Techniques for Parameter Estimation

``Millionaires should always gamble, poor men never,'' J.M. Keynes

``If I wanted to gamble, I would buy a casino,'' P. Getty

Parameter Estimation Problem

Example: Spring model

$$m\ddot{u} + c\dot{u} + ku = F_0 \cos \omega t$$

has the solution

$$u(t) = c_1 e^{r_1 t} + c_2 e^{r_2 t} + \frac{F_0}{\sqrt{m^2(\omega_0^2 - \omega^2)^2 + c^2\omega^2}} \cos(\omega t - \delta)$$

where r_1 and r_2 are solutions of the characteristic equation, $\omega_0^2 = k/m$, δ satisfies $\cos \delta = m(\omega_0^2 - \omega^2)/\Delta$, and $\Delta = \sqrt{m^2(\omega_0^2 - \omega^2)^2 + c^2\omega^2}$.

Note: Nonlinear dependence on the parameters q = (m,c,k)

Admissible Parameter Space:

$$\mathcal{Q} = \{(m, c, k) \,|\, 0 < m < M, 0 \leq c < C, 0 < k < k\}$$

First-Order System with Observations:

$$\frac{dx}{dt} = Ax(t;q) + F(t)$$

$$y(t;q) = Cx(t;q)$$

Parameter Estimation Problem

Parameter Estimation Problem (Scalar): Find $q \in Q$ that minimizes

$$J(q) = \sum_{j=1}^{n} [y_j - y(t_j;q)]^2$$

$$\Rightarrow \hat{q} = \arg \min_{q \in Q} \sum_{j=1}^{n} [y_j - y(t_j;q)]^2$$

where $y(t_j;q)$ are observed model values determined by

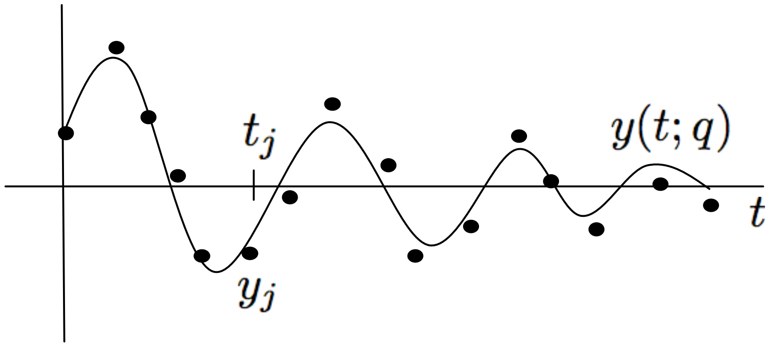
$$\frac{dx}{dt} = Ax(t;q) + F(t)$$

$$y(t;q) = Cx(t;q)$$

and y_j denotes data collected at times $t_j, j = 1, \cdots, n$.

Issues:

- Optimization techniques
- Accommodation of errors or noise in the model and data



Note: *Numerical Methods for Model Calibration*, MA 798C, Fall 2008, TH 10:15-11:30

MATLAB Optimization Routines

Note: There is significant documentation for the Optimization Toolbox

Minimization:

- fmincon: Constrained nonlinear minimization
- fminsearch: Unconstrained nonlinear minimization (Nelder-Mead)
- fminunc: Unconstrained nonlinear minimization (gradient-based trust region)
- quadprog: Quadratic programming

Equation Solving:

- fsolve: Nonlinear equation solving
- fzero: scalar nonlinear equation solving

Least Squares:

- lsqlin: Constrained linear least squares
- lsqnonlin: Nonlinear least squares
- lsqnonneg: Nonnegative linear least squares

Kelley's Routines: Available at the webpage http://www4.ncsu.edu/~ctk/

Tie between Optimization and Root Finding

Problem 1: minimize $f(x)$, $f : \mathbb{R}^n \to \mathbb{R}$

Problem 2: solve $F(x) = 0$ where $F : \mathbb{R}^n \to \mathbb{R}^n$

Note:

- If x^* solves (1), it also solves (2) with $F(x) = \nabla f(x)$
- If x^* solves (2), it solves (1) with $f(x) = \|F(x)\|^2 = F(x)^T F(x)$

Newton's Method (n=1): Let x_j approximate the root p with $F'(x_j) \neq 0$. Then

$$F(x) = F(x_j) + F'(x_j)(x - x_j) + \frac{(x - x_j)^2}{2} F''(\xi)$$

$$\Rightarrow 0 \approx F(x_j) + F'(x_j)(p - x_j)$$

$$\Rightarrow p \approx x_j - \frac{F(x_j)}{F'(x_j)}$$

Iteration: $x_{j+1} = x_j - \frac{F(x_j)}{F'(x_j)}$

Note: Quadratic convergence if function is sufficiently smooth and 'reasonable' initial value

Tie between Optimization and Root Finding

Newton's Method (n>1): Consider $F(x) = \nabla f(x) = 0$

Iteration: $x_{j+1} = x_j + s_j$ where s_j solves

$$F(x_j) + F'(x_j)s_j = 0$$

$$\Rightarrow x_{j+1} = x_j - H(x_j)^{-1}\nabla f(x_j)$$

Hession:

$$F'(x) = H(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}$$