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)

Theory

Methods
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

- The 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, 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)
• No guarantee of converging to a desired root (when other roots are present)

• Recall, $g(t) = 0$ may contain approximations, 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 (\( p = 2 \))

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

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

- Replace $g'(t^q)$ in Newton’s method with an estimate (a few choices for this)
- Standard technique/method 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 $p \approx 1.618$
- Often/typically faster than Newton, since only $g$ (not $g'$) is needed while only a few extra iterations are required for the same 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 \( t_M = \frac{t_L + t_R}{2} \), and if \( g(t_L)g(t_M) < 0 \), set \( t_R = t_M \)
  • Otherwise, set \( t_L = t_M \) knowing that \( g(t_M)g(t_R) < 0 \) is true

• Iterate until \( t_R - t_L < \varepsilon \)

• 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)
• Bisection can be used to continue to shrink the interval, whenever Newton/Secant would fail to stay inside the current 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

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

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

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

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

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

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

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

- Thus, $\Delta c^q$ is often (instead) used as a search direction, i.e. $c^{q+1} = c^q + \alpha^q \Delta c^q$

- The parameterized line $c^{q+1}(\alpha) = c^q + \alpha \Delta c^q$ is used as a 1D (input) domain

- Find $\alpha^q$ such that $F(c^{q+1}(\alpha^q)) = 0$ 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 a solution

• **Option 1**: find simultaneous roots of the vector valued $F(c^{q+1}(\alpha)) = 0$

• **Option 2**: find roots of or minimize $g(\alpha) = \frac{1}{2} F^T (c^{q+1}(\alpha)) F(c^{q+1}(\alpha))$
Nonlinear Systems Problems

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

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

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

• Minimize the scalar cost function $\hat{f}(c)$ by finding the critical points where $\nabla \hat{f}(c) = J^T_{\hat{f}}(c) = F(c) = 0$

• $F'(c^q)\Delta c^q = -F(c^q)$ gives the search direction, where $F'(c) = J_F(c) = H^T_{\hat{f}}(c)$

• That is, solve $H^T_{\hat{f}}(c^q)\Delta c^q = -J^T_{\hat{f}}(c^q)$ 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 $g(\alpha) = \frac{1}{2}J^T_{\hat{f}}(c^{q+1}(\alpha))J^T_{\hat{f}}(c^{q+1}(\alpha))$ to find or make progress toward critical points of $\hat{f}(c)$

• **Option 3:** minimize $\hat{f}(c^{q+1}(\alpha))$ directly
Optimization Problems

- Solve $H_f^T(c^q)\Delta c^q = -J_f^T(c^q)$ 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:** For vector valued $J_f^T(c^{q+1}(t))$, 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 $g(t) = \frac{1}{2}J_f^T(c^{q+1}(t))J_f^T(c^{q+1}(t)) = 0$ to find or make progress toward critical points of $\hat{f}(c)$
  - Here, $g'(t) = \frac{1}{2}J_f^T(c^{q+1}(t))H_f^T(c^{q+1}(t))\Delta c^q + \frac{1}{2}((\Delta c^q)^T H_f^T(c^{q+1}(t))J_f^T(c^{q+1}(t))$
  - Both terms are scalars, so $g'(t) = J_f^T(c^{q+1}(t))H_f^T(c^{q+1}(t))\Delta c^q$

- **Option 3:** Minimize $\hat{f}(c^{q+1}(t))$ directly (see unit 16)