Computational Methods

Systems of Nonlinear Equations
Systems of Nonlinear Equations

- Systems of linear equations can often be used to describe or approximate simple systems
  - Efficient direct and iterative solution algorithms
- A range of systems cannot be modeled linearly and require nonlinear equations
  - Iterative methods for single equations do not directly translate to systems of equations
    - Bracketing in multi-dimensional spaces is very difficult
    - Fixed point functions are harder to define and convergence is more difficult to assess
Fixed Point Methods

- The Fixed point problem for multi-dimensional space can be defined analogous to the one for single equations

\[ \bar{x} = g(\bar{x}) \]

- Fixed point methods converge in the neighborhood of a solution if the spectral radius of the Jacobian matrix of \( g(x) \) at the solution is less than 1

\[ \rho(J_g(x^*)) < 1 \quad , \quad \rho(A) = \max |\lambda_i| \leq \|A^k\|^{1/k} \]

- If the Jacobian at the solution is 0 then convergence is at least quadratic
Multivariate Newton’s Method

- In multiple dimensions the “derivative” of a system of functions is defined by the Jacobian matrix

\[
J_f(\vec{x}) = \begin{pmatrix}
\frac{\partial f_1(\vec{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\vec{x})}{\partial x_n} \\
\vdots & \ddots & \vdots \\
\frac{\partial f_m(\vec{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\vec{x})}{\partial x_n}
\end{pmatrix}
\]

- Newton’s method can be redefined

\[
g(\vec{x}) = \vec{x} - J_f(\vec{x})^{-1} f(\vec{x})
\]

- To avoid the matrix inversion the iteration can be performed in 2 steps

\[
J_f(\vec{x})\vec{s} = -f(\vec{x}), \quad g(\vec{x}) = \vec{x} + \vec{s}
\]
Multivariate Newton’s Method

- The Multivariate Newton’s Method converges quadratic if the Jacobian matrix is nonsingular
  - Has to start close enough to the solution to ensure the spectral radius condition for convergence
- Each iteration of Newton’s method requires a function computation, the computation of the Jacobian matrix and the solution of a linear system
  - Complexity per iteration is $O(n^3)$
Broyden’s Method

- When the Jacobian matrix is not available we need a way to approximate it while still maintaining performance
  - In scalar functions this leads to the secant method
  - In multi-variate systems the next best thing is Broyden’s Method
    - Assume the best available approximation of the Jacobian at time $i-1$
    - $A_{i-1}$
    - Then the approximate fixed point step is
    $$x_i = x_{i-1} - A_{i-1}^{-1}F(x_{i-1})$$
Broyden’s Method

Now we have to compute $A_i$

- $A$ should respect the derivative and orthogonality relation
  
  $A_i \delta_i \approx \Delta_i$

  $\delta_i = x_i - x_{i-1}$, $\Delta_i = f(x_i) - f(x_{i-1})$

  
  $A_i \omega = A_{i-1} \omega$ for $\delta_i^T \omega = 0$

  From this follows

  $A_i = A_{i-1} + \frac{(\Delta_i - A_{i-1} \delta_i) \delta_i^T}{\delta_i^T \delta_i}$

- Sherman-Morrison formula

  $A_i^{-1} = A_{i-1}^{-1} + \frac{(\delta_i - A_{i-1} \Delta_i) \delta_i^T A_{i-1}^{-1}}{\delta_i^T A_{i-1}^{-1} \Delta_i}$

  Requires no matrix inversion (reduces iteration to $O(n^2)$)
Systems of Nonlinear Equations

- Systems of nonlinear equations can be solved using iterative fixed point methods
  - Existence of solution and convergence are difficult to determine
- Different iterative methods can be used
  - Newton’s method
    - Requires $O(n^3)$ operations per iteration
    - Quadratic convergence
  - Broyden’s method
    - Analogous to Secant method for single equation
    - With Sherman-Morrison update reduces to $O(n^2)$ per iteration