1D Root Finding
Part II Roadmap

• Part I – Linear Algebra (units 1-12) \( Ac = b \)

• Part II – Optimization (units 13-20)
  • (units 13-16) Optimization -> Nonlinear Equations -> 1D roots/minima
  • (units 17-18) Computing/Avoiding Derivatives
  • (unit 19) Hack 1.0: “I give up” \( H = I \) and \( J \) is mostly 0 (descent methods)
  • (unit 20) Hack 2.0: “It’s an ODE!?" (adaptive learning rate and momentum)
Fixed Point Iteration

• Find roots of $g(t)$, i.e. where $g(t) = 0$

• Let $\hat{g}(t) = g(t) + t$ and iterate $t^{q+1} = \hat{g}(t^q)$ until convergence

• A converged $t^*$ satisfies $t^* = \hat{g}(t^*) = g(t^*) + t^*$ implying that $g(t^*) = 0$

• Converges when: $|g'(t^*)| < 1$, the initial guess is close enough to $t^*$, and $g$ is sufficiently smooth

• $e^{q+1} = t^{q+1} - t^* = \hat{g}(t^q) - \hat{g}(t^*) = g'(^\hat{t})(t^q - t^*) = g'(^\hat{t})e^q$ for some $^\hat{t}$ between $t^{q+1}$ and $t^*$ (by the Mean Value Theorem)

• When all $g'(^\hat{t})$ have $|g'(^\hat{t})| \leq C < 1$, then $|e^q| \leq C^q |e^0|$ proves convergence
Convergence Rate

- Consider $\|e^{q+1}\| \leq C \|e^q\|^p$ as $q \to \infty$ where $C \geq 0$
  - When $p = 1$, $C < 1$ is required and the convergence rate is linear
  - When $p > 1$, the convergence rate is superlinear
  - When $p = 2$, the convergence rate is quadratic

- Statements only apply asymptotically (once convergence is happening)
- Might converge to a different non-desired root (when other roots are present)

- Solving $g(t) = 0$ may only approximate the problem being solved, so it’s not clear how accurate the root finder needs to be anyways
1D Newton’s Method

• Solve $g'(t^q)\Delta t = -g(t^q)$ and update $t^{q+1} = t^q + \Delta t = t^q - \frac{g(t^q)}{g'(t^q)}$

• Stop when $|g(t^q)| < \epsilon$, which implies $|t^{q+1} - t^q| < \frac{\epsilon}{|g'(t^q)|}$
  - Thus, poorly conditioned when $g'(t^*)$ is small
  - Especially problematic for repeated roots where $g'(t^*) = 0$

• Quadratic convergence rate ($p = 2$), when not degenerate

• Requires computing $g$ and $g'$ every iteration; but, computing derivatives isn’t always straightforward/cheap (see units 17/18 on Computing/Avoiding Derivatives)
1D Newton’s Method

\[ t^{q+1} = t^q - \frac{g(t^q)}{g'(t^q)} \] or alternatively \( g'(t^q) = \frac{g(t^q) - 0}{t^q - t^{q+1}} = \frac{\Delta g}{\Delta t} \)
Secant Method

- Replace $g'(t^q)$ in Newton’s method with an estimate (a few choices for this)
- The standard approach draws a line through previous iterates
- Estimate $g'(t^q) \approx \frac{g(t^q) - g(t^{q-1})}{t^q - t^{q-1}}$
- Then $t^{q+1} = t^q - g(t^q) \frac{t^q - t^{q-1}}{g(t^q) - g(t^{q-1})}$

- Superlinear convergence rate with $p \approx 1.618$, when not degenerate
- Typically/often faster than Newton, since $g'$ is not needed and only a few extra iterations are required to obtain the same accuracy (for a reasonable accuracy)
Secant Method

\[ t^{q+1} = t^q - g(t^q) \frac{t^q - t^{q-1}}{g(t^q) - g(t^{q-1})} \] based on \( g'(t^q) \approx \frac{g(t^q) - g(t^{q-1})}{t^q - t^{q-1}} \)
Bisection Method

- If \( g(t_L)g(t_R) < 0 \), then (assuming continuity) the sign change indicates a root in the interval \([t_L, t_R]\)

- Let \( t_M = \frac{t_L + t_R}{2} \),
  - If \( g(t_L)g(t_M) < 0 \), set \( t_R = t_M \)
  - Otherwise, set \( t_L = t_M \) knowing that \( g(t_R)g(t_M) < 0 \) is true

- Iterate until \( t_R - t_L < \epsilon \)

- Guaranteed to converge to a root in the interval (unlike Newton/Secant)

- The interval shrinks in size by a factor of two each iteration; so, linear convergence rate \( p = 1 \) with \( C = \frac{1}{2} \)
Bisection Method

- If \( g(t_L)g(t_M) < 0 \), set \( t_R = t_M \); otherwise, set \( t_L = t_M \)
Mixed Methods

• Given an interval with a root indicated by $g(t_L)g(t_R) < 0$
• Iterate with Newton/Secant as long as the iterates stay inside the interval
  • When iteration attempts to leave the interval, use prior iterates to shrink the interval as much as possible (while still guaranteeing a root)
• If Newton/Secant attempt to leave the current interval, instead use Bisection to continue shrinking the interval

• Leverages the speed of Newton/Secant, while still guaranteeing convergence via Bisection

• Many/various strategies exist
Function/Derivative Requirements

• All methods require evaluation of the function $g$

• Newton also requires the derivative $g'$ (as do mixed methods using Newton)
Useful Derivatives

\[ \frac{\partial}{\partial t} c^{q+1}(t) = \Delta c^q, \text{ since } c^{q+1}(t) = c^q + t\Delta c^q \]

\[ \frac{\partial}{\partial t} F(c^{q+1}(t)) = J_F(c^{q+1}(t))\Delta c^q \text{ and } \frac{\partial}{\partial t} F^T(c^{q+1}(t)) = (\Delta c^q)^T J_F^T(c^{q+1}(t)) \]

- \[ \frac{\partial}{\partial t} F_i(c^{q+1}(t)) = (J_F)_i(c^{q+1}(t)) \Delta c^q \] where the \( F_i(c^{q+1}(t)) \) are the scalar row entries of \( F(c^{q+1}(t)) \)

- Scalar \( \hat{f}(c^{q+1}(t)) \) has system \( J_{\hat{f}}^T(c^{q+1}(t)) = 0 \) for critical points

\[ \frac{\partial}{\partial t} J_{\hat{f}}^T(c^{q+1}(t)) = H_{\hat{f}}^T(c^{q+1}(t))\Delta c^q \text{ and } \frac{\partial}{\partial t} J_{\hat{f}}(c^{q+1}(t)) = (\Delta c^q)^T H_{\hat{f}}(c^{q+1}(t)) \]

- \[ \frac{\partial}{\partial t} \left( J_{\hat{f}}^T \right)_i(c^{q+1}(t)) = \left( H_{\hat{f}}^T \right)_i(c^{q+1}(t))\Delta c^q \]
Recall: Line Search (Unit 14)

• Given the linearization errors in \( F'(c^q)\Delta c^q = (\beta - 1)F(c^q) \), the resulting \( \Delta c^q \) can lead to a poor estimate for \( c^{q+1} \) via \( c^{q+1} = c^q + \Delta c^q \)

• Instead, \( \Delta c^q \) is often just used as a search direction, i.e. \( c^{q+1} = c^q + \alpha^q \Delta c^q \)

• The 1D (parameterized) line \( c^{q+1}(\alpha) = c^q + \alpha \Delta c^q \) is the new domain

• Find an \( \alpha \) with \( F(c^{q+1}(\alpha)) = 0 \) simultaneously for all equations

• **Safe Set** methods restrict \( \alpha \) in various ways, e.g. \( 0 \leq \alpha \leq 1 \)
Recall: Line Search (Unit 14)

• Since $F$ is vector valued, consider $g(\alpha) = F(c^{q+1}(\alpha))^T F(c^{q+1}(\alpha)) = 0$
• Since $g(\alpha) \geq 0$, solutions to $F(c^{q+1}(\alpha)) = 0$ are minima of $g(\alpha)$
• $g(\alpha)$ might be strictly positive (with no $g(\alpha) = 0$), but minimizing $g(\alpha)$ might still help to make progress towards an $\alpha$ with $F(c^{q+1}(\alpha)) = 0$

• **Option 1**: find simultaneous roots of the vector valued $F(c^{q+1}(\alpha)) = 0$
• **Option 2**: find roots of or minimize $g(\alpha) = \frac{1}{2} F^T(c^{q+1}(\alpha)) F(c^{q+1}(\alpha))$, to find or make progress towards an $\alpha$ with $F(c^{q+1}(\alpha)) = 0$
Nonlinear Systems Problems

- Solve $J_F(c^q)Δc^q = (β - 1)F(c^q)$ for $Δc^q$ and use $c^{q+1}(t) = c^q + tΔc^q$ in $F(c^{q+1}(t)) = 0$

- **Option 1**: find simultaneous (for all $i$) roots for all the $g_i(t) = F_i(c^{q+1}(t)) = 0$
  - Here, $g'_i(t) = (J_F)_i(c^{q+1}(t))Δc^q$

- **Option 2**: find roots of $g(t) = \frac{1}{2}F^T(c^{q+1}(t))F(c^{q+1}(t)) = 0$
  - Here, $g'(t) = \frac{1}{2}F^T(c^{q+1}(t))J_F(c^{q+1}(t))Δc^q + \frac{1}{2}(Δc^q)^TJ_F^T(c^{q+1}(t))F(c^{q+1}(t))$
  - Since both terms are scalars, $g'(t) = F^T(c^{q+1}(t))J_F(c^{q+1}(t))Δc^q$
Recall: Optimization Problems (Unit 14)

- Minimize the scalar cost function $\hat{f}(c)$ by finding the critical points where $\nabla \hat{f}(c) = J^T_{\hat{f}}(c) = F(c) = 0$
- $F'(c^q)\Delta c^q = (\beta - 1)F(c^q)$ gives the search direction (as usual)
- Here, $F'(c) = J_F(c) = H^T_{\hat{f}}(c)$
- So, solve $H^T_{\hat{f}}(c^q)\Delta c^q = (\beta - 1)J^T_{\hat{f}}(c^q)$ to find the search direction $\Delta c^q$
- **Option 1**: find simultaneous roots of the vector valued $J^T_{\hat{f}}(c^{q+1}(\alpha)) = 0$, which are critical points of $\hat{f}(c)$
- **Option 2**: find roots of or minimize $g(\alpha) = \frac{1}{2}J^2_{\hat{f}}(c^{q+1}(\alpha))J^T_{\hat{f}}(c^{q+1}(\alpha))$, to find or make progress towards critical points of $\hat{f}(c)$
- **Option 3**: minimize $\hat{f}(c^{q+1}(\alpha))$ directly
Optimization Problems

• Solve \( H_f^T(c^q)\Delta c^q = (\beta - 1)J_f^T(c^q) \) for \( \Delta c^q \) and use \( c^{q+1}(t) = c^q + t\Delta c^q \) in \( J_f^T(c^{q+1}(t)) = 0 \)

• Option 1: find simultaneous (for all \( i \)) roots for all the \( g_i(t) = (J_f^T)_i(c^{q+1}(t)) = 0 \) to find the critical points of \( \hat{f}(c) \)
  • Here, \( g_i'(t) = (H_f^T)_i(c^{q+1}(t))\Delta c^q \)

• Option 2: find roots of \( g(t) = \frac{1}{2}J_f(c^{q+1}(t))J_f^T(c^{q+1}(t)) = 0 \) to find or make progress towards critical points of \( \hat{f}(c) \)
  • Here, \( g'(t) = \frac{1}{2}J_f(c^{q+1}(t))H_f^T(c^{q+1}(t))\Delta c^q + \frac{1}{2}(\Delta c^q)^TH_f(c^{q+1}(t))J_f^T(c^{q+1}(t)) \)
  • Since both terms are scalars, \( g'(t) = J_f(c^{q+1}(t))H_f^T(c^{q+1}(t))\Delta c^q \)

• Option 3: minimize \( \hat{f}(c^{q+1}(t)) \) directly (see unit 16)