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 can not 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 mutli-dimensional space can be defined analogous to the one for single equations

$$\vec{x} = g(\vec{x})$$

  - 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

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

  - 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

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

- 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 $J_f(\vec{x})\vec{s} = -f(\vec{x}) \quad , \quad g(\vec{x}) = \vec{x} + \vec{s}$

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 a 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

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

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

    - 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

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

  - 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