Lecture 23 Outline

Friday, November 15, 2019 11:53 AM

IVP + BVP

Root Finding

Bisection; Regula Falsi; Newton-Raphson;

Secant Method; Fixed Point

IVP & BVP

Friday, November 15, 2019 11:55 AM

Many PDE problems are IVP + BVP

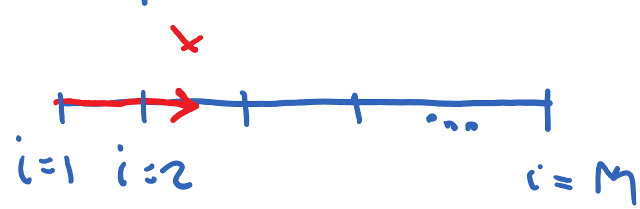
Example: Time-evolving heat problem (diffusion)

$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u = 0, \quad \alpha > 0$$

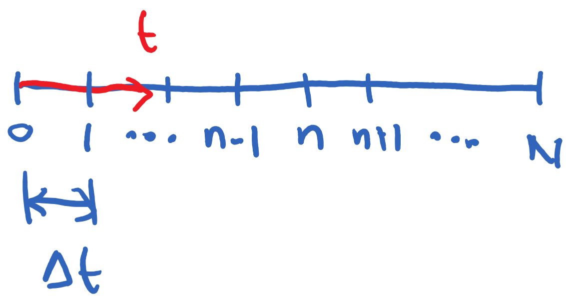
Describes how the temperature $u(x,t)$ evolves over time due to conduction

Need to combine IVP and BVP concepts

1D grid over space



1D time points



$$u(t_n, x_i) = u_i^n \quad \text{time step; not power}$$

$$\frac{\partial u}{\partial t} - \alpha^2 \frac{\partial^2 u}{\partial x^2} = 0$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \alpha^2 \underbrace{\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}}_{\text{Central difference in space at } t_n} = 0 \qquad \text{Forward Euler in time}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \alpha^2 \underbrace{\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2}}_{\text{Central difference in space at } t_{n+1}} = 0 \qquad \text{Backward Euler in time}$$

Many other schemes are possible

Example:

Let $\dfrac{du}{dt} = F\left(x, t, u, \dfrac{\partial u}{\partial x}, \dfrac{\partial^2 u}{\partial x^2}, \ldots\right)$

Denote $F_i^n = F\left(x_i, t_n, u_i^n, \dfrac{\partial u_i^n}{\partial x}, \dfrac{\partial^2 u_i^n}{\partial x^2}, \ldots\right)$

Forward Euler $\quad \dfrac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^n \quad \mathcal{O}(\Delta t)$

Backward Euler $\quad \dfrac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^{n+1} \quad \mathcal{O}(\Delta t)$

Crank-Nicholson $\quad \dfrac{u_i^{n+1} - u_i^n}{\Delta t} = \dfrac{1}{2}\left(F_i^n + F_i^{n+1}\right)$

$\mathcal{O}(\Delta t^2)$

Root Finding

Saturday, November 16, 2019 3:50 PM

Nonlinear equations of one variable

Recall that $g(x)$ is a linear function

if $g(x)+g(y)=g(x+y)$

Example: $g(x)=ax$, $a\in\mathbb{R}$

$$g(x)+g(y)=ax+ay=a(x+y)=g(x+y)$$

$\therefore$ linear

Example: $g(x)=ax^2$, $a\in\mathbb{R}$

$$g(x)+g(y)=ax^2+ay^2\neq a(x+y)^2=g(x+y)$$

$\therefore$ non-linear

Consider next several methods for solving $g(x)=a$

Rewrite this as $f(x)=g(x)-a$

Then find the roots of $f(x)=0$

Methods: ① Bisection

② Regula falsi

③ Newton-Raphson

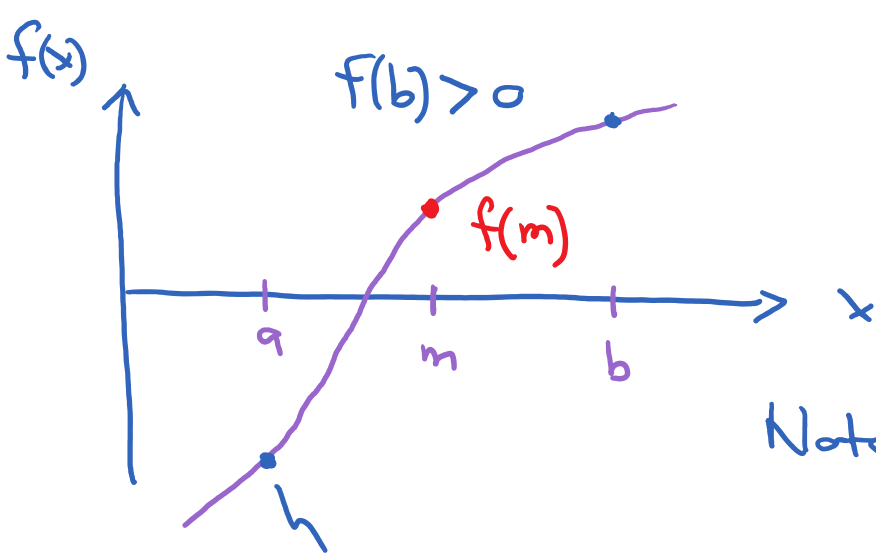
④ Secent

⑤ Fixed point

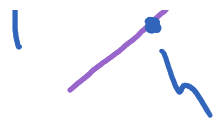
① Bisection Method: Requires that a zero exists in the range $[a, b]$

How can one check this requirement?

Simply require that $f(a) f(b) < 0$



Note: $f(a) f(b) < 0$



$f(a) < 0$

$f(a)f(b) < 0$

Let $m = \dfrac{a+b}{2}$

If $f(a)f(m) < 0$, redo with range $[a, m]$; otherwise redo with range $[m, b]$

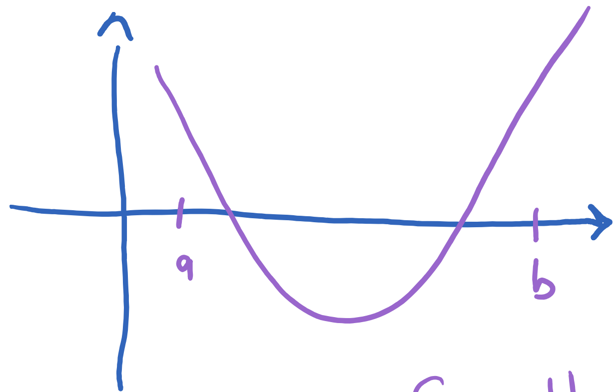
Keep going with these iterations until

$|f(m)| < \varepsilon$ ← error tolerance

Convergence is linear, because the bound on the root decreases by 1/2 for each iteration

Issue: One must have $f(a)f(b) < 0$ for this scheme to work

→ If $f'(x) = 0$ anywhere in $[a, b]$, then the root may be missed then the root may be missed



Can these roots be found?

but if $f(a)f(b) < 0$ is true, then this approach will always find the root (perhaps slowly)

If there are multiple roots within $[a, b]$, then we have no idea which one will be chosen

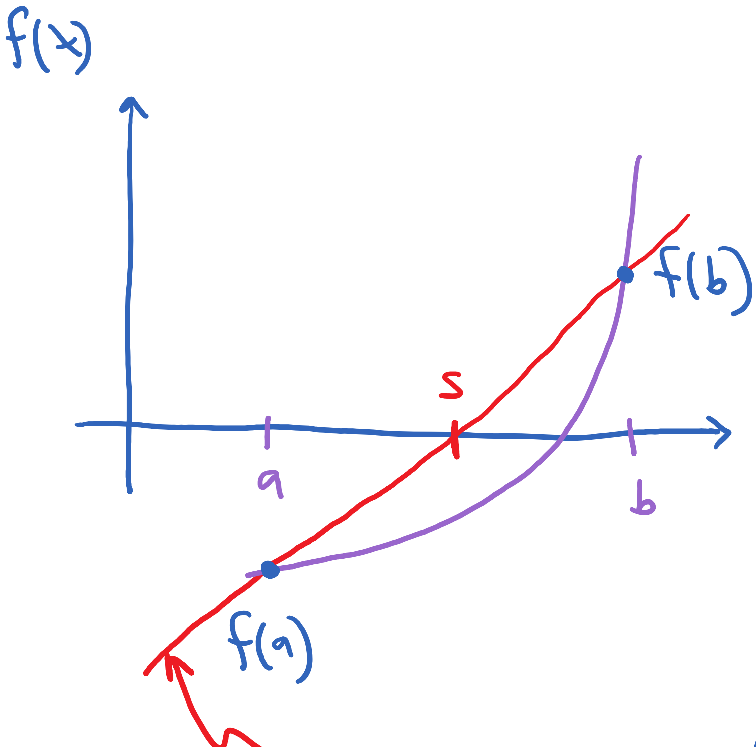
② Regula falsi (rule of false position)

Modification of bisection method

Let $f(a)f(b) < 0$ for range $[a, b]$

Instead of checking $[a, \frac{a+b}{2}]$, check whether $f(a)\,f(s) < 0$, where

$$s = b - \left(\frac{b-a}{f(b)-f(a)}\right) f(b)$$



$$y(x) = f(b) - \left(\frac{f(b)-f(a)}{b-a}\right)(b-x)$$

Then, $y(s) = f(b) - \left(\frac{f(b)-f(a)}{b-a}\right)(b-s) = 0$

$$(b-s) = \frac{b-a}{f(b)-f(a)} f(b)$$

$$s = b - \left(\frac{b-a}{f(b)-f(a)}\right) f(b) \quad //$$

If $f(a)f(s) < 0$, then use $[a, s]$ for next iteration; otherwise, use $[s, b]$

Still has only linear convergence

If $f(a)f(b) < 0$ → Guaranteed to converge!

③ Newton-Raphson Method

Let x_1 be a point near the root x^*

Then, from Taylor series,

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{1}{2} f''(x_1)(x - x_1)^2 + \ldots$$

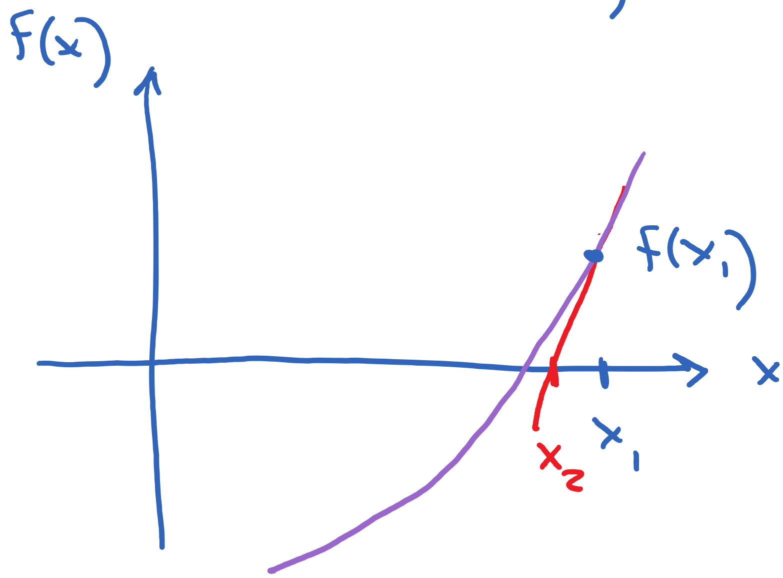
Approximate as

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \mathcal{O}(x - x_1)^2$$

and solve for approximation to root

$$f(x_2) = f(x_1) + f'(x_1)(x_2 - x_1) = 0$$

$$\rightarrow \quad x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$



Each iteration is then

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Consider convergence chacteristics

Let x^* be the true root and x_i, x_{i+1} be estimates at iterations i, $i+1$, such that

$$|x^* - x_i| = \delta \ll 1$$

Define errors $e_i = x^* - x_i$, $e_{i+1} = x^* - x_{i+1}$

However, we know

$$f(x^*) = 0 = f(x_i) + f'(x_i)(x^* - x_i) + \frac{f''(\xi)}{2}(x^* - x_i)^2$$

for some $\xi \in (x^*, x_i)$ such that

$$\frac{f''(\xi)}{2}(x^* - x_i)^2 \approx \frac{f''(x_i)}{2}(x^* - x_i)^2 + \text{H.O.T.}$$

In Newton-Raphson

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \Rightarrow f(x_i) = f'(x_i)(x_i - x_{i+1})$$

Then,

$$f(x^*) = 0 = f(x_i) + f'(x_i)(x^* - x_i) + \frac{f''(\xi)}{2}(x^* - x_i)^2$$

$$0 = f'(x_i)(x_i - x_{i+1}) + f'(x_i)(x^* - x_i) + \frac{f''(\xi)}{2}(x^* - x_i)^2$$

$$0 = f'(x_i)(x^* - x_{i+1}) + \frac{f''(\xi)}{2}(x^* - x_i)^2$$

$$0 = f'(x_i)\, e_{i+1} + \frac{f''(\xi)}{2} e_i^2$$

$$0 = f'(x_i)\, e_{i+1} + \frac{f''(\xi)}{2} e_i^2$$

$$\rightarrow \quad e_{i+1} = -\frac{f''(\xi)}{2f'(x_i)} e_i^2$$

$$\rightarrow \quad e_{i+1} \propto e_i^2 \longrightarrow \text{2nd order convergence}$$

If $e_i \sim 10^{-3}$

$e_{i+1} \sim 10^{-6}$

$e_{i+2} \sim 10^{-12}$

Issues: The initial guess at the root, x_0, must be "close" to x^*

This means that one must test for divergence, as well as convergence

So, convergence occurs if $|f(x_i)| < \varepsilon$

Divergence occurs, if

# of iterations is large

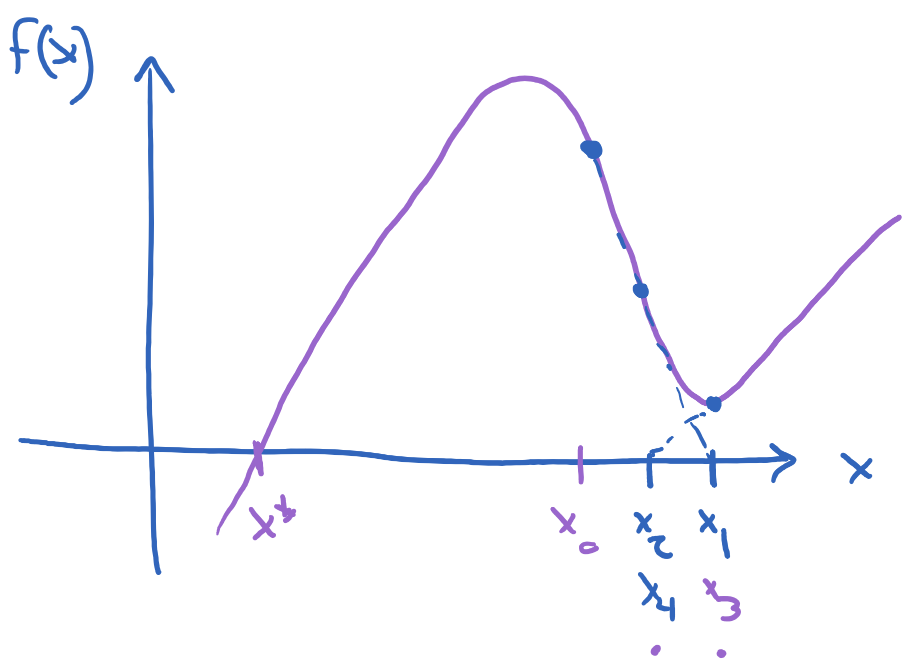
or $|f'(x_i)| < \varepsilon_1$

or $|x_{i+1} - x_i| > \delta$

Why check $|f'(x_i)| < \varepsilon_1$?

Because $x_{i+1} = x_i - \dfrac{f(x_i)}{f'(x_i)}$

One may never converge if x_0 is too far from x^* or if one gets oscillations



x_4 x_3

$\vdots$ $\vdots$

Final issue: $f'(x)$ might be difficult or expensive to evaluate

④ Secant Method: Tries to alleviate issue if $f'(x)$ is not known or expensive to evaluate

Approximate $f'(x_i) \approx \dfrac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$

Then,

$$x_{i+1} = x_i - \left(\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \right) f(x_i)$$

Rate of convergence is ≈ 1.62

Some of the same issues as Newton-Raphson

⑤ Fixed Point Method

A fixed point is one where

$x = h(x)$, e.g., $y(x) = \sqrt{x}$, $x = 1$

Let $f(x)$ have a linear and nonlinear part

$f(x) = x - g(x) \Rightarrow f(x) = 0$ as

$x - g(x) = 0 \rightarrow x = g(x)$

Iteration is then $x_{i+1} = g(x_i)$

Converges if $|x_{i+1} - g(x_{i+1})| < \varepsilon$

or $|f(x_{i+1})| < \varepsilon$

Convergence

Let x^* be the root, such that $x^* = g(x^*)$

with $x_{i+1} = g(x_i)$

Then $x^* - x_{i+1} = g(x^*) - g(x_i)$

and $$\frac{e_{i+1}}{e_i} = \frac{x^* - x_{i+1}}{x^* - x_i} = \frac{g(x^*) - g(x_i)}{x^* - x_i}$$

The mean value theorem of calculas states that if $g(x)$ is continuous over $[x^*, x_{i+1}]$, then there exists a $\xi \in [x^*, x_i]$ such that

$$g'(\xi) = \frac{g(x^*) - g(x_i)}{x^* - x_i}$$

$$\Rightarrow \frac{e_{i+1}}{e_i} = g'(\xi) \Rightarrow e_{i+1} = g'(\xi) e_i$$

$\Rightarrow$ Convergence occurs if $|g'(\xi)| < 1$