Discretization of Derivatives

Partial Differential Equations

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Objectives

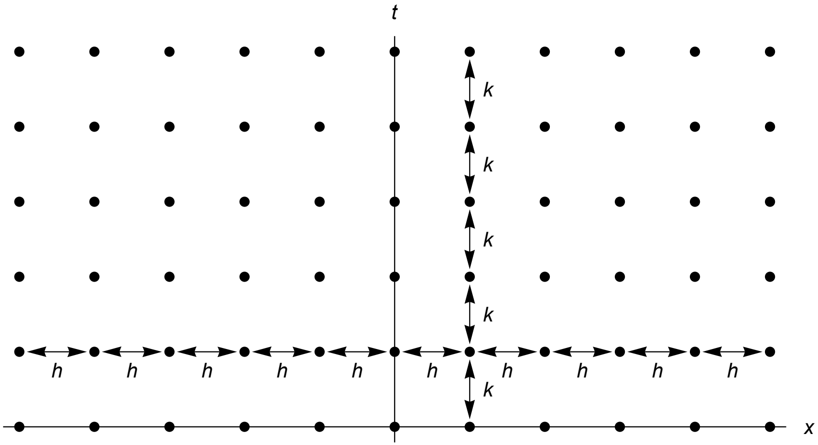
In this lesson we will:

- review Taylor's theorem,
- develop forward, backward, and centered difference formulas for the first derivative, and
- develop the midpoint formula for the second derivative.

Discretization

- Finite difference methods replace the *xt*-plane with a regularly spaced grid of points. as illustrated in
- This collection of regularly spaced points is often referred to as a **discretization** of the plane.
- The horizontal spacing of the points is denoted as h while the vertical spacing is denoted as k.
- A particular point in the discrete plane will be located by its coordinates $(i\,h, j\,k)$ where i and $j \in \mathbb{Z}$.
- If u is a real-valued function of (x, t) then the approximation of this function at the point with coordinates $(i\,h, j\,k)$ will be compactly denoted as u_i^j.

Illustration



Taylor's Theorem

The solution of an ordinary or partial differential equation by the finite difference method is a matter of developing formulas to approximate the derivatives or partial derivatives of functions at the discrete grids of points described above. The underlying mechanism which makes these approximations possible is **Taylor's theorem**.

Theorem

If function f is $n+1$ times continuously differentiable on (a, b) and if $a < x_0 < b$ then for any $x \in (a, b)$,

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n + \frac{f^{(n+1)}(z)}{(n+1)!}(x - x_0)^{n+1}$$

where z lies between x_0 and x.

Taylor Polynomial and Remainder

The expression

$$P_n(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

is called the n**th Taylor polynomial approximation** of $f(x)$ centered at x_0 and

$$R_n(x) = \frac{f^{(n+1)}(z)}{(n+1)!}(x - x_0)^{n+1}$$

is called the n**th Taylor remainder**.

If there exists a constant M_n such that

$$\max_{a \le z \le b} \left| \frac{f^{(n+1)}(z)}{(n+1)!} \right| \le M_n,$$

then the absolute error in approximating $f(x)$ on interval (a, b) by $P_n(x)$ is bounded by $E_n(x) = M_n |x - x_0|^{n+1}$.

Forward and Backward Difference

Suppose $U(x)$ is twice continuously differentiable on an open interval containing x_0, then

$$U(x_0 + h) = U(x_0) + U'(x_0)h + U''(z)\frac{h^2}{2!}$$

where z lies between x_0 and $x_0 + h$. Rearranging terms yields the equation

$$U'(x_0) = \frac{U(x_0 + h) - U(x_0)}{h} - U''(z)\frac{h}{2!}.$$

When $h > 0$ this produces the **forward difference** approximation to $U'(x_0)$ or equivalently,

$$U'(x_0) \approx \frac{U(x_0 + h) - U(x_0)}{h}.$$

If $h < 0$, this is called the **backward difference** approximation to $U'(x_0)$. The error term $U''(z)h/2!$ is described as being $O(h)$ (pronounced "big oh of h") as $h \to 0$. Since $U(x)$ is assumed to be twice continuously differentiable near x_0, when h is sufficiently small,

$$\left|\frac{U''(z)}{2!}h\right| \leq M\,|h|\,,$$

where M is a positive constant.

Centered Difference

If $U(x)$ is three times times continuously differentiable on (a, b) and $a < x_0 < b$ then

$$U'(x_0) = \frac{U(x_0 + h) - U(x_0 - h)}{2h} + U'''(v)\frac{h^2}{3!},$$

for some $a < v < b$.

The approximation

$$U'(x_0) \approx \frac{U(x_0 + h) - U(x_0 - h)}{2h}$$

is known as the **centered difference formula** and has an error term which is $O(h^2)$.

Second Derivative

Suppose $U(x)$ is four times times continuously differentiable on (a, b) and $a < x_0 < b$, then

$$U''(x_0) = \frac{U(x_0 + h) - 2U(x_0) + U(x_0 - h)}{h^2} + U^{(4)}(v)\frac{h^2}{12}$$

for some $a < v < b$.

The approximation

$$U''(x_0) \approx \frac{U(x_0 + h) - 2U(x_0) + U(x_0 - h)}{h^2}$$

is known as the **second derivative midpoint formula** and has an error term which is $O(h^2)$.

Application: Heat Equation

If u is a function of (x, t) the discrete approximation to the homogeneous heat equation

$$u_t = u_{xx}$$

can be expressed using the forward difference formula in t and the second derivative midpoint formula in x as

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