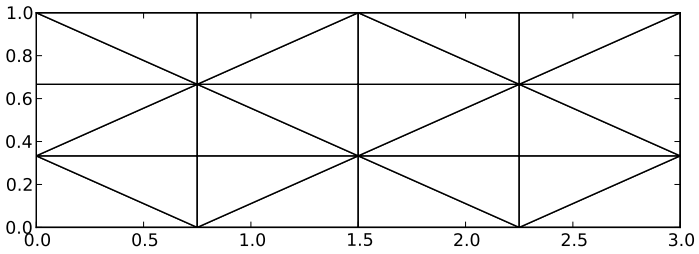
- triangles
- quadrilaterals

3D:

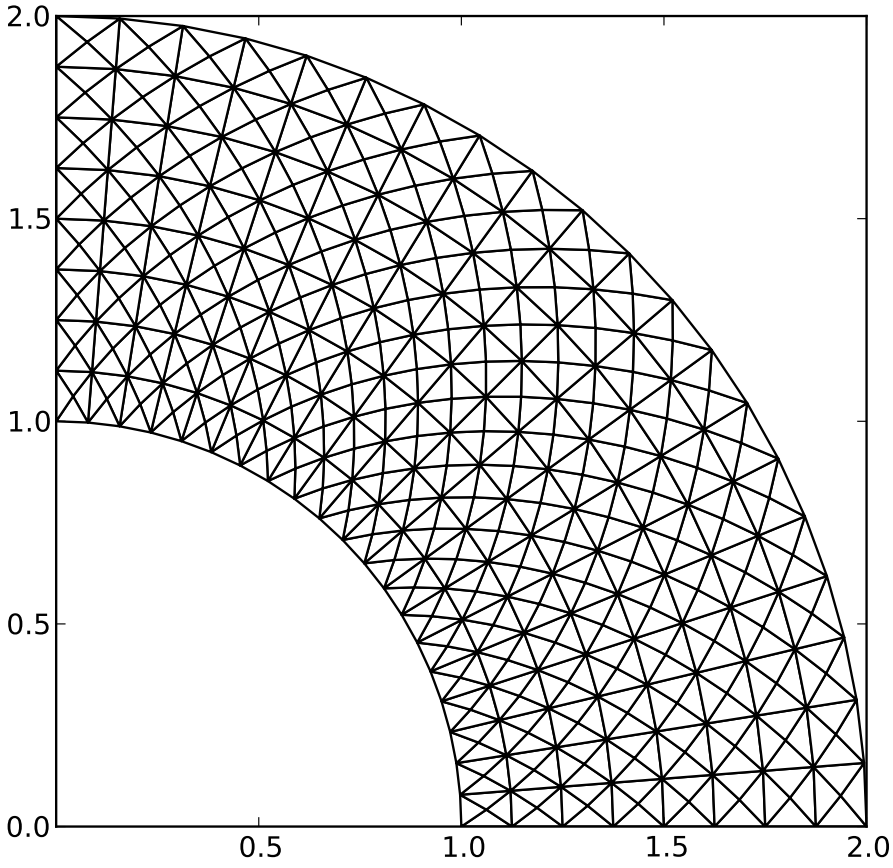
- tetrahedra
- hexahedra

Rectangular domain with 2D P1 elements

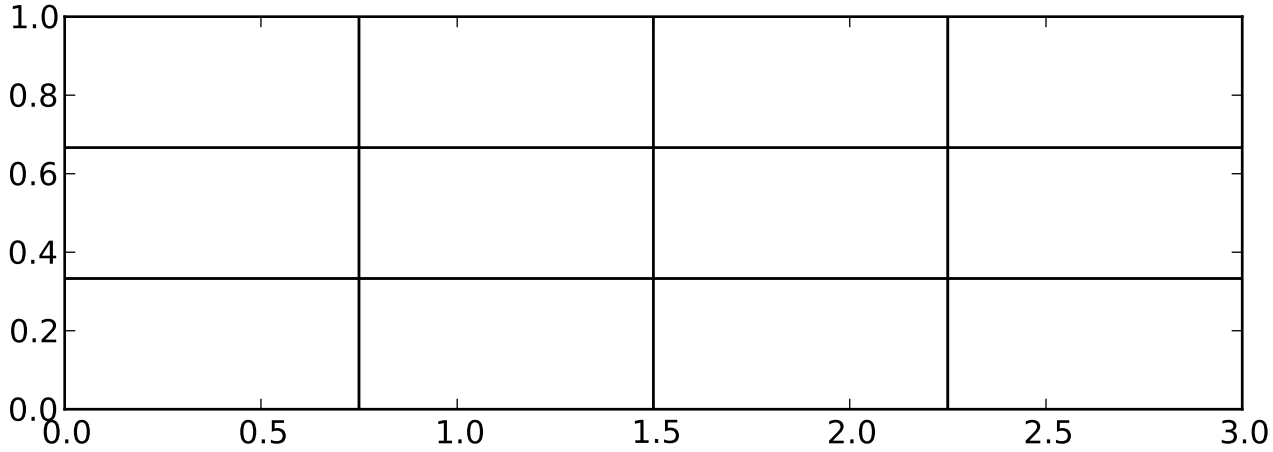




Deformed geometry with 2D P1 elements

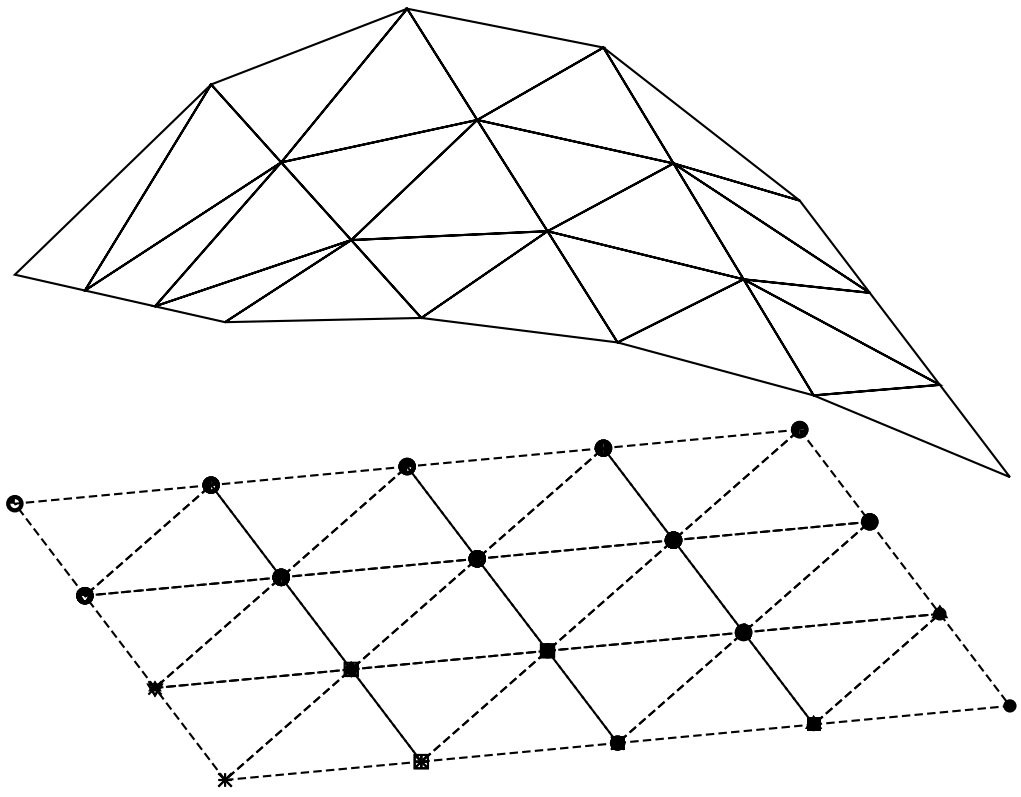


Rectangular domain with 2D Q1 elements



Basis functions over triangles in the physical domain

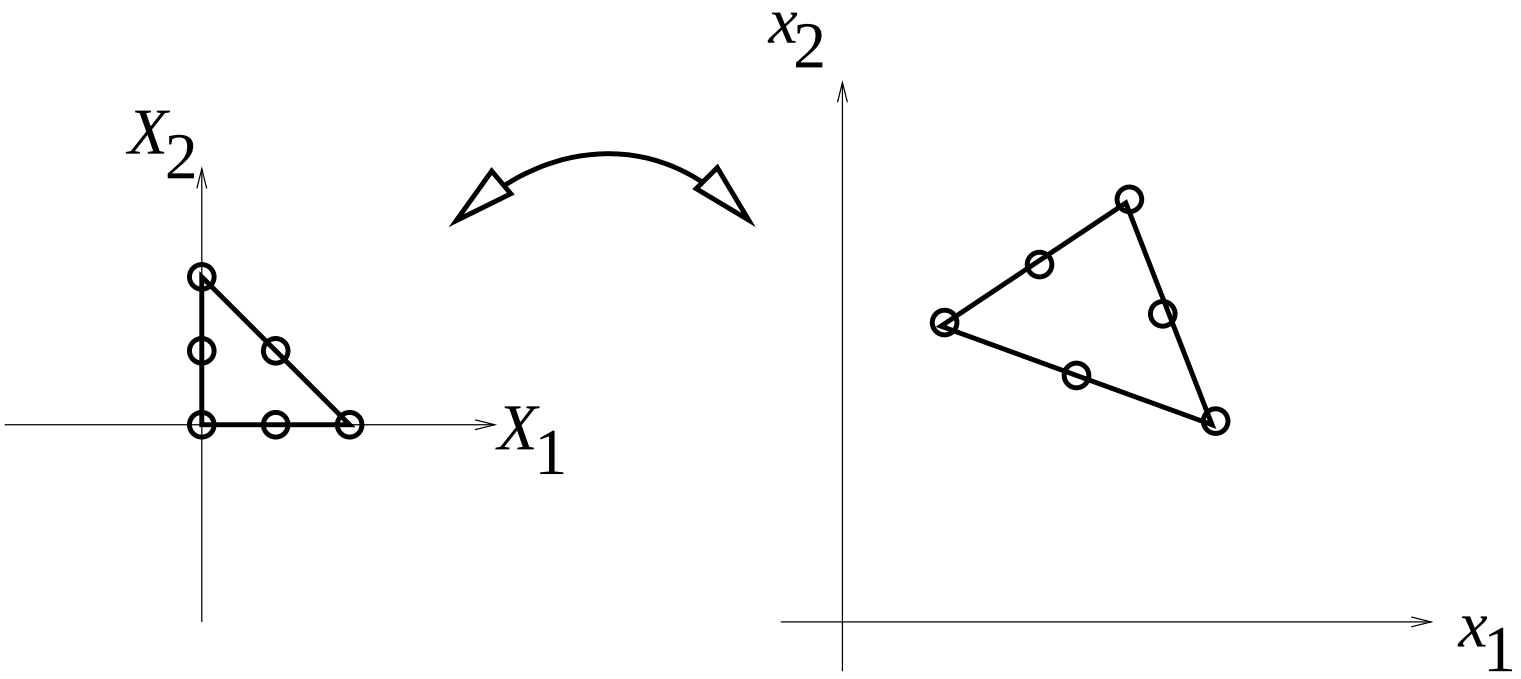
The P1 triangular 2D element: u is linear $ax + by + c$ over each triangular cell



Basic features of 2D P1 elements

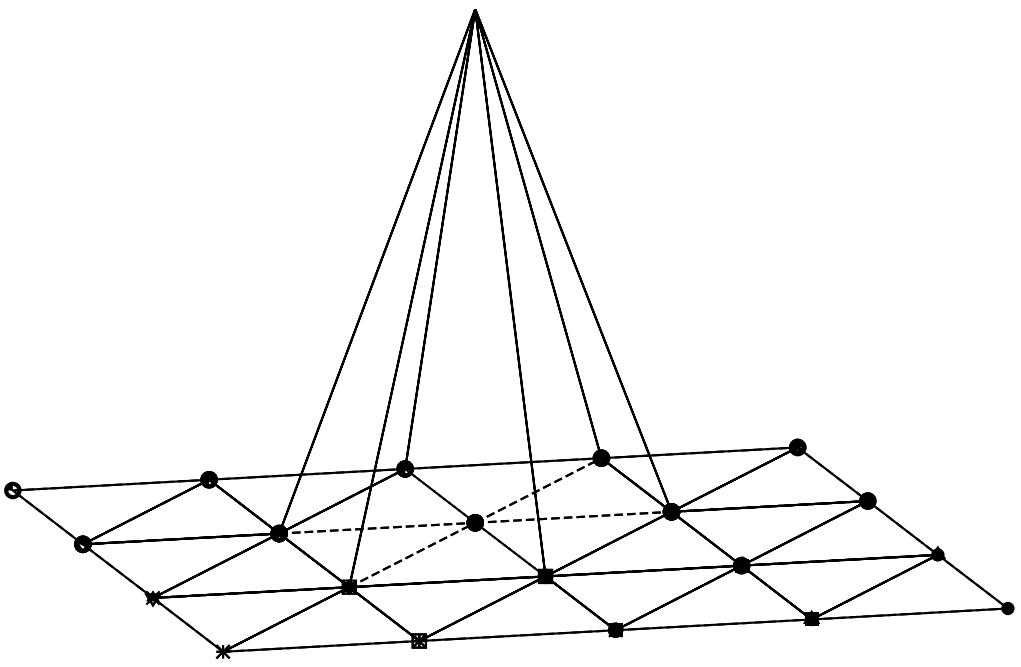
- $\varphi_r(X, Y)$ is a linear function over each element
- Cells = triangles
- Vertices = corners of the cells
- Nodes = vertices
- Degrees of freedom = function values at the nodes

Linear mapping of reference element onto general triangular cell



φ_i: pyramid shape, composed of planes

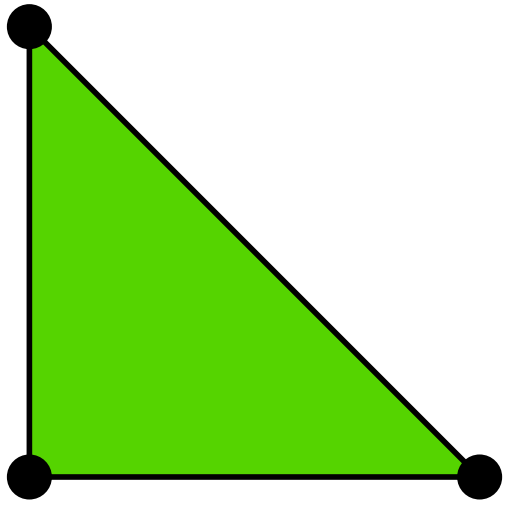
- $\varphi_i(X, Y)$ varies linearly over an element
- $\varphi_i = 1$ at vertex (node) i, 0 at all other vertices (nodes)



Element matrices and vectors

- As in 1D, the contribution from one cell to the matrix involves just a few numbers, collected in the element matrix and vector
- $\varphi_i \varphi_j \neq 0$ only if i and j are degrees of freedom (vertices/nodes) in the same element
- The 2D P1 has a 3×3 element matrix

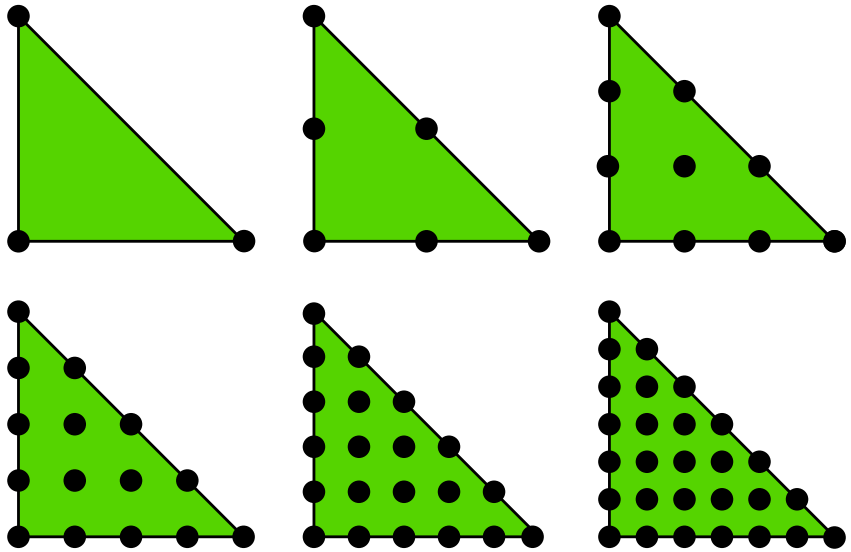
Basis functions over triangles in the reference cell



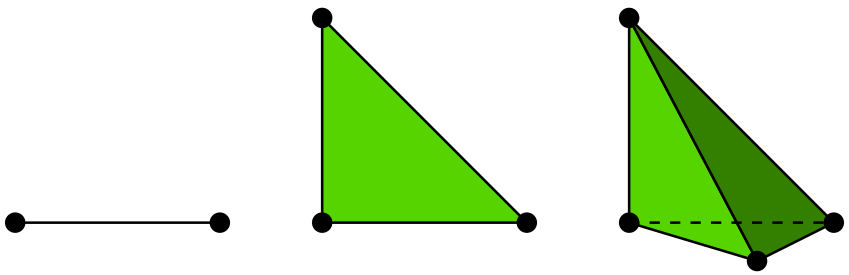
$$\tilde{\varphi}_0(X, Y) = 1 - X - Y \tag{86}$$
$$\tilde{\varphi}_1(X, Y) = X \tag{87}$$
$$\tilde{\varphi}_2(X, Y) = Y \tag{88}$$

Higher-degree $\tilde{\varphi}_r$ introduce more nodes (dof = node values)

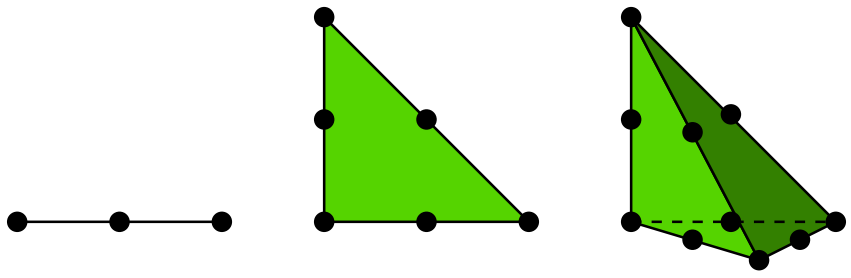
2D P1, P2, P3, P4, P5, and P6 elements



P1 elements in 1D, 2D, and 3D



P2 elements in 1D, 2D, and 3D



- Interval, triangle, tetrahedron: *simplex* element (plural quick-form: *simplices*)
- Side of the cell is called *face*
- Thetrahedron has also *edges*

Affine mapping of the reference cell; formula

Mapping of local $\mathbf{X} = (X, Y)$ coordinates in the reference cell to global, physical $\mathbf{x} = (x, y)$ coordinates:

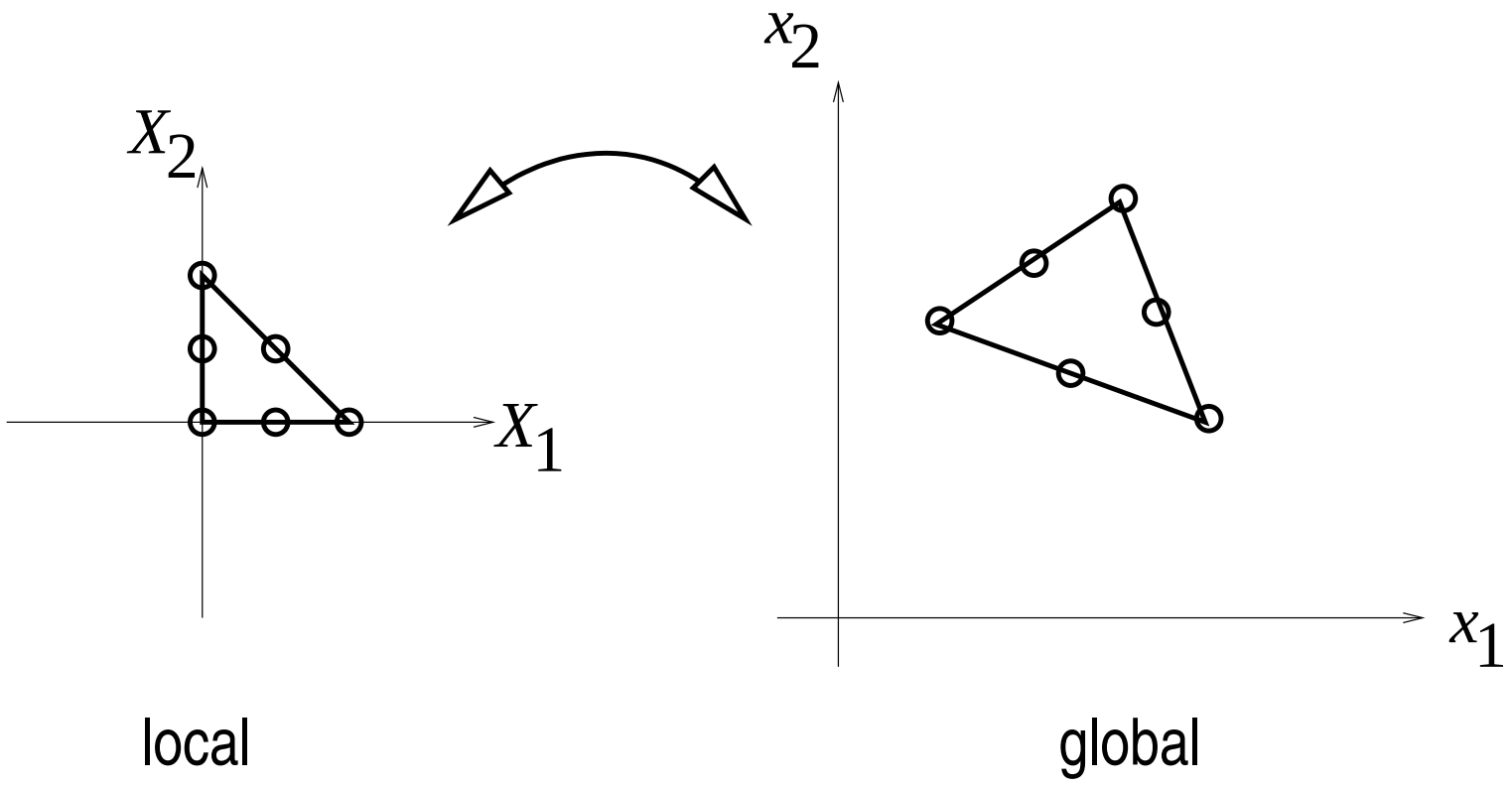
$$\mathbf{x} = \sum_r \tilde{\varphi}_r^{(1)}(\mathbf{X})\mathbf{x}_{q(e,r)} \tag{89}$$

where

- r runs over the local vertex numbers in the cell
- $\mathbf{x}_i$ are the (x, y) coordinates of vertex i
- $\tilde{\varphi}_r^{(1)}$ are P1 basis functions

This mapping preserves the straight/planar faces and edges.

Affine mapping of the reference cell; figure

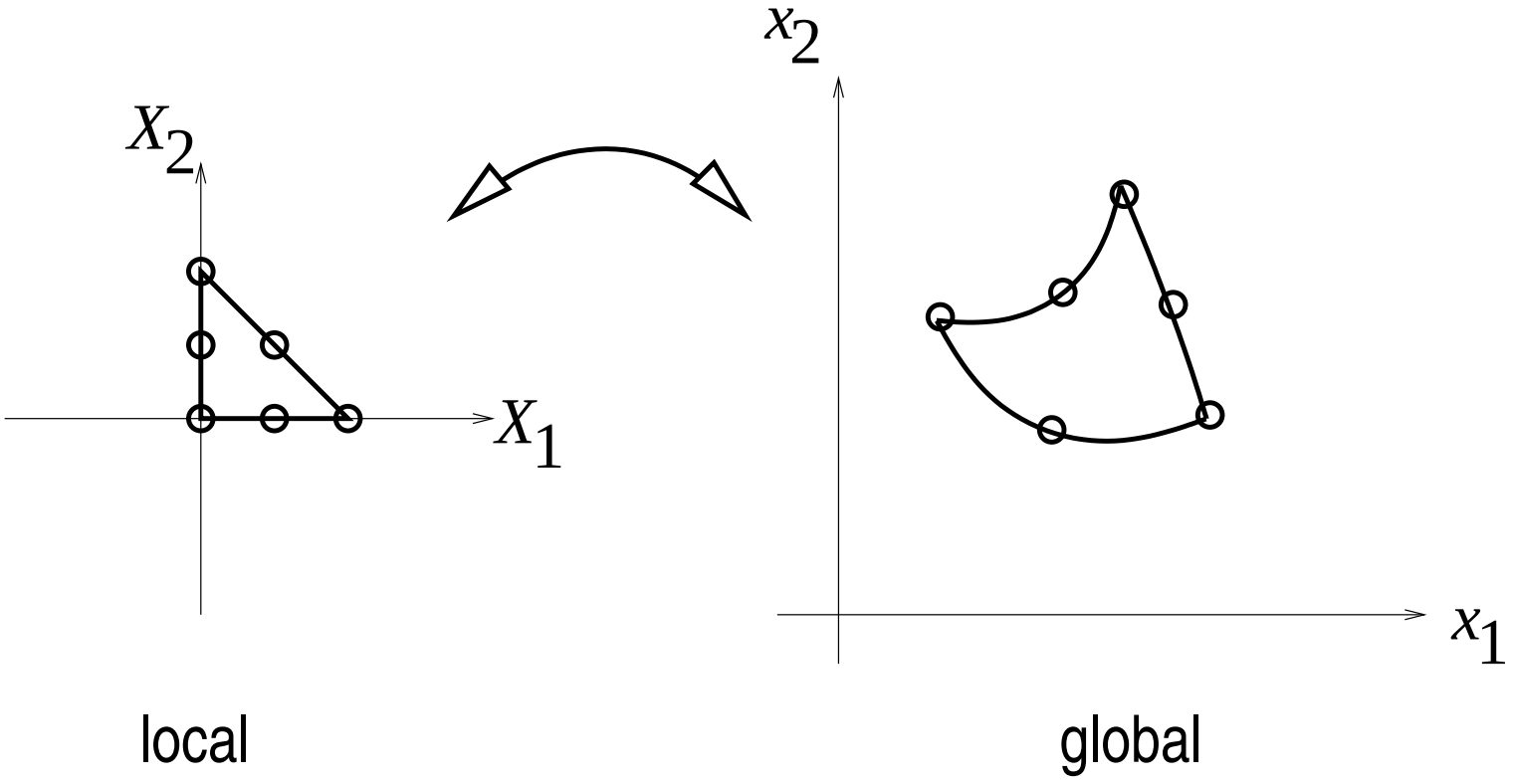


Isoparametric mapping of the reference cell

Idea: Use the basis functions of the element (not only the P1 functions) to map the element

$$\mathbf{x} = \sum_r \tilde{\varphi}_r(\mathbf{X})\mathbf{x}_{q(e,r)} \tag{90}$$

Advantage: higher-order polynomial basis functions now map the reference cell to a *curved* triangle or tetrahedron.



Computing integrals

Integrals must be transformed from $\Omega^{(e)}$ (physical cell) to $\tilde{\Omega}^r$ (reference cell):

$$\int_{\Omega^{(e)}} \varphi_i(\mathbf{x})\varphi_j(\mathbf{x})\,\mathrm{d}x = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\mathbf{X})\tilde{\varphi}_j(\mathbf{X})\det J\;\mathrm{d}X \tag{91}$$

$$\int_{\Omega^{(e)}} \varphi_i(\mathbf{x})f(\mathbf{x})\,\mathrm{d}x = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\mathbf{X})f(\mathbf{x}(\mathbf{X}))\det J\;\mathrm{d}X \tag{92}$$

where $\mathrm{d}x = dxdy$ or $\mathrm{d}x = dxdydz$ and $\det J$ is the determinant of the Jacobian of the mapping $\mathbf{x}(\mathbf{X})$.

$$J = \begin{bmatrix} \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} \\ \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y} \end{bmatrix}, \quad \det J = \frac{\partial x}{\partial X}\frac{\partial y}{\partial Y} - \frac{\partial x}{\partial Y}\frac{\partial y}{\partial X} \tag{93}$$

Affine mapping (89): $\det J = 2\Delta$, $\Delta =$ cell volume

!slide **Remark on going from 1D to 2D/3D**

Finite elements in 2D and 3D builds on the same *ideas* and *concepts* as in 1D, but there is simply much more to compute because the specific mathematical formulas in 2D and 3D are more

Differential equation models

Our aim is to extend the ideas for approximating f by u, or solving

$$u = f$$

to real differential equations.
Three methods:

1. least squares
2. Galerkin/projection
3. collocation (interpolation)

Method 2 will be totally dominating!

Abstract differential equation

$$\mathcal{L}(u) = 0, \quad x \in \Omega \tag{94}$$

Examples:

$$\mathcal{L}(u) = \frac{d^2u}{dx^2} - f(x), \tag{95}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) + f(x), \tag{96}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) - au + f(x), \tag{97}$$

$$\mathcal{L}(u) = \frac{d}{dx}\left(\alpha(u)\frac{du}{dx}\right) + f(u, x) \tag{98}$$

Abstract boundary conditions

$$\mathcal{B}_0(u) = 0, \ x = 0, \quad \mathcal{B}_1(u) = 0, \ x = L \tag{99}$$

Examples:

$$\mathcal{B}_i(u) = u - g, \qquad \text{Dirichlet condition} \tag{100}$$

$$\mathcal{B}_i(u) = -\alpha \frac{du}{dx} - g, \qquad \text{Neumann condition} \tag{101}$$

$$\mathcal{B}_i(u) = -\alpha \frac{du}{dx} - h(u - g), \qquad \text{Robin condition} \tag{102}$$

Reminder about notation

- $u_e(x)$ is the symbol for the *exact* solution of $\mathcal{L}(u_e) = 0$
- $u(x)$ denotes an *approximate* solution
- $V = \text{span}\{\psi_0(x), \ldots, \psi_N(x)\}$: we seek $u \in V$
- V has basis $\{\psi_i\}_{i \in I}$
- $I = \{0, \ldots, N\}$ is an index set
- $u(x) = \sum_{j \in I} c_j \psi_j(x)$
- Inner product: $(u, v) = \int_\Omega uv \, \mathrm{d}x$
- Norm: $||u|| = \sqrt{(u, u)}$

Residual-minimizing principles

- When solving $u = f$ we knew the error $e = f - u$ and could use principles for minimizing the error
- When solving $\mathcal{L}(u_e) = 0$ we do not know u_e and cannot work with the error $e = u_e - u$
- We only have the *error in the equation*: the residual R

Inserting $u = \sum_j c_j \psi_j$ in $\mathcal{L} = 0$ gives a residual

$$R = \mathcal{L}(u) = \mathcal{L}(\sum_j c_j \psi_j) \neq 0 \tag{103}$$

Goal: minimize R wrt $\{c_i\}_{i \in I}$ (and hope it makes a small e too)

$$R = R(c_0, \ldots, c_N; x)$$

The least squares method

Idea: minimize

$$E = ||R||^2 = (R, R) = \int_\Omega R^2 dx \tag{104}$$

Minimization wrt $\{c_i\}_{i \in I}$ implies

$$\frac{\partial E}{\partial c_i} = \int_\Omega 2R \frac{\partial R}{\partial c_i} dx = 0 \quad \Leftrightarrow \quad (R, \frac{\partial R}{\partial c_i}) = 0, \quad i \in I \tag{105}$$

$N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i \in I}$

The Galerkin method

Idea: make R orthogonal to V,

$$(R, v) = 0, \quad \forall v \in V \tag{106}$$

This implies

$$(R, \psi_i) = 0, \quad i \in I, \tag{107}$$

$N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i \in I}$

The Method of Weighted Residuals

Generalization of the Galerkin method: demand R orthogonal to some space W, possibly $W \neq V$:

$$(R, v) = 0, \quad \forall v \in W \tag{108}$$

If $\{w_0, \ldots, w_N\}$ is a basis for W:

$$(R, w_i) = 0, \quad i \in I \tag{109}$$

- $N + 1$ equations for $N + 1$ unknowns $\{c_i\}_{i \in I}$
- Weighted residual with $w_i = \partial R / \partial c_i$ gives least squares

Terminology: test and Trial Functions

- ψ_j used in $\sum_j c_j \psi_j$: *trial function*
- ψ_i or w_i used as weight in Galerkin's method: *test function*

The collocation method

Idea: demand $R = 0$ at $N + 1$ points

$$R(x_i; c_0, \ldots, c_N) = 0, \quad i \in I \tag{110}$$

Note: The collocation method is a weighted residual method with delta functions as weights

$$\text{property of } \delta(x): \quad \int_\Omega f(x)\delta(x - x_i)dx = f(x_i), \quad x_i \in \Omega \tag{111}$$

$$0 = \int_\Omega R(x; c_0, \ldots, c_N)\delta(x - x_i)\,\mathrm{d}x = R(x_i; c_0, \ldots, c_N)$$

Examples on using the principles

Goal.

Exemplify the least squares, Galerkin, and collocation methods in a simple 1D problem with global basis functions.

The first model problem

$$-u''(x) = f(x), \quad x \in \Omega = [0, L], \quad u(0) = 0, \ u(L) = 0 \tag{112}$$

Basis functions:

$$\psi_i(x) = \sin\left((i+1)\pi\frac{x}{L}\right), \quad i \in I \tag{113}$$

The residual:

$$\begin{aligned} R(x; c_0, \ldots, c_N) &= u''(x) + f(x), \\ &= \frac{d^2}{dx^2}\left(\sum_{j\in I} c_j\psi_j(x)\right) + f(x), \\ &= -\sum_{j\in I} c_j\psi_j''(x) + f(x) \end{aligned} \tag{114}$$

Boundary conditions

Since $u(0) = u(L) = 0$ we must ensure that all $\psi_i(0) = \psi_i(L) = 0$. Then

$$u(0) = \sum_j c_j \psi_j(0) = 0, \quad u(L) = \sum_j c_j \psi_j(L)$$

- u known: Dirichlet boundary condition
- u' known: Neumann boundary condition
- Must have $\psi_i = 0$ where Dirichlet conditions apply

The least squares method; principle

$$(R, \frac{\partial R}{\partial c_i}) = 0, \quad i \in I$$

$$\frac{\partial R}{\partial c_i} = \frac{\partial}{\partial c_i} \left(\sum_{j \in I} c_j \psi_j''(x) + f(x) \right) = \psi_i''(x) \qquad (115)$$

Because:

$$\frac{\partial}{\partial c_i} \left(c_0 \psi_0'' + c_1 \psi_1'' + \cdots + c_{i-1} \psi_{i-1}'' + c_i \psi_i'' + c_{i+1} \psi_{i+1}'' + \cdots + c_N \psi_N'' \right) =$$

The least squares method; equation system

$$(\sum_j c_j \psi_j'' + f, \psi_i'') = 0, \quad i \in I, \tag{116}$$

Rearrangement:

$$\sum_{j \in I} (\psi_i'', \psi_j'') c_j = -(f, \psi_i''), \quad i \in I \tag{117}$$

This is a linear system

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

with

$$\begin{aligned} A_{i,j} &= (\psi_i'', \psi_j'') \\ &= \pi^4 (i+1)^2 (j+1)^2 L^{-4} \int_0^L \sin\left((i+1)\pi \frac{x}{L}\right) \sin\left((j+1)\pi \frac{x}{L}\right) dx \\ &= \begin{cases} \frac{1}{2} L^{-3} \pi^4 (i+1)^4 & i = j \\ 0, & i \neq j \end{cases} \end{aligned} \tag{118}$$

Orthogonality of the basis functions gives diagonal matrix

Useful property:

$$\int_0^L \sin\left((i+1)\pi\frac{x}{L}\right)\sin\left((j+1)\pi\frac{x}{L}\right)\,dx = \delta ij, \quad \Rightarrow (\psi_i'', \psi_j'') = \delta_{ij}, \quad \delta_{ij} = \tag{120}$$

With diagonal $A_{i,j}$ we can easily solve for c_i:

$$c_i = \frac{2L}{\pi^2(i+1)^2}\int_0^L f(x)\sin\left((i+1)\pi\frac{x}{L}\right)\,dx \tag{121}$$

Least squares method; solution

Let's sympy do the work ($f(x) = 2$):

```
from sympy import *
import sys

i, j = symbols('i j', integer=True)
x, L = symbols('x L')
f = 2
a = 2*L/(pi**2*(i+1)**2)
c_i = a*integrate(f*sin((i+1)*pi*x/L), (x, 0, L))
c_i = simplify(c_i)
print c_i
```

$$c_i = 4\frac{L^2\left((-1)^i + 1\right)}{\pi^3\left(i^3 + 3i^2 + 3i + 1\right)}$$

$$u(x) = \sum_{k=0}^{N/2} \frac{8L^2}{\pi^3(2k+1)^3} \sin\left((2k+1)\pi\frac{x}{L}\right) . \qquad (122)$$

- Fast decay: $c_2 = c_0/27$, $c_4 = c_0/125$
- Only one term might be good enough

$$u(x) \approx \frac{8L^2}{\pi^3} \sin\left(\pi\frac{x}{L}\right) .$$

The Galerkin method; principle

$$(u'' + f, v) = 0, \quad \forall v \in V,$$

or

$$(u'', v) = -(f, v), \quad \forall v \in V \tag{123}$$

This is a *variational formulation* of the differential equation problem.
$\forall v \in V$ means for all basis functions:

$$(\sum_{j \in I} c_j \psi_j'', \psi_i) = -(f, \psi_i), \quad i \in I \tag{124}$$

The Galerkin method; solution

Since $\psi_i'' \propto \psi_i$, Galerkin's method gives the same linear system and the same solution as the least squares method (in this particular example).

The collocation method

$R = 0$ or the differential equation must be satisfied at $N+1$ points:

$$-\sum_{j \in I} c_j \psi_j''(x_i) = f(x_i), \quad i \in I \tag{125}$$

This is a linear system $\sum_j A_{i,j} = b_i$ with entries

$$A_{i,j} = -\psi_j''(x_i) = (j+1)^2 \pi^2 L^{-2} \sin\left((j+1)\pi \frac{x_i}{L}\right), \quad b_i = 2$$

Choose: $N = 0$, $x_0 = L/2$

$$c_0 = 2L^2/\pi^2$$

Comparison of the methods

- Exact solution: $u(x) = x(L - x)$
- Galerkin or least squares ($N = 0$): $u(x) = 8L^2\pi^{-3}\sin(\pi x/L)$
- Collocation method ($N = 0$): $u(x) = 2L^2\pi^{-2}\sin(\pi x/L)$.
- Max error in Galerkin/least sq.: $-0.008L^2$
- Max error in collocation: $0.047L^2$

Integration by parts

Second-order derivatives will hereafter be integrated by parts

$$\int_0^L u''(x)v(x)dx = -\int_0^L u'(x)v'(x)dx + [vu']_0^L$$
$$= -\int_0^L u'(x)v'(x)dx + u'(L)v(L) - u'(0)v(0) \quad (126)$$

Motivation:

- Lowers the order of derivatives
- Gives more symmetric forms (incl. matrices)
- Enables easy handling of Neumann boundary conditions
- Finite element basis functions φ_i have discontinuous derivatives (at cell boundaries) and are not suited for terms with φ_i''

Boundary function; principles

- What about nonzero Dirichlet conditions?
- E.g. $u(L) = D$

Boundary function; example

$u(0) = C$ and $u(L) = D$. Choose

$$B(x) = L^{-1}(C(L-x) + Dx): \qquad B(0) = C,\ B(L) = D$$

$$u(x) = L^{-1}(C(L-x) + Dx) + \sum_{j \in I} c_j \psi_j(x), \qquad (127)$$

$$u(0) = C, \quad u(L) = 0$$

Abstract notation for variational formulations

The finite element literature (and much FEniCS documentation) applies an abstract notation for the variational formulation:

*Find $(u - B) \in V$ such that

$$a(u, v) = L(v) \quad \forall v \in V$$

Example on abstract notation

Given a variational formulation for $-u'' = f$:

$$\int_\Omega u'v'dx = \int_\Omega fvdx \quad \text{or} \quad (u', v') = (f, v) \quad \forall v \in V$$

Abstract formulation: finn $(u - B) \in V$ such that

$$a(u, v) = L(v) \quad \forall v \in V$$

We identify

$$a(u, v) = (u', v'), \quad L(v) = (f, v)$$

Bilinear and linear forms

- $a(u, v)$ is a *bilinear form*
- $L(v)$ is a *linear form*

Linear form means

$$L(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 L(v_1) + \alpha_2 L(v_2),$$

Bilinear form means

$$a(\alpha_1 u_1 + \alpha_2 u_2, v) = \alpha_1 a(u_1, v) + \alpha_2 a(u_2, v),$$
$$a(u, \alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 a(u, v_1) + \alpha_2 a(u, v_2)$$

In nonlinear problems: Find $(u - B) \in V$ such that $F(u; v) = 0 \ \forall v \in V$

The linear system associated with abstract form

$$a(u, v) = L(v) \quad \forall v \in V$$

is equivalent to

$$a(u, \psi_i) = L(\psi_i) \quad i \in I$$

Insert $u = \sum_j c_j \psi_j$ and use linearity:

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

This is a linear system

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

with

$$A_{i,j} = a(\psi_j, \psi_i)$$
$$b_i = L(\psi_i)$$

Equivalence with minimization problem

If $a(u, v) = a(v, u)$,

$$a(u, v) = L(v) \quad \forall v \in V,$$

is equivalent to minimizing the functional

$$F(v) = \frac{1}{2}a(v, v) - L(v)$$

over all functions $v \in V$. That is,

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

- Much used in the early days of finite elements
- Still much used in structural analysis and elasticity
- Not as general as Galerkin's method (since $a(u, v) = a(v, u)$)

Examples on variational formulations

Goal.

Derive variational formulations for many prototype differential equations in 1D that include

- variable coefficints
- mixed Dirichlet and Neumann conditions
- nonlinear coefficients

Variable coefficient; problem

$$-\frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) = f(x), \quad x \in \Omega = [0, L],\ u(0) = C,\ u(L) = D\,. \tag{128}$$

- Variable coefficient $\alpha(x)$
- *Nonzero* Dirichlet conditions at $x = 0$ *and* $x = L$
- Must have $\psi_i(0) = \psi_i(L) = 0$
- $V = \text{span}\{\psi_0, \ldots, \psi_N\}$
- $v \in V$: $v(0) = v(L) = 0$

$$u(x) = B(x) + \sum_{j \in I} c_j \psi_i(x)$$

$$B(x) = C + \frac{1}{L}(D - C)x$$

Variable coefficient; variational formulation (1)

$$R = -\frac{d}{dx}\left(a\frac{du}{dx}\right) - f$$

Galerkin's method:

$$(R, v) = 0, \quad \forall v \in V,$$

or with integrals:

$$\int_\Omega \left(\frac{d}{dx}\left(\alpha\frac{du}{dx}\right) - f\right) v \,\mathrm{d}x = 0, \quad \forall v \in V\,.$$

Variable coefficient; variational formulation (2)

Integration by parts:

$$-\int_\Omega \frac{d}{dx}\left(\alpha(x)\frac{du}{dx}\right) v \,\mathrm{d}x = \int_\Omega \alpha(x)\frac{du}{dx}\frac{dv}{dx}\,\mathrm{d}x - \left[\alpha\frac{du}{dx}v\right]_0^L.$$

Boundary terms vanish since $v(0) = v(L) = 0$

Variational formulation.

Find $(u - B) \in V$ such that

$$\int_\Omega \alpha(x)\frac{du}{dx}\frac{dv}{dx}dx = \int_\Omega f(x)v dx, \quad \forall v \in V,$$

Compact notation:

$$(\alpha u', v') = (f, v), \quad \forall v \in V$$

Variable coefficient; abstract notation

$$a(u, v) = L(v) \quad \forall v \in V,$$

$$a(u, v) = (\alpha u', v'), \quad L(v) = (f, v)$$

Variable coefficient; linear system

$v = \psi_i$ and $u = B + \sum_j c_j \psi_j$:

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

Reorder to form linear system:

$$\sum_{j \in I} (\alpha \psi_j', \psi_i') c_j = (f, \psi_i) + (a(D - C)L^{-1}, \psi_i'), \quad i \in I\,.$$

This is $\sum_j A_{i,j} c_j = b_i$ with

$$A_{i,j} = (a\psi_j', \psi_i') = \int_\Omega \alpha(x)\psi_j'(x), \psi_i'(x)\,\mathrm{d}x,$$

$$b_i = (f, \psi_i) + (a(D - C)L^{-1}, \psi_i') = \int_\Omega \left(f(x)\psi_i(x) + \alpha(x)\frac{D - C}{L}\psi_i'(x) \right.$$

First-order derivative in the equation and boundary condition; problem

[[[