Partial differential equations

All previously discussed equations are ordinary differential equations (ODE). An equation of two or more variables containing also partial derivatives is a partial differential equation (PDE).

A numerical solution will usually contain a huge amount of numbers. The solution should be somehow visualized.

There are several very different analytical methods either to solve the equations or convert them to a more tractable form.

Integral transforms:

Laplace transform

$$\mathcal{L}f(x) = \int e^{-st} f(t) \mathrm{d}t.$$

There is no simple formula for the inverse transform, and it is not unique.

The direct transform is stable, but the inverse transform is numerically unstable.

Fourier transform, for e.g. convolution type problems.

Separation of variables:

Take the Laplace equation

$$\nabla^2 f = 0.$$

In rectangular coordinates try a trial solution (ansatz)

$$f(x, y, z) = X(x)Y(y)Z(z),$$

where X depends only on x etc.

Substitution to the original equation gives

$$\nabla^2 f = YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} = 0.$$

Divide by XYZ and rearrange terms:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} - \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}.$$

The left hand side depends on x only and the right hand side on y and z. This is possible only if both sides have the same constant value, say C:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = C$$
$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -C$$

In the same way the latter equation can be split into two separate equations:

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = D$$
$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -C - D$$

Thus the equation is replaced by three ordinary differential equations.

The kind of the trial solution depends on the type of the equation.

Green's functions:

Let \mathcal{L} be a linear but otherwise arbitrary operator (like d/dx). The Green's function G corresponding to \mathcal{L} is defined as

$$\mathcal{L}G(x, x') = \delta(x - x').$$

Then

$$\mathcal{L}G(x, x')f(x) = \delta(x - x')f(x).$$

Integrating this we get

$$\int \mathcal{L}G(x, x')f(x)dx' = \int \delta(x - x')f(x)dx' = f(x).$$

Assume we have an equation

$$\mathcal{L}u(x) = f(x).$$

Use the previous equation to express f(x):

$$\mathcal{L}u(x) = f(x) = \int \mathcal{L}G(x, x')f(x)dx'.$$

Since \mathcal{L} is linear we can take it outside the integral:

$$\mathcal{L}u(x)' = \mathcal{L} \int G(x, x') f(x) \mathrm{d}x'$$

Thus the equation is satisfied by

$$u(x) = \int G(x, x') f(x) \mathrm{d}x'.$$

The problem now is to find the function G corresponding to \mathcal{L} .

Types of PDE's

Very many phenomena can be described with second order linear equations

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu + g = 0.$$

Depending on the coefficients of the derivatives the equation is

- 1 elliptic, if $b^2 4ac < 0$,
- 2 parabolic, if $b^2 4ac = 0$,
- 3 hyperbolic, if $b^2 4ac > 0$.

The classification is not very important from the numerical point of view. However

- hyperbolic and parabolic equations often describe evolution with time, and are therefore initial value problems with some boundary values also

- elliptic equations often describe a "static" situation with given boundary values.

The usual numerical solution methods are

- difference methods
- element methods

An example of a simple partial differential equation in two dimension is the Laplace equation, which in rectangular coordinates is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

In the Laplace equation a = c = 1 and b = 0, hence $b^2 - 4ac = -4$, and the equation is elliptic.

If the right-hand side is nonzero, we have the Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y).$$

For example the gravitational potential V satisfies the Poisson equation

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = \nabla^2 V = -4\pi G \rho(x, y, z),$$

where ρ is the density and G the constant of gravitation.

Difference method/elliptic equations

The elliptic equations describing a "steady state" are the most strightforward to solve by numerical methods.

Replace partial derivatives by finite differences. Use symmetric expressions for the differences.

$$\frac{\partial u(x_i, y_j)}{\partial x} = \frac{u(x_{i+1}, y_j) - u(x_{i-1}, y_j)}{2\Delta x},$$

$$\frac{\partial u(x_i, y_j)}{\partial y} = \frac{u(x_i, y_{j+1}) - u(x_i, y_{j-1})}{2\Delta y},$$

$$\frac{\partial^2 u(x_i, y_j)}{\partial x^2} = \frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{(\Delta x)^2},$$

$$\frac{\partial^2 u(x_i, y_j)}{\partial y^2} = \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1})}{(\Delta y)^2}.$$

Denote $u_{i,j} = u(x_i, y_j)$ and use the same step in both directions, $h = \Delta x = \Delta y$. Then

$$\frac{\partial^2 u_{i,j}}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2},\\ \frac{\partial^2 u_{i,j}}{\partial y^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2}.$$

The Laplace equation is now

or

$$\nabla^2 u_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2} = 0$$
$$\frac{1}{h^2} (u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}) = 0.$$

The Laplace operator can be expressed as a diagram

$$\nabla^2 = \frac{1}{h^2} \begin{bmatrix} 1 & \\ 1 & -4 & 1 \\ & 1 & \end{bmatrix}.$$

The differences can be more accurately described by using a larger number of neighboring points. A nine point method:

$$\nabla^2 = \frac{1}{6h^2} \begin{bmatrix} 1 & 4 & 1\\ 4 & -20 & 4\\ 1 & 4 & 1 \end{bmatrix}.$$

In three dimensions we could use e.g.

$$\nabla^2 = \frac{1}{h^2} \begin{bmatrix} 1 & 1 \\ & | & / \\ 1 & - & -6 & - & 1 \\ & / & | \\ 1 & 1 & & \end{bmatrix}.$$

The boundary conditons can specify different thing. Common versions are e.g.:

Dirichlet boundary conditions: the function to be solved is known along the whole boundary of the area.

Neumann boundary conditions give the values of the normal gradients along the boundary.

A rather boring often used example: a rectangular slab with one edge kept at 100 degrees temperature and other edges at 0 degrees.

To make things really simple, use only three grid points:

Evaluate the Laplace operator at each grid point:

$$\frac{1}{h^2}(0+0+u_2+0-4u_1) = 0$$
$$\frac{1}{h^2}(u_1+0+u_3+0-4u_2) = 0$$
$$\frac{1}{h^2}(u_2+0+100+0-4u_3) = 0$$
$$\begin{pmatrix} -4 & 1 & 0\\ 1 & -4 & 1\\ 0 & 1 & -4 \end{pmatrix} \begin{pmatrix} u_1\\ u_2\\ u_3 \end{pmatrix} = \begin{pmatrix} 0\\ 0\\ 100 \end{pmatrix}.$$

or

A denser grid might be

u_1	u_2	u_3	u_4	u_5	u_6
u_7	u_8	u_9	u_{10}	u_{11}	u_{12}
u_{13}	u_{14}	u_{15}	u_{16}	u_{17}	u_{18}

When there are many grid points, the coefficient matrix is something like this:

•••										
1			1	-4	1			1		
	1			1	-4	1			1	
		1			1	-4	1			1
•••										

The difference from ODE's is that the nonzero diagonals are not all adjacent. Yet, the matrix can be stored as a band matrix.

In elimination also the zeros between the nonzero diagonals are replaced by nonzero values.

The more grid points there are, the smaller is the fraction of nonzero elements.

Usually the number of points is large, and then one should use sparse matrix methods to save space.

Due to the large number of equations, elimination methods can lead to serious round-off errors. Then iterative methods can be better.

Liebmann iteration

Write the set of equations

$$\begin{pmatrix} -4 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & -4 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 100 \end{pmatrix}.$$

in such a way that the left-hand side contains the diagonal elements of the original set:

$$u_1 = \frac{u_2}{4},$$

$$u_2 = \frac{u_1 + u_3}{4},$$

$$u_3 = \frac{u_2 + 100}{4}.$$

These iteration formulas are used to update the solution vector u, until the solution does not change too much. The iteration can be terminated when e.g. the largest change of the elements of u is sufficiently small. From the graph of the Laplace operator we get immediately formulas suitable for the iteration:

$$\nabla^2 u = \frac{1}{h^2} \begin{bmatrix} 1 & 1 \\ 1 & -4 & 1 \\ & 1 \end{bmatrix} u_{ij} = 0,$$

from which

$$u_{ij} = \frac{1}{4}(u_{i,j+1} + u_{i,j-1} + u_{i-1,j} + u_{i+1,j}).$$

The initial value can be obtained e.g. by solving the equation with a very coarse grid. This solution is then used to interpolate approximate values for a denser grid. Convergence of the Liebmann iteration can be slow. Convergence can be accelerated using an *overrelaxation method*.

Use a superscript to denote the iteration in which the value has been calculated:

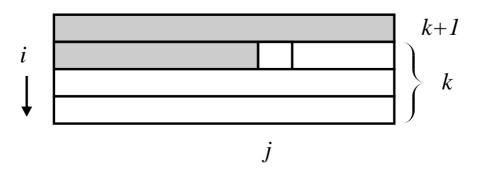
$$u_{ij}^{k+1} = \frac{1}{4} (u_{i,j+1}^k + u_{i,j-1}^{k+1} + u_{i-1,j}^{k+1} + u_{i+1,j}^k).$$

Add and subtract u_{ij}^k :

$$u_{ij}^{k+1} = u_{ij}^{k} + \left(\frac{u_{i,j+1}^{k+1} + u_{i,j-1}^{k+1} + u_{i-1,j}^{k+1} + u_{i+1,j}^{k} - 4u_{ij}^{k}}{4}\right).$$

The expression in parentheses is a correction that is used to update u_{ij} . When the solution has been found, that expression is zero.

The old values u_{ij}^k can be replaced by the new iterates u_{ij}^{k+1} .



Often the correction is too small, and therefore the values of u converge very slowly towards the correct solution. The convergence can be accelerated by increasing the correction term in an appropriate way:

$$u_{ij}^{k+1} = u_{ij}^k + \omega \left(\frac{u_{i,j+1}^k + u_{i,j-1}^{k+1} + u_{i-1,j}^{k+1} + u_{i+1,j}^k - 4u_{ij}^k}{4} \right).$$

The constant ω in in the range [1,2]. When the number of points becomes very big, the optimal value $\rightarrow 2$.

(In the case of a rectangular grid and Dirichlet's boundary value the optimal value is

$$\omega = \frac{4}{2 + \sqrt{4 - c^2}},$$

where

$$c = \cos\frac{\pi}{n} + \cos\frac{\pi}{m},$$

and n and m are the numbers of grid points in x and y directions, respectively.)

Difference method/parabolic equations

These often describe the evolution of some system in time. Hence initial values are needed in addition to some boundary conditions.

Typical example is the diffusion equation that can be used to describe many things like heat transfer, liquid flow or flow of electric current:

$$\frac{\partial u}{\partial t} = c \frac{\partial^2 u}{\partial x^2}$$

The solution requires initial values, u(x, t = 0) = g(x), where g is a known function, and boundary conditions u(x = 0, t) = a, u(x = 1, t) = b.

Replace again the derivatives by finite differences:

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{h^2} (u_{i+1}^k - 2u_i^k + u_{i-1}^k),$$
$$\frac{\partial u}{\partial t} = \frac{1}{\Delta t} (u_i^{k+1} - u_i^k).$$

Thus we get the discretised equations

$$u_i^{k+1} = u_i^k + \frac{c\Delta t}{h^2} (u_{i+1}^k - 2u_i^k + u_{i-1}^k).$$

The right-hand side term u_i^k vanishes if $2c\Delta t/h^2 = 1$. It can be shown (but we shall not do it here) that this gives a limit for the stability of the equation. The equation is stable only if $2c\Delta t/h^2 < 1$.

This *Courant* condition takes different forms for different equations, but the idea is the same: If the spatial step is shortened, also the time step must be decreased. Essentially it means that in one time step differences have no time to propagate further away than one spatial step.

If we want to make weather predictions more precide by halving the distance between the grid points (in 3D) the number of grid points will increase 8-fold. But also the time step must be halved, so the total amount of work will increase by a factor 16.

The method is explicit: at each time step only the values computed at the previous time step are needed. The error is $\mathcal{O}(\Delta t) + \mathcal{O}(h^2)$.

Implicit methods are more accurate with respect of time. For example, the Crank-Nicholson method:

$$u_i^{k+1} = u_i^k + \frac{c\Delta t}{2h^2}(u_{i+1}^{k+1} - 2u_i^{k+1} + u_{i-1}^{k+1} + u_{i+1}^k - 2u_i^k + u_{i-1}^k).$$

The error is $\mathcal{O}((\Delta t)^2) + \mathcal{O}(h^2)$, and the method is stable for all Δt .

A disadvantage is that at each time step a tridiagonal set of equations must be solved.

Difference method/hyperbolic equations

A typical example is the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

Discretisation gives

$$\frac{u_i^{k+1} - 2u_i^k + u_i^{k-1}}{(\Delta t)^2} = c^2 \frac{u_{i+1}^k - 2u_i^k + u_{i-1}^k}{h^2}$$

or

$$u_i^{k+1} = 2u_i^k - u_i^{k-1} + \frac{c^2(\Delta t)^2}{h^2}(u_{i+1}^k - 2u_i^k + u_{i-1}^k).$$

If the time step is chosen so that $c\Delta t = h$, we have

$$u_i^{k+1} = -u_i^{k-1} + u_{i+1}^k + u_{i-1}^k.$$

The equation can describe e.g. a vibrating string. Initially we need the deviations u_i^0 at t = 0.

To calculate u_i^1 we also need the value of u_i^{-1} , i.e. before the initial time. Thus the velocity at t = 0 is needed. In the case of a vibrating string the string is initially just released from the displaced position, and the velocity is 0. Thus for the first time interval $u_i^1 = (u_{i+1}^0 + u_{i-1}^0)/2$.

Element methods

The Finite Element Methods (FEM) are quit different from difference methods. They are widely used in structural analysis, hydro/aerodynamics and multiphysics problems like magnetohydrodynamics combining Maxwell and Navier–Stokes equations.

The element method is pretty complicated to implement. Fortunately, there are several reliable programs (mostly commercial). See e.g. CSC's web pages.

Elmer

Elmer is an open source multiphysical simulation software mainly developed by CSC. Elmer development was started 1995 in collaboration with Finnish Universities, research institutes and industry. After it's open source publication in 2005, the use and development of Elmer has become international.

Elmer includes physical models of fluid dynamics, structural mechanics, electromagnetics, heat transfer and acoustics, for example. These are described by partial differential equations which Elmer solves by the Finite Element Method (FEM).

For concurrent information visit the discussion forum and wiki at http://www.elmerfem.org.

The basic ideas are:

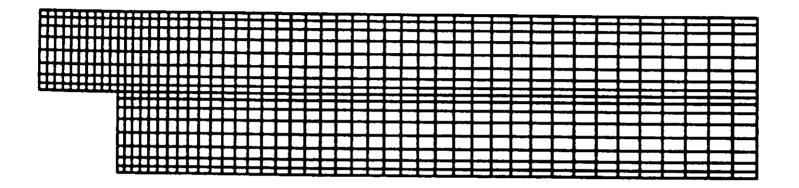
- Divide the region into small elements (grid generation)
- In each element, the solution is described by a simple basis function (like a polynomial). Each basis function is nonzero in a small area only.
- The solution is obtained as a linear combination of the basis functions.
- At the boundary of two elements the two basis functions have the same values at the nodal points (e.g. at the apices of a triangular element). It may also be required that then derivatives have the same values at the nodes.
- Coefficients of the basis functions are obtained as a solution of an optimization problem. Finding the solution means solving a (usually large) set of linear equations.

Shapes and sizes of the elements can be chosen quite freely. The method is easy to apply even in complicated geometries.

In critical areas small elements can be used for accuracy, and in less interesting areas large elements for speed.

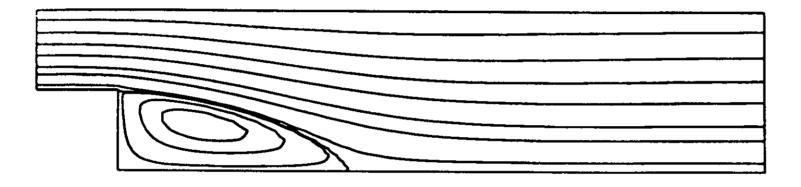
In principle, the problem is converted to an optimization problem that can always be solved. Therefore the method is more stable than difference methods.

Flow over a step. The element grid can be denser around the step where the flow is more complicated.



FEM programs are usually accompanied by routines to display the results in different graphical forms.

The flow over a step and the velocity vectors of the flow:



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Variational calculus

Assume we want to find a function y = y(x) in the range $x \in [x_1, x_2]$ such that the integral

$$J = \int_{x_1}^{x_2} f(y, y', x) \,\mathrm{d}x$$

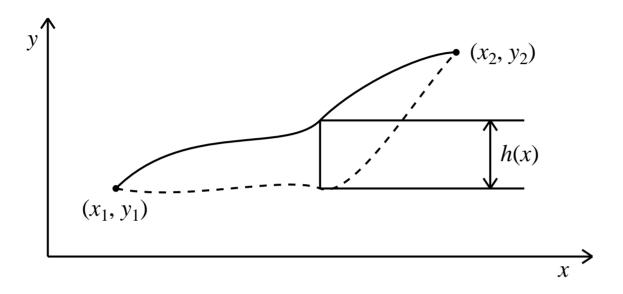
of a known function f = f(y, y', x), where y' = dy/dx, attains its extremum. Assume also that the endpoints $y_1 = y(x_1)$ and $y_2 = y(x_2)$ are fixed.

Let y(x,0) be the function we are looking for. Other possible functions can be expressed as

$$y(x,a) = y(x,0) + ah(x),$$
 (1)

where h is an arbitrary function vanishing at the endpoints of the interval $[x_1, x_2]$.

We are looking for the path giving an extremum (solid line). The function h = h(x) is an arbitrary deviation from the optimal path.



The value of J obviously depends on a:

$$J(a) = \int f(y(x,a), y'(x,a), x) \,\mathrm{d}x.$$

In order to J have an extremum at a = 0 we must have $\frac{\partial J}{\partial a} = 0.$

$$\left. \frac{\partial J}{\partial a} \right|_{a=0} = 0.$$

Evaluate this derivative:

$$\frac{\partial J}{\partial a} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} \frac{\partial y}{\partial a} + \frac{\partial f}{\partial y'} \frac{\partial y'}{\partial a} \right) \, \mathrm{d}x.$$

The latter term is

$$\int_{x_1}^{x_2} \frac{\partial f}{\partial y'} \frac{\partial y'}{\partial a} dx$$

= $\int_{x_1}^{x_2} \frac{\partial f}{\partial y'} \frac{\partial y}{\partial x \partial a} dx$
= $\int_{x_1}^{x_2} \frac{\partial f}{\partial y'} \frac{\partial y}{\partial a} - \int_{x_1}^{x_2} \frac{d}{dx} \left(\frac{\partial f}{\partial y'}\right) \frac{\partial y}{\partial a} dx.$

Here $\partial y/\partial a = h(x)$, which vanishes at the end points. Hence we get

$$\frac{\partial J}{\partial a} = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) \frac{\partial y}{\partial a} \, \mathrm{d}x. \tag{(*)}$$

Denote by δX the variation of X, defined as

$$\delta X = \frac{\partial X}{\partial a} \bigg|_{a=0} \mathrm{d}a.$$

(This is just an abbreviation for this expression.)

Multiply equation (*) by da and evaluate both sides at a = 0:

$$\delta J = \int_{x_1}^{x_2} \left(\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial y'} \right) \, \delta y \, \mathrm{d}x.$$

This must vanish for f to give an extremum. Since $\delta y = h(x) da$ is arbitrary, the integral can vanish only if the integrand is identically zero:

$$\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial y'} = 0.$$

This is known as Lagrange's or Euler's equation.

Back to the method: we now know that the functional

$$F[v] = \int v(x, y, y') \, dx$$

attains an extremum when \boldsymbol{v} satisfies the Lagrange equation

$$\frac{\partial v}{\partial y} - \frac{d}{dx}\frac{\partial v}{\partial y'} = 0.$$

Take

$$v = (y'(x))^2 + 2f(x)y(x),$$

whence

$$\frac{\partial v}{\partial y} = 2f(x),$$
$$\frac{\partial v}{\partial y'} = 2y'$$
$$\frac{d}{dx}\frac{\partial v}{\partial y'} = 2y''.$$

The Lagrange equation is now

2f(x) - 2y''(x) = 0

or

$$y'' = f(x).$$

The differential equation

$$y'' = f(x)$$

can be solved as a variational problem by finding the minimum for the functional

$$F[v] = \int y'^2 + 2f(x)y \, dx$$

Similarly, the Poisson equation

$$\nabla^2 u = f(x, y, z)$$

can be solved by minimising the functional

$$F[u] = \int \left(\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial z} \right)^2 + 2f(x, y, z)u \right) \, dx \, dy \, dz.$$

Approximate the solution by a linear combination of the basis functions ϕ_i :

$$v = \sum_{j} a_{j} \phi_{j}.$$

The functional to be minimised is then

$$F[v] = \int \left((\sum_j a_j \phi'_j)^2 + 2f(x) \sum_j a_j \phi_j \right) dx.$$

The minimum is given by the equations

$$\frac{\partial F[v]}{\partial a_i} = 0.$$

$$\frac{\partial F[v]}{\partial a_i} = \int \left(2\phi'_i (\sum_j a_j \phi'_j) + 2f(x)\phi_i \right) dx$$
$$= 2\sum_j a_j \int \phi'_i \phi'_j dx + 2\int f(x)\phi_i dx,$$

whence

$$\sum_{j} a_j \int \phi'_i \phi'_j \, dx = -\int f(x)\phi_i.$$

Fa = b,

We get a set of equations

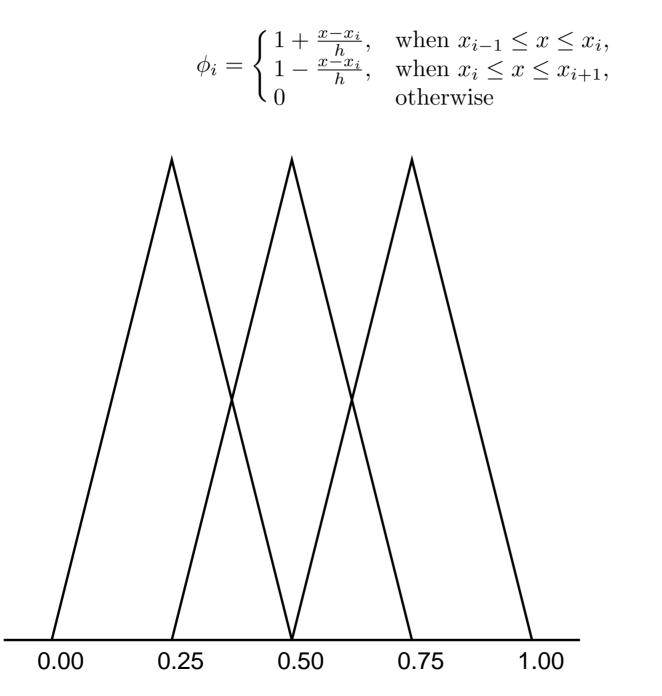
where

$$F_{ij} = \int \phi'_i \phi'_j \, dx,$$

$$b_i = -\int f(x)\phi_i \, dx.$$

Example: try to solve the equation y'' = x with the boundary conditions y(0) = y(1) = 0.

We use the basis functions



The elements of the coefficient matrix are

$$\int \phi'_i \phi'_j \, dx = \begin{cases} -\frac{1}{h}, & \text{when } i = j \pm 1, \\ \frac{2}{h}, & \text{when } i = j, \\ 0, & \text{otherwise} \end{cases}$$

$$\int_{0}^{1} f\phi_{1} dx = \int_{0}^{h} x \left(1 + \frac{x - h}{h}\right) dx + \int_{h}^{2h} x \left(1 - \frac{x - h}{h}\right) dx$$
$$= \frac{h^{2}}{3} + \frac{2h^{2}}{3} = h^{2},$$
$$\int_{0}^{1} f\phi_{2} dx = 2h^{2},$$
$$\int_{0}^{1} f\phi_{3} dx = 3h^{2}.$$

For simplicity, take h = 0.25; thus there are only three basis functions.

The minimisation problem leads to the set of equations

$$\frac{1}{0.25} \begin{pmatrix} 2 & -1 & 0\\ -1 & 2 & -1\\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} a_1\\ a_2\\ a_3 \end{pmatrix} = -0.25^2 \begin{pmatrix} 1\\ 2\\ 3 \end{pmatrix}.$$

The solution of this is

$$a = \begin{pmatrix} -0.0391\\ -0.0625\\ -0.0547 \end{pmatrix}.$$

For example, $y(0.5) = a_2\phi_2(0.5) = a_2 = -0.0625$.

The exact solution is $y = \frac{1}{6}(x^3 - x)$, whence y(0.5) = -0.0625.