Lecture 16

Two point-boundary value problems

- Rayleigh-Ritz method.

Integral equations

- General definitions
- Volterra equations
- Singular kernels

Rayleigh-Ritz method:

Up to now our approach to both differentiation and integration has been to use finite differences. The Rayleigh-Ritz method departs significantly from this point of view. Its idea is the basic concept behind more sophisticated methods that we will see in the context of PDE's, like finite element methods.

The central idea is to reduce the boundary value problem to a minimization of a functional in a given functional space. The solution is therefore the function that minimizes the value of the functional.

The method consists in approximating the (infinite dimensional) space of functions in which one searches the minimum to a finite dimensional set. This casts the problem in a way amenable to numerical solution.

You have probably encountered this idea before, for instance when people look for fundamental states in quantum mechanics with trial wavefunctions (e.g. Hartree-Fock).

Suppose you want to solve the boundary-value problem,

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=f(x) \qquad 0\le x\le 1$$

With $\quad y(0)=y(1)=0$

This equation corresponds, for instance, to the deflection y(x) of a beam of unit length with variable cross section represented by q(x) and under the influence of the stresses p(x) and f(x), and we assume p,q,f to be continuous and non-vanishing.

It can easily be shown that a function y(x) solves this equation if it minimizes the integral,

$$I(y)=\int_0^1\left\{p(x)[y'(x)]^2+q(x)[y(x)]^2-2f(x)y(x)\right\}dx$$

Let us now consider a finite set of functions $\phi_i(x)$, $i=1,2,\ldots,n$ such that they are linearly independent and $\phi_i(0)=\phi_i(1)=0$.

An approximate solution to the differential equation is obtained by minimizing the integral with respect to the finite number of parameters c_i

$$\phi(x) = \sum_{i=1}^{n} c_i \phi_i(x)$$

$$I(\phi) = \int_0^1 \left\{ p(x)\left[\sum_{\mathrm{i=1}}^{\mathrm{n}} c_i \phi_i'(x)\right]^2 + q(x)\left[\sum_{\mathrm{i=1}}^{\mathrm{n}} c_i \phi_i(x)\right]^2 - 2f(x)\left[\sum_{\mathrm{i=1}}^{\mathrm{n}} c_i \phi_i(x)\right]\right\} dx$$

To minimize, we require, $\quad \dfrac{\partial I}{\partial c_i} = 0 \qquad i = 1,2,\ldots n$

Which yields,

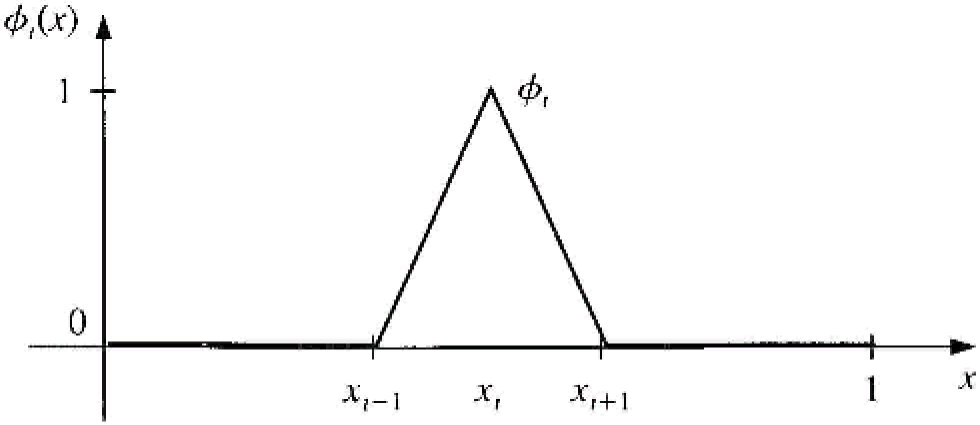
$$0 = \int_0^1 \left\{ 2p(x)\left[\sum_{\mathrm{i=1}}^{\mathrm{n}} c_i \phi_i'(x)\right]\phi_j'(x) + 2q(x)\left[\sum_{\mathrm{i=1}}^{\mathrm{n}} c_i \phi_i(x)\right]\phi_j(x) - 2f(x)\phi_j(x)\right\} dx$$

This can be viewed as a linear system: Ac=b with,

$$a_{ij} = \int_0^1 \left[p(x)\phi'_i(x)\phi'_j(x) + q(x)\phi_i(x)\phi_j(x)\right] dx \qquad b_j = \int_0^1 f(x)\phi_i(x)\, dx$$

To make the construction work, we need to pick an explicit and reasonable basis of functions. One possible choice is to consider functions that are piece-wise polynomial.

$$\phi_i(x) = \begin{cases} 0, & 0 \le x \le x_{i-1}, \\ \dfrac{x - x_{i-1}}{h_{i-1}}, & x_{i-1} < x \le x_i, \\ \dfrac{x_{i+1} - x}{h_i}, & x_i < x \le x_{i+1}, \\ 0, & x_{i+1} < x \le 1, \end{cases}$$



In this example, we take piecewise linear functions. The derivative of these functions is not continuous, but it is finite. Given how the functions are defined, one has,

$$\phi_i(x)\phi_j(x) = 0 \quad \text{and} \quad \phi_i'(x)\phi_j'(x) = 0$$

Unless j is equal to i-1,i+1 or i. If we therefore go back to the matrix of the system of equations, we see that it is tri-diagonal,

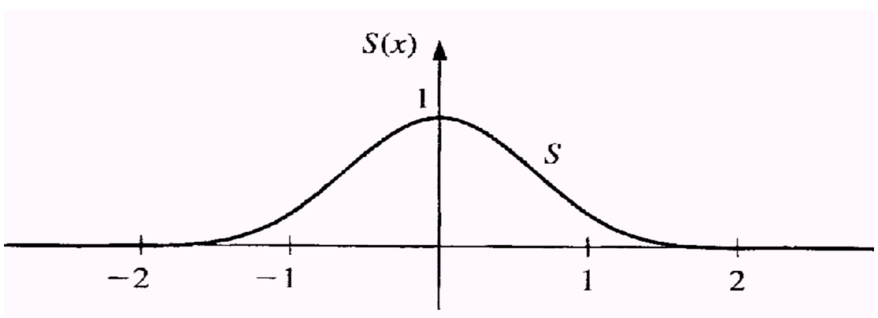
$$a_{ij} = \int_0^1 \left[p(x)\phi'_i(x)\phi'_j(x) + q(x)\phi_i(x)\phi_j(x) \right] dx$$

From here on, the calculations are straightforward. However, one has to ponder a few details.

Computing the matrix requires computing some integrals. Unless one is lucky, this has to be accomplished numerically. One should arrange the calculations in such a way as to not repeat similar integrals.

If one goes this way, the resulting solution is of course, a function that will inherit properties from the basis of functions one chose. With the basis we showed, the result will be a continuous function with discontinuous derivatives.

A possible basis of smoother functions is given by considering "splined triangles". That is, consider functions,



These functions are 1 at 0, have vanishing first and second derivatives at +/-2.

If you recall our discussion of splines, you'll remember that we had these conditions to be met:

- $S(x)$ is a cubic polynomial, denoted $S_j(x)$ in the subinterval $[x_j, x_{j+1}]$ for each $j=0,1,\dots n-1$.
- $S_j(x_j)=f(x_j)$ for each $j=0,1,\dots n$
- $S_{j+1}(x_{j+1})=S_j(x_{j+1})$ for each $j=0,1,\dots n-2$
- $S'_{j+1}(x_{j+1})=S'_j(x_{j+1})$ for each $j=0,1,\dots n-2$
- $S''_{j+1}(x_{j+1})=S''_j(x_{j+1})$ for each $j=0,1,\dots n-2$
- One of the following set of boundary conditions are satisfied,
  I) $S''(x_0)=S''(x_n)=0$ (free or "natural" boundary)
  II) $S'(x_0)=f'(x_0)$ and $S'(x_n)=f'(x_n)$ ("clamped" boundary)

What we are doing now is requesting both I) and II) to be true. So something else has to give. We relinquish the second condition and only request that S=1 at x=0. The resulting spline is,

$$S(x)=\begin{cases} 0, & x\le -2,\\ \frac{1}{4}(2+x)^3, & -2\le x\le -1,\\ \frac{1}{4}\left[(2+x)^3-4(1+x)^3\right], & -1<x\le 0,\\ \frac{1}{4}\left[(2-x)^3-4(1-x)^3\right], & 0<x\le 1,\\ \frac{1}{4}(2-x)^3, & 1<x\le 2,\\ 0, & 2<x. \end{cases}$$

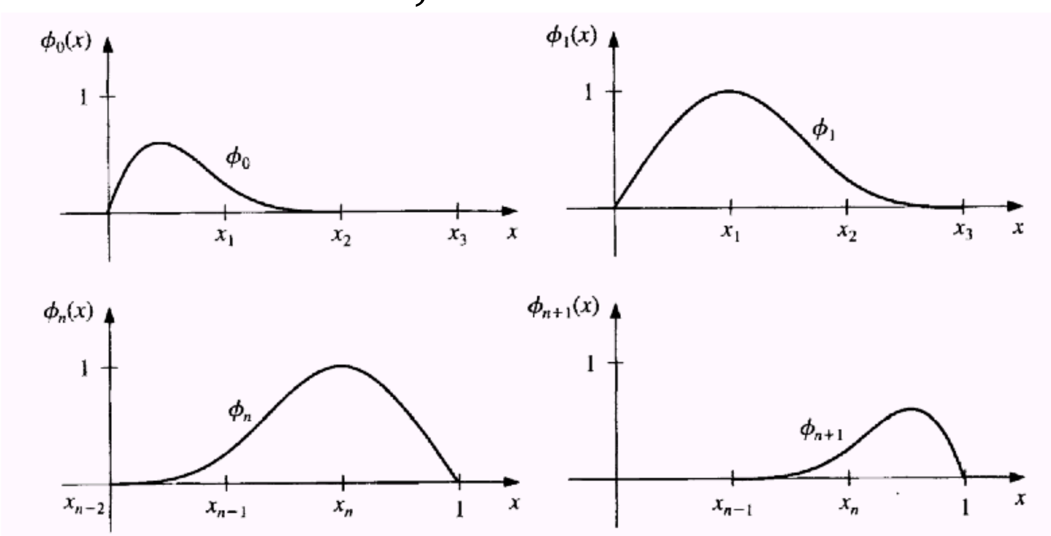
So choosing such splines we construct a basis in the same way as we did with the triangles. The only glitch is that since the splines require 5 points, we need to do special arrangements at the endpoints.

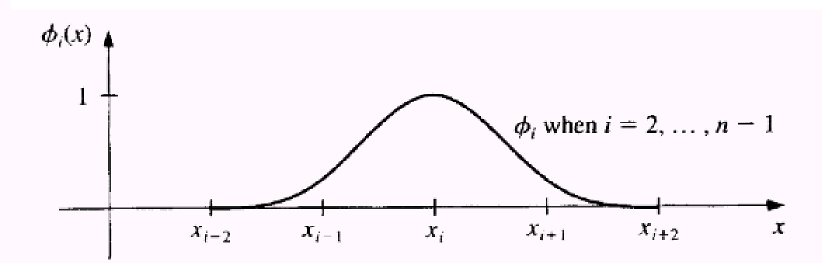
One possible such arrangement is given by,

$$\phi_i(x) = \begin{cases} S\left(\frac{x}{h}\right) - 4S\left(\frac{x+h}{h}\right), & i = 0, \\ S\left(\frac{x-h}{h}\right) - S\left(\frac{x+h}{h}\right), & i = 1, \\ S\left(\frac{x-ih}{h}\right), & 2 \le i \le n-1, \\ S\left(\frac{x-nh}{h}\right) - S\left(\frac{x-(n+2)h}{h}\right), & i = n, \\ S\left(\frac{x-(n+1)h}{h}\right) - 4S\left(\frac{x-(n+2)h}{h}\right), & i = n+1. \end{cases}$$

And since the splines connect five adjacent points, one would end up with a matrix that is band-diagonal with 5 bands.

Which look like,





Integral equations:

There is close resemblance between integral equations and linear systems of equations. Such resemblance becomes a correspondence when one attacks the problem numerically and discretizes the equations.

"Fredholm equation of the first kind"

$$g(t) = \int_a^b K(t,s) f(s)\, ds \quad \longleftrightarrow \quad \mathbf{K} \cdot \mathbf{f} = \mathbf{g}$$

You are trying to solve for f(s) with g(t) given. K(t,s) is the "kernel". Because kernels "smooth out" properties of f(s) the inverse problem can be quite unstable to solve.

"Fredholm equation of the second kind"

Eigenvalue problem

$$f(t) = \lambda \int_a^b K(t,s) f(s)\, ds + g(t) \longleftrightarrow (\mathbf{K} - \sigma \mathbf{1}) \cdot \mathbf{f} = \mathbf{g}$$

Volterra equations are special cases of the Fredholm equations that correspond to the case in which the kernel is zero for s>t. In such cases the equation is written,

$$g(t) = \int_a^t K(t,s) f(s)\, ds \longleftrightarrow \sum_{j=1}^{k} K_{kj} f_j = g_k$$

With K a lower triangular matrix.

As we wrote them, all these equations are linear. The non-linear versions correspond to an integrand K(t,s,f(s)) and are considerably harder to solve except in the case of Volterra equations, as we will see.

The key to solving these kinds of equations is to use a quadrature scheme for the integral. Then one only requires to evaluate things at a finite number of points and we turn the equations into systems of linear equations.

For instance, consider a Fredholm equation of the second kind,

$$f(t) = \lambda \int_a^b K(t,s) f(s)\, ds + g(t)$$

The Nystrom method consists in choosing a quadrature rule,

$$\int_a^b y(s)\, ds = \sum_{j=1}^{N} w_j y(s_j)$$

Where the s_j are the abscissas and w_j are the weights of the method chosen. Evaluating at the quadrature points we have, $\widetilde{K}_{ij} = K_{ij} w_j$

$$f(t_i) = \lambda \sum_{j=1}^{N} w_j K(t_i, s_j) f(s_j) + g(t_i)$$

$$\left(\mathbf{1} - \lambda \widetilde{\mathbf{K}}\right) \cdot \mathbf{f} = \mathbf{g}$$

So we have a linear system of equations. If one wishes to know the solution at points other than the t_i, then one simply uses the above expression at the point. This maintains the accuracy of the quadrature. This is Nystrom's observation.

```
 SUBROUTINE fred2(n,a,b,t,f,w,g,ak)
      INTEGER n,NMAX
      REAL a,b,f(n),t(n),w(n),g,ak
      EXTERNAL ak,g
      PARAMETER (NMAX=200)
CU    USES ak,g,gauleg,lubksb,ludcmp
      INTEGER i,j,indx(NMAX)
      REAL d,omk(NMAX,NMAX)
      if(n.gt.NMAX) pause 'increase NMAX in fred2'
      call gauleg(a,b,t,w,n)
      do 12 i=1,n
        do 11 j=1,n
          if(i.eq.j)then
            omk(i,j)=1.
          else
            omk(i,j)=0.
          endif
          omk(i,j)=omk(i,j)-ak(t(i),t(j))*w(j)
11      continue
        f(i)=g(t(i))
12    continue
      call ludcmp(omk,n,NMAX,indx,d)
      call lubksb(omk,n,NMAX,indx,f)
      return
      END
```

User-supplied routines for kernel and “RHS”

Gauss quadrature, returns weights and abscissas

Setup, solve linear equations

Volterra equation of the second kind,

$$f(t) = \int_a^t K(t,s) f(s)\, ds + g(t)$$

Trapezoid rule, $\quad t_i = a + ih, \quad i = 0, 1, \ldots, N, \qquad h \equiv \frac{b-a}{N}$

$$f_0 = g_0$$

$$(1 - \tfrac{1}{2} h K_{ii}) f_i = h \left(\tfrac{1}{2} K_{i0} f_0 + \sum_{j=1}^{i-1} K_{ij} f_j \right) + g_i,$$

And the solution can be found immediately.

If the equation is non-linear then we would solve for f_i using Newton-Raphson using as initial guess f_{i-1}.

Singular kernels:

Many common kernels in physics have singularities in certain regions of the domain. Here are some strategies to deal with this:

- Change of variables.
- If K(s,t)=w(s)K'(s,t) with w(s) having the singular portion, one can then use a Gaussian quadrature scheme with w(s) as weight function.
- If the kernel is highly peaked, compared to the rate of variation of f(s), then one can use a polynomial approximation to f(s) near the peak and just compute a few "moments" of the kernel. The more peaked the kernel is, the better the approximation!
- A common situation is that the kernel is infinite at t=s. In such case one can analytically subtract,

$$\begin{aligned}\int_a^b K(t,s)f(s)\,ds &= \int_a^b K(t,s)[f(s)-f(t)]\,ds + \int_a^b K(t,s)f(t)\,ds\\ &= \int_a^b K(t,s)[f(s)-f(t)]\,ds + r(t)f(t)\end{aligned}$$

One therefore loses the diagonal terms K_{ii}

Summary

- Rayleigh-Ritz: convert differential equation to minimization of an action problem.
- Integral equations are related to linear systems of equations when discretized.
- For singular kernels, change variables of use weights or approximations.