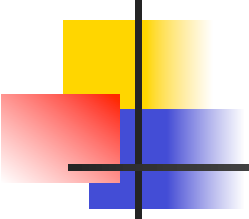


Computational Methods

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 multi-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

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

- 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

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

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

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

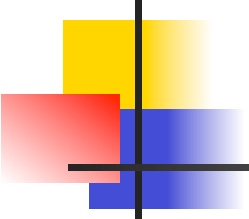
- From this follows

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

- 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