Overview

Motivation:

- Root refinement: apply function approximation
  - → linear approximants: secant, Newton
  - → quadratic approximants: Halley, Brent

- Bisection has linear order of convergence. Are there faster methods?
- Observations:
  - Bisection only uses function values at interval endpoints
  - Function behavior over the interval is not used
- Idea: approximate the function over an interval

$$f(x)=0 \leftrightarrow f(x) \cong g(x)=0$$

- Choices:
  - g first-degree polynomial interpolant
  - g second-degree polynomial interpolant
  - g first-degree Taylor polynomial (series truncation)
  - g second-degree Taylor polynomial (series truncation)

- Instead of $f(x)=0$ solve $g(x)=0$ with $f\cong g$, g linear approximant
- Goal construct approximation sequence $\{x_n\}_{n\in\mathbb{N}}$, $x_n\to z$, $f(z)=0$
- Linear approximant = polynomial of degree $m=1$, requires 2 data points

$$\mathcal{D}=\{(x_i, y_i=f(x_i)), i=n-1,n\}$$

$$p(t)=\sum_{i=0}^{1} y_{n-1+i}\,\ell_{n-1+i}(t)=y_{n-1}\frac{t-x_n}{x_{n-1}-x_n}+y_n\frac{t-x_{n-1}}{x_n-x_{n-1}}$$

- Find next term in approximation sequence $\{x_n\}_{n\in\mathbb{N}}$ by setting $p(x_{n+1})=0\Rightarrow$

$$y_{n-1}(x_{n+1}-x_n)-y_n\,(x_{n+1}-x_{n-1})=0\Rightarrow$$

$$x_{n+1}=\frac{x_{n-1}\,y_n-x_n\,y_{n-1}}{y_n-y_{n-1}}=x_n-\frac{y_n}{y_n-y_{n-1}}(x_n-x_{n-1})$$

- The above is known as the *secant method*, and requires 1 function evaluation per iteration, same as bisection.

- Error analysis: define $e_n = x_n - z$
- Replace in secant iteration formula $x_{n+1} = x_n - \frac{y_n}{y_n - y_{n-1}}(x_n - x_{n-1})$

$$e_{n+1} = e_n - \frac{y_n}{y_n - y_{n-1}}(e_n - e_{n-1}) \quad (1)$$

- Assume $f \in C^2$, and use Taylor series expansions around root z ($f(z) = 0$)

$$y_n = f'(z)e_n + \frac{1}{2}f''(z)e_n^2 + \cdots, \; y_{n-1} = f'(z)e_{n-1} + \frac{1}{2}f''(z)e_{n-1}^2 + \cdots$$

- Replace in (1) (use notation $f' = f'(z)$, $f'' = f''(z)$, $c = f''/(2f')$)

$$\frac{y_n}{y_n - y_{n-1}} \cong \frac{f'(z)e_n + \frac{1}{2}f''(z)e_n^2}{f'(z)(e_n - e_{n-1}) + \frac{1}{2}f''(z)(e_n - e_{n-1})^2} \Rightarrow$$

$$e_{n+1} = e_n\left[1 - \frac{f' + \frac{1}{2}f''e_n}{f' + \frac{1}{2}(e_n + e_{n-1})f''}\right] = e_n\left[1 - \frac{1 + c\,e_n}{1 + (e_n + e_{n-1})c}\right] \Rightarrow$$

- Recall that for small δ

$$\frac{1}{1+\delta} = 1 - \delta + \delta^2 - \cdots$$

- Apply to with $\delta = e_{n-1}/(1+ce_n)$

$$e_{n+1} = e_n\left[1 - \frac{1+c\,e_n}{1+(e_n+e_{n-1})c}\right] = e_n\left[1 - \frac{1}{1+c\delta}\right] \cong e_n\,c\delta = \frac{c\,e_{n-1}e_n}{1+ce_n}$$

  Assume e_n is small such that $1+ce_n \cong 1$ to obtain $e_{n+1} = ce_{n-1}\,e_n$

- At what order does $\{e_n\}$ converge to zero? For large enough n

$$|e_n| \cong r\;|e_{n-1}|^p,\; |e_{n+1}| \cong r\;|e_n|^p => r^{p+1}|e_{n-1}|^{p^2} = |c|\;r\;|e_{n-1}|^{p+1}$$

- Since $e_n \to 0$, obtain $p^2 - p - 1 = 0$ with solution $p = \phi = (1+\sqrt{5})/2 \cong 1.62$
- Secant converges at rate p faster than linear, slower than quadratic

- Instead of $f(x)=0$ solve $g(x)=0$ with $f\cong g$, g linear approximant
- Goal construct approximation sequence $\{x_n\}_{n\in\mathbb{N}}$, $x_n\to z$, $f(z)=0$
- Linear approximant = Taylor polynomial of degree $m=1$

$$p(t)=f(x_n)+f'(x_n)(t-x_n)$$

- Find next term in approximation sequence $\{x_n\}_{n\in\mathbb{N}}$ by setting $p(x_{n+1})=0\Rightarrow$

$$f(x_n)+f'(x_n)(x_{n+1}-x_n)=0\Rightarrow$$

$$x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)}$$

- The above is known as the *Newton method*, and requires 1 function evaluation and 1 derivative evaluation per iteration, more expensive than secant or bisection.

- Error analysis: define $e_n = x_n - z$
- Replace in Newton iteration formula $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

$$e_{n+1} = e_n - \frac{f(x_n)}{f'(x_n)} \tag{2}$$

- Assume $f \in C^2$, and use Taylor series expansions around root z ($f(z) = 0$)

$$f(x_n) = f' e_n + \frac{1}{2} f'' e_n^2 + \cdots, \; f'(x_n) = f' + f''(z) e_n + \frac{1}{2} f'''(z) e_n^2 + \cdots$$

- Replace in (2) to obtain

$$e_{n+1} = e_n - \frac{f' e_n + \frac{1}{2} f'' e_n^2 + \cdots +}{f' + f'' e_n + \cdots} \cong \frac{1}{2} \frac{f''}{f'} e_n^2$$

- Newton's method is *second order* (as long as $f' \neq 0$)
- If $f' = f'(z) = 0$ (double roots) convergence drops to first order

- Instead of $f(x)=0$ solve $g(x)=0$ with $f \cong g$, g quadratic approximant
- Goal construct approximation sequence $\{x_n\}_{n\in\mathbb{N}}$, $x_n \to z$, $f(z)=0$
- Quadratic approximant = polynomial of degree $m=2$, Newton form

$$p(t)=y_{n-2}+[y_{n-1},y_{n-2}](t-x_{n-2})+[y_n,y_{n-1},y_{n-2}](t-x_{n-2})(t-x_{n-1})$$

- Find next term in approximation sequence $\{x_n\}_{n\in\mathbb{N}}$ by setting $p(x_{n+1})=0 \Rightarrow$

$$x_{n+1}=x_n-\frac{2y_n}{w\pm\sqrt{w^2-4y_n[y_n,y_{n-1},y_{n-2}]}},$$

- The w quantity involves divided differences

$$w=[y_n,y_{n-1}]+[y_n,y_{n-2}]-[y_{n-1},y_{n-2}]$$

- This is *Muller's method*, and requires 1 function evaluation per iteration and has order of convergence 1.84 (superlinear, better than secant 1.62)

- Instead of $f(x)=0$ solve $g(x)=0$ with $f \cong g$, g quadratic approximant
- Quadratic approximant = Taylor polynomial of degree $m=2$

$$p(t) = f(x_n) + f'(x_n)(t-x_n) + \frac{1}{2} f''(x_n)(t-x_n)^2$$

- Find next term in approximation sequence $\{x_n\}_{n\in\mathbb{N}}$ by setting $p(x_{n+1})=0 \Rightarrow$

$$x_{n+1} = x_n - \frac{2f(x_n)f'(x_n)}{2[f'(x_n)]^2 - f(x_n)f''(x_n)}$$

- The above is known as the *Halley's method*, and requires 1 function evaluation and 2 derivative evaluations per iteration, more expensive than Newton, but has cubic order of convergence.