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 $g(t)$ 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 $t^* = \hat{g}(t^*) = g(t^*) + t^*$, and so $g(t^*) = 0$

• Converges when $|g'(t^*)| < 1$ for a close enough initial guess (when $g$ 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 the desired root (when others are present)

• Recall, $g(t) = 0$ may contain approximations, so it’s not clear how accurate the root finder needs to be
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 multiple 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)
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 (when continuous) 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 $t_R - t_L < \epsilon$

- 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)
• 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 function evaluation $g$

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

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

- \( \frac{\partial}{\partial t} F \left( c^{q+1}(t) \right) = J_F \left( c^{q+1}(t) \right) \Delta c^q \) and \( \frac{\partial}{\partial t} F^T \left( c^{q+1}(t) \right) = (\Delta c^q)^T J_F^T \left( c^{q+1}(t) \right) \)
  - \( \frac{\partial}{\partial t} F_i \left( c^{q+1}(t) \right) = (J_F)_i \left( c^{q+1}(t) \right) \Delta c^q \) where \( F_i \left( c^{q+1}(t) \right) \) 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

- \( \frac{\partial}{\partial t} J_{\hat{f}}^T \left( c^{q+1}(t) \right) = H_{\hat{f}}^T \left( c^{q+1}(t) \right) \Delta c^q \) and \( \frac{\partial}{\partial t} J_{\hat{f}} \left( c^{q+1}(t) \right) = (\Delta c^q)^T H_{\hat{f}} \left( c^{q+1}(t) \right) \)
  - \( \frac{\partial}{\partial t} \left( J_{\hat{f}}^T \right)_i \left( c^{q+1}(t) \right) = \left( H_{\hat{f}}^T \right)_i \left( c^{q+1}(t) \right) \Delta c^q \)
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 $g'(t) = F^T(c^{q+1}(t))J_F(c^{q+1}(t))\Delta c^q$
Optimization Problems

• Solve $H^T_{\hat{f}}(c^q)\Delta c^q = -J^T_{\hat{f}}(c^q)$ for $\Delta c^q$ and use $c^{q+1}(t) = c^q + t\Delta c^q$ in $J^T_{\hat{f}}(c^{q+1}(t)) = 0$

• Option 1: For vector valued $J^T_{\hat{f}}(c^{q+1}(t))$, find simultaneous (for all $i$) roots for all the $g_i(t) = (J^T_{\hat{f}})_i(c^{q+1}(t)) = 0$ to find the critical points of $\hat{f}(c)$
  • Here, $g'_i(t) = (H^T_{\hat{f}})_i(c^{q+1}(t))\Delta c^q$

• Option 2: Find roots of $g(t) = \frac{1}{2}J^T_{\hat{f}}(c^{q+1}(t))J^T_{\hat{f}}(c^{q+1}(t)) = 0$ to find or make progress toward critical points of $\hat{f}(c)$
  • Here, $g'(t) = \frac{1}{2}J_{\hat{f}}(c^{q+1}(t))H^T_{\hat{f}}(c^{q+1}(t))\Delta c^q + \frac{1}{2}(\Delta c^q)^TH_{\hat{f}}(c^{q+1}(t))J^T_{\hat{f}}(c^{q+1}(t))$
  • Both terms are scalars, so $g'(t) = J_{\hat{f}}(c^{q+1}(t))H^T_{\hat{f}}(c^{q+1}(t))\Delta c^q$

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