CS5016
Computational Methods and Applications

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PDEs and Finding Roots

Scribe 07

What is a PDE?

An equation involving one or more derivatives of an unknown function. If all derivatives are taken w.r.t a several independent variable, we get a partial differential equation (PDE). The well known 1D heat equation

$$\frac{\partial u(x,t)}{\partial t} - \mu \frac{\partial^2 u(x,t)}{\partial x^2} = f(x,t), \qquad x \in (a,b), \ t > 0$$

where $\mu > 0$ is the coefficient representing thermal diffusivity.

Boundary Value Problem

Differential eqns in an open multidimensional region $\Omega \subset \mathbb{R}^d$ for which the value of the unknown solution (or its derivatives) is prescribed on the boundary $\partial\Omega$ of the multidimensional region.

$$\frac{\partial u(x,t)}{\partial t} - \mu \frac{\partial^2 u(x,t)}{\partial x^2} = f(x,t), \qquad x \in (a,b); \ t > 0$$

with the initial condition

$$u(x,0) = g(x) \quad \forall x \in [a,b]$$

and boundary condition

$$u(a,t) = u(b,t) = 0 \quad \forall t > 0$$

Approximation By Finite Differences

Consider the following approximation for $h > 0$

$$\frac{\partial u(x,t)}{\partial x} \approx g(x,t) = \frac{u(x+h/2,t) - u(x-h/2,t)}{h}$$

Then we have

$$\frac{\partial^2 u(x,t)}{\partial x^2} \approx \frac{g(x+h/2,t) - g(x-h/2,t)}{h}$$

$$\approx \frac{u(x+h,t) - u(x,t)}{h^2} - \frac{u(x,t) - u(x-h,t)}{h^2}$$

$$= \frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2}$$

Let us partition the interval $[a,b]$ into interval $I_j = [x_j, x_{j+1}]$ of length h for $j = 0, 1, \dots, N$ with $x_0 = a$ and $x_N = b$.

Let $u_j(t)$ denote the approx. of $u(x_j, t)$, $j \in \{0, \dots N\}$. Then forall $t > 0$, we should have $\forall j \in \{1, \dots, N-1\}$

$$\frac{du_j(t)}{dt} - \frac{\mu}{h^2}\left(u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\right) = f_j(t)$$

with init condition $u_0(t) = 0$ and $u_N(t) = 0$, $f_j(t) = f(x_j, t)$, and $u_j(0) = g(x_j)$

Giving us the following system of ODE

$$\frac{du(t)}{dt} = \frac{\mu}{h^2} A u(t) + f(t)$$

with $u(0) = g$

Handling Problem with 2 Spatial Dimensions

we have $u(x,t)$ when $x \in \mathbb{R}^2$. The heat equation is given as

$$\frac{\partial u(x,t)}{\partial t} - \mu \frac{\partial^2 u(x,t)}{\partial x_1^2} - \mu \frac{\partial^2 u(x,t)}{\partial x_2^2} = f(x,t) \quad \forall x \in \Omega$$

with initial condition $u(x,0) = g(x)$ and boundary condition $u(x,t) = 0 \;\; \forall x \in \partial\Omega, t \geq 0$

Approximate Ω as a grid of points such that $x_{1,i} = x_{1,0} + ih$ and $x_{2,j} = x_{2,0} + jh$

Then,

$$\frac{\partial^2 u}{\partial x_1^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}, \quad \frac{\partial^2 u}{\partial x_2^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2}$$

$$\Rightarrow \frac{\partial u(x,t)}{\partial t} = \frac{\mu}{h^2}\left(u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{i,j}\right) + f(x,t)$$

$$\equiv u(i,j)' = \frac{\mu}{h^2}\left(u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{i,j}\right) + f(x,t)$$

$$u' = A^* u + f$$
$$= \frac{\mu}{h^2} A u + f$$

$$\frac{du}{dt} - \frac{\mu}{h^2} A u = f$$

Solution: $u e^{\int -\frac{\mu}{h^2} A\, dt} = \int f e^{\int -\frac{\mu}{h^2} A\, dt} + C$

Root Finding Algorithms

An algorithm for finding zeros/roots of continuous functions. A zero of a function $f: R \to R$ is a number x such that $f(x) = 0$. As generally, zeros of a function cannot be computed exactly nor expressed in closed form, root finding algos provide approximations to zeros.

Most root finding algorithms do not guarentee that they will find all the roots. In particular, if such an algo does not find a root, that does not mean no root exists.

→ This can happen due to a variety of reasons, such as the choice of the initial guess, the characteristics of the eqn being solved, or the limitations of the algorithm itself. Hence it may be necessary to try diff algorithms or improve the initial guess inorder to find the roots.

The Bisection Method

Consider a continuous fn $f: R \to R$ and an interval $[a,b]$. If $f(a) \cdot f(b) \leq 0$ then function f has at least one zero in the interval $[a,b]$. i.e., $\exists$ a pt $x^* \in [a,b]$ s.t. $f(x^*) = 0$.

Pseudocode

```
while |a-b| > ε do
    let c = (a+b)/2
    if sgn(f(c)) == sgn(f(a)) then
        a = c
    else
        b = c
    end if
end while
return (a+b)/2
```

Each iteration of the while loop reduces the interval size by a factor of 2. So, number of iterations reqd to achieve an accuracy of ε is prop. to $\log_2(\frac{1}{\varepsilon})$.

So the time complexity $O(\log(1/\varepsilon))$.

$n \leq n_{1/2} \equiv \left\lceil \log_2\left(\frac{\varepsilon_0}{\varepsilon}\right)\right\rceil$. ε is reqd tolerance and ε_0 is initial bracket size, $|b-a|$.

Newton-Raphson Method

Consider a differentiable function $f: \mathbb{R} \to \mathbb{R}$. If the f satisfies sufficient assumptions and the initial guess x_0 is close, a root can be found using the following iterative method.

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

Conditions f should satisfy:

- f must be continuous and differentiable at least once in the interval $[a,b]$.
- The initial guess x_0 should be chosen such that $f(x_0)$ and $f'(x_0)$ are non-zero.
- f' should be continuous on $[a,b]$ and non-zero at the root
- f'' should exist and be continuous on $[a,b]$.
- f'' should not change sign on $[a,b]$ where the root lies.

If $F: \mathbb{R}^k \to \mathbb{R}^k$ multivariate vector valued function then the iteration is given by

$$x_{k+1} = x_k - J(x_k)^{-1} F(x_k)$$

where $J(x_k)$ is the Jacobian Matrix of F.

Jacobian matrix is a matrix of all its first order partial derivatives.

scipy.optimize in the SciPy module offers methods to find zeroes of function.