Lecture 9 Solving nonlinear system

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Outline

Examples

- The root of polynomials

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 = 0$$

- Polynomial system

$$\begin{cases} p_1(x_1, x_2, \cdots, x_n) & = & 0 \\ p_2(x_1, x_2, \cdots, x_n) & = & 0 \\ \cdots & \cdots & \cdots \\ p_n(x_1, x_2, \cdots, x_n) & = & 0 \end{cases}$$

- Some transcendental equation for example

$$x = \tan x$$

  or systems.

- Equations obtained from the discretization of nonlinear ordinary differential equations (ODEs) or partial differential equations (PDEs).

Iterations

- Iterative methods

  Object: construct sequence $\{\boldsymbol{x}_k\}_{k=1}^{\infty}$, such that $\boldsymbol{x}_k$ converge to a fixed vector $\boldsymbol{x}^*$, and $\boldsymbol{x}^*$ is the solution of the linear system.

- General iteration idea:

  If we want to solve equations

$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{0},$$

and the equation $\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x})$ has the same solution as it, then construct

$$\boldsymbol{x}_{k+1} = \boldsymbol{f}(\boldsymbol{x}_k).$$

If $\boldsymbol{x}_k \to \boldsymbol{x}^*$, then $\boldsymbol{x}^* = \boldsymbol{f}(\boldsymbol{x}^*)$, thus the root of $\boldsymbol{g}(\boldsymbol{x})$ is obtained.

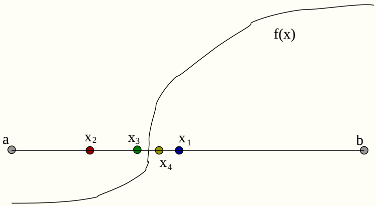
Bisection method

- Suppose we have interval $[a, b]$ and function $f(x)$

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

then there exists a root $c \in [a, b]$ such that $f(c) = 0$.

- In order to minimized the worst case possibility, the section point must be $\frac{a+b}{2}$. So the length of the interval will be halved successively.
- A linear convergence method $C = \frac{1}{2}$.



Bisection method

Algorithm

1. Set initial interval $a_0 = a, b_0 = b$, $k = 0$;
2. Choose $m = \frac{a_k+b_k}{2}$. If $f(m) = 0$, over; if $f(m)f(a_k) < 0$, set
$$a_{k+1} = a_k, \quad b_{k+1} = m$$
otherwise
$$a_{k+1} = m, \quad b_{k+1} = b_k$$
and set $k = k + 1$.
3. Repeat the above procedure until $|b_k - a_k| \leq \epsilon_0$.

Bisection method

Example: compute the minimal positive solution of the equation

$$\cos(x) + \frac{1}{1 + e^{-2x}} = 0$$

with bisection method.

Newton's method

- Taylor expansion at current iteration point x_0

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \cdots$$

- Local linear approximation

$$f(x) \approx g(x) = f(x_0) + f'(x_0)(x - x_0)$$

- Compute the root of $g(x)$, we have

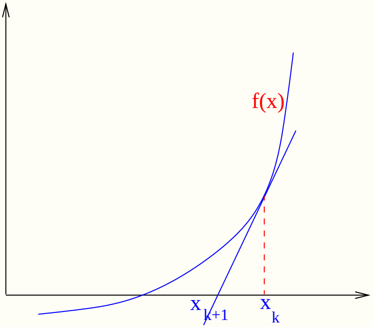
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

- Newton's method

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

Newton's method

- Graphical explanation



- Example: compute the minimal positive solution of the equation

$$\cos(x) + \frac{1}{1 + e^{-2x}} = 0$$

with Newton's method.

Newton's method

Theorem

If $f'(x^*) \neq 0$, then Newton's method converges with second order if x^0 is close to x^* sufficiently.

Drawbacks of Newton's method:

1. one needs to compute the derivative which is a huge cost (especially for high dimensional case).
2. The initial state x_0 must be very close to x^*.

Secant method

- To overcome the drawback of Newton's method on the evaluation of the derivative, introduce the secant method.
- Suppose we have iteration point x_{k-1}, x_k then

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

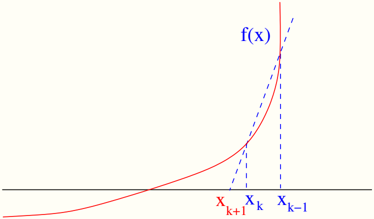
- Secant method

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

- Secant method needs two starting points.

Secant method

- Graphical explanation



- Example: compute the minimal positive solution of the equation

$$\cos(x) + \frac{1}{1 + e^{-2x}} = 0$$

with secant method.

Secant method

Theorem

If $f'(x^*) \neq 0$, then Secant's method converges with order $\frac{\sqrt{5}+1}{2} \approx 1.618$ if x_0, x_1 is close to x^* sufficiently.

Secant method can NOT be applied to high dimensional case directly.

Outline

Newton's method

- Taylor expansion at current iteration point $\boldsymbol{x}_0$

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x}_0) + \nabla F(\boldsymbol{x}_0) \cdot (\boldsymbol{x} - \boldsymbol{x}_0) + \cdots$$

- Local linear approximation

$$\boldsymbol{F}(\boldsymbol{x}) \approx \boldsymbol{G}(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x}_0) + \nabla \boldsymbol{F}(\boldsymbol{x}_0) \cdot (\boldsymbol{x} - \boldsymbol{x}_0)$$

where $\nabla \boldsymbol{F}$ is the Jacobian matrix defined as $(\nabla \boldsymbol{F})_{ij} = \frac{\partial F_i}{\partial x_j}$.

- Compute the solution of $\boldsymbol{G}(\boldsymbol{x}) = 0$, then

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 - \nabla \boldsymbol{F}(\boldsymbol{x}_0)^{-1} \cdot \boldsymbol{F}(\boldsymbol{x}_0)$$

- Newton's method

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \nabla \boldsymbol{F}(\boldsymbol{x}_k)^{-1} \cdot \boldsymbol{F}(\boldsymbol{x}_k)$$

Newton's method

- Example: compute one solution of the equation

$$\begin{cases} (x_1+3)(x_2^3-7)+18 &= 0 \\ \sin(x_2 e^{x_1}-1) &= 0 \end{cases}$$

with Newton's method, initial $[-0.5, 1.4]$.

Newton's method

Theorem

If $\nabla \boldsymbol{F}(\boldsymbol{x}^*)$ is nonsingular, then Newton's method converges with second order if $\boldsymbol{x}^0$ is close to $\boldsymbol{x}^*$ sufficiently.

Drawbacks of Newton's method:

1. one needs to compute the Jacobian matrix which is a huge cost.
2. The initial state $\boldsymbol{x}_0$ must be very close to $\boldsymbol{x}^*$.

Broyden's method

- Consider the local linear approximation of $\boldsymbol{F}$ at $\boldsymbol{x}_k$

$$\boldsymbol{F}(\boldsymbol{x}) \approx \boldsymbol{F}(\boldsymbol{x}_k) + \nabla \boldsymbol{F}(\boldsymbol{x}_k)(\boldsymbol{x} - \boldsymbol{x}_k)$$

- Take $\boldsymbol{x} = \boldsymbol{x}_{k-1}$, and define

$$\boldsymbol{g}_k = \boldsymbol{F}(\boldsymbol{x}_{k-1}) - \boldsymbol{F}(\boldsymbol{x}_k), \quad \boldsymbol{A}_k = \nabla \boldsymbol{F}(\boldsymbol{x}_k), \quad \boldsymbol{y}_k = \boldsymbol{x}_{k-1} - \boldsymbol{x}_k$$

then we have

$$\boldsymbol{A}_k \cdot \boldsymbol{y}_k = \boldsymbol{g}_k$$

- Similar as quasi-Newton's method for handling $\boldsymbol{A}_k$, take

$$\boldsymbol{A}_k = \boldsymbol{A}_{k-1} + \boldsymbol{C}_k$$

where $\boldsymbol{C}_k$ is a correction matrix.

Broyden's method

- Take C_k as a rank one matrix

$$\boldsymbol{C}_k = \boldsymbol{u}_k \boldsymbol{y}_k^T$$

where $\boldsymbol{u}_k$ is undetermined.

- Thus we have

$$\boldsymbol{A}_{k-1} \cdot \boldsymbol{y}_k + \boldsymbol{u}_k \boldsymbol{y}_k^T \boldsymbol{y}_k = \boldsymbol{g}_k$$

then

$$\boldsymbol{u}_k = \frac{\boldsymbol{g}_k - \boldsymbol{A}_{k-1} \cdot \boldsymbol{y}_k}{\boldsymbol{y}_k^T \boldsymbol{y}_k}$$

i.e. we have

$$\boldsymbol{A}_k = \boldsymbol{A}_{k-1} + \frac{\boldsymbol{g}_k - \boldsymbol{A}_{k-1} \cdot \boldsymbol{y}_k}{\boldsymbol{y}_k^T \boldsymbol{y}_k} \boldsymbol{y}_k^T$$

Remark on Broyden's method

- For the rank one correction of a matrix

$$\boldsymbol{B} = \boldsymbol{A} + \boldsymbol{x}\boldsymbol{y}^T$$

If $\boldsymbol{A}$ is invertible, and $\boldsymbol{y}^T\boldsymbol{A}\boldsymbol{x} \neq -1$, we have

$$\boldsymbol{B}^{-1} = \boldsymbol{A}^{-1} - \frac{\boldsymbol{A}^{-1}\boldsymbol{x}\boldsymbol{y}^T\boldsymbol{A}^{-1}}{1 + \boldsymbol{y}^T\boldsymbol{A}^{-1}\boldsymbol{x}}$$

- The formula above gives a efficient strategy to implement the quasi-Newton's method

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \boldsymbol{A}_k^{-1} \cdot \boldsymbol{F}(\boldsymbol{x}_k)$$

with $\boldsymbol{A}_k^{-1}$ is known.

- Broyden's method is a locally superlinear convergence method.

Introduction to homotopy method

- In order to overcome the difficulty of the local convergence, we consider the homotopy method.
- Introduce a linear homotopy

$$\boldsymbol{H}(\boldsymbol{x},t) = (1-t)\boldsymbol{F}_0(\boldsymbol{x}) + t\boldsymbol{F}(\boldsymbol{x})$$

  If $t=0$, $\boldsymbol{H}(\boldsymbol{x},0) = \boldsymbol{F}_0(\boldsymbol{x})$ which is often chosen a easily solved system.
  If $t=1$, $\boldsymbol{H}(\boldsymbol{x},1) = \boldsymbol{F}(\boldsymbol{x})$ which is the equations we would like to solve;
- Some choices of $\boldsymbol{F}_0(\boldsymbol{x})$:

$$\boldsymbol{F}_0(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x}-\boldsymbol{x}_0), \quad \boldsymbol{A} \text{ is nonsingular}$$

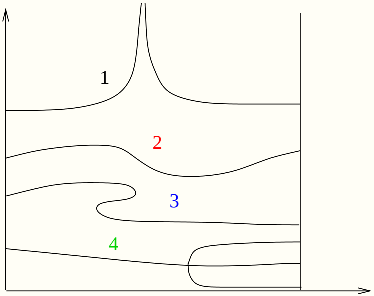
$$\boldsymbol{F}_0(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x}) - \boldsymbol{F}(\boldsymbol{x}_0)$$

Introduction to homotopy method

- Set up a sequence
$$0 = \lambda_0 < \lambda_1 < \cdots < \lambda_n = 1$$
The gap
$$\max |\lambda_i - \lambda_{i-1}| \leq \text{Tolerance}$$
- If we have the solution $\boldsymbol{x}_i$ for system $\boldsymbol{H}(\boldsymbol{x}, \lambda_i)$, then as an initial point, compute the solution $\boldsymbol{x}_{i+1}$ for system $\boldsymbol{H}(\boldsymbol{x}, \lambda_{i+1})$ by Newton-like method. Because $\lambda_i - \lambda_{i+1}$ is small, it is supposed $\boldsymbol{x}_i$ is close to $\boldsymbol{x}_{i+1}$.
- This method is very successful in solving the roots for polynomial system.

Homotopy method

- Graphical interpretation (顺藤摸瓜)



- Difficulties: The continuation pathway may be very complicate.
  1. Turning point: case 3 in figure.
  2. Going to infinity: case 1 in figure.
  3. Bifurcation point: case 4 in figure.

Homework assignment

Compute one solution of the equation

$$\begin{cases} (x_1+3)(x_2^3-7)+18 & = & 0 \\ \sin(x_2 e^{x_1}-1) & = & 0 \end{cases}$$

with Broyden's method, initial $[-0.5, 1.4]$.