CS5321 Numerical Optimization

10 Least Squares Problem

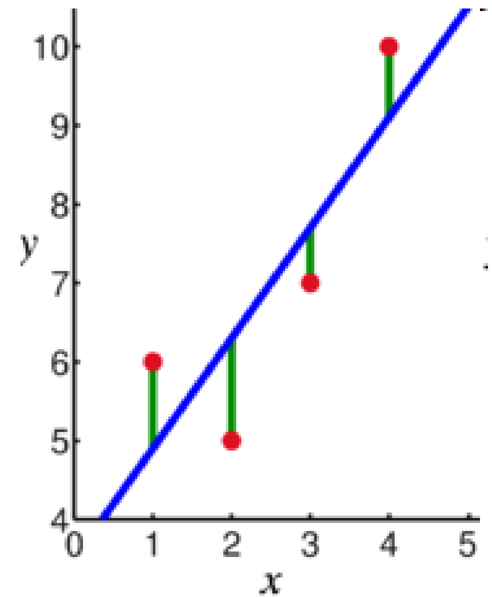
Least-squares problems

- Linear least-squares problems
  - QR method
- Nonlinear least-squares problems
  - Gradient and Hessian of nonlinear LSP
  - Gauss--Newton method
  - Levenberg--Marquardt method
  - Methods for large residual problem

Example of linear least square

- $y = \beta_1 + \beta_2 x$ (from Wikipedia)

$$\begin{aligned} \beta_1 + 1\beta_2 &= 6 \\ \beta_1 + 2\beta_2 &= 5 \\ \beta_1 + 3\beta_2 &= 7 \\ \beta_1 + 4\beta_2 &= 10 \end{aligned}$$



$$[6-(\beta_1+1\beta_2)]^2+[5-(\beta_1+2\beta_2)]^2+[7-(\beta_1+3\beta_2)]^2+[10-(\beta_1+4\beta_2)]^2$$

- $\beta_1 = 3.5$, $\beta_2 = 1.4$. The line is $y = 3.5 + 1.4x$

Linear least squares problems

- A linear least-squares problem is $f(x) = {}^1/_2 ||Ax - y||^2$.
- It's gradient is $\nabla f(x) = A^\mathrm{T}(Ax - y)$
- The optimal solution is at $\nabla f(x) = 0$, $A^\mathrm{T}Ax = A^\mathrm{T}y$
  - $A^\mathrm{T}Ax = A^\mathrm{T}y$ is called the *normal* equation.
- Perform QR decomposition on matrix $A = QR$.

$$A^T A x = R^T Q^T Q R x = R^T Q^T y$$

  - R^T is invertible. The solution $x = R^{-1}Q^T y$.

Example of nonlinear LS

$$\phi(x,t) = x_1 + t x_2 + t^2 x_3 + x_4 e^{-x_5 t}$$

- Find $(x_1, x_2, x_3, x_4, x_5)$ to minimize $\frac{1}{2}\sum_{j=1}^{m}[\phi(x,t_j) - y_j]^2$

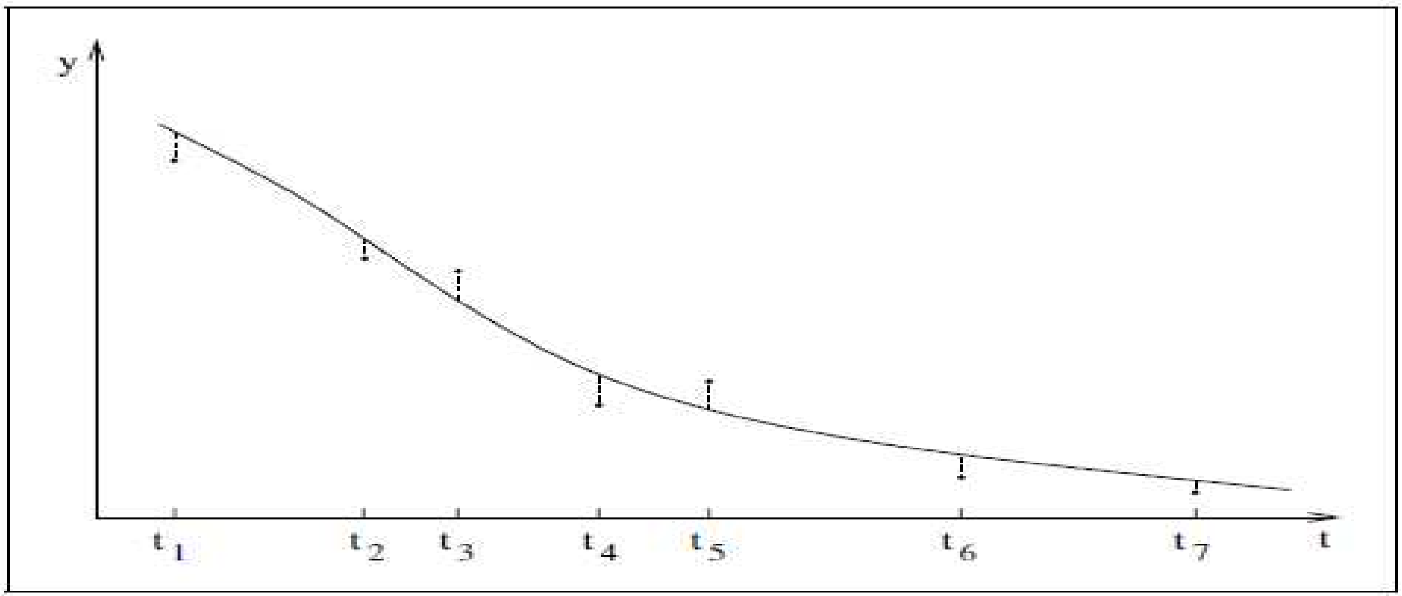


Figure 10.1 Deviation between the model (10.7) (smooth curve) and the observed measurements are indicated by the vertical bars.

Gradient and Hessian of LSP

- The object function of least squares problem is $f(x) = \frac{1}{2}\sum_{j=1}^{m} r_j^2(x)$ where r_i are n variable functions.
- Define $R(x) = \begin{pmatrix} r_1(x) \\ r_2(x) \\ \vdots \\ r_m(x) \end{pmatrix}$ The Jacobian $J(x) = \begin{pmatrix} \nabla r_1(x)^T \\ \nabla r_2(x)^T \\ \vdots \\ \nabla r_m(x)^T \end{pmatrix}$
- Gradient $\nabla f(x) \;=\; \sum_{j=1}^{m} r_j(x)\nabla r_j(x) = J(x)^T R(x)$

  Hessian $\nabla^2 f(x) \;=\; J(x)^T J(x) + \sum_{j=1}^{m} r_j(x)\nabla^2 r_j(x)^T$

Gauss-Newton method

$$\nabla^2 f(x) = J(x)^T J(x) + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)^T$$

- Gauss-Newton uses the Hessian approximation

$$\nabla^2 f(x) \approx J(x)^T J(x)$$

  - It's a good approximation if ||R|| is small.
  - This is the matrix of the normal equation
  - Usually with the line search technique
- Replace $f(x) = \frac{1}{2}\sum_{j=1}^{m} r_j^2(x)$ with $f(x) = \frac{1}{2}\|Jp + R\|^2$

Convergence of Gauss-Newton

- Suppose each r_j is Lipschitz continuously differentiable in a neighborhood $\mathcal{N}$ of $\{x|f(x)\leq f(x_0)\}$ and the Jacobians $J(x)$ satisfy $||J(x)z||\geq\gamma||z||$. Then the Gauss-Newton method, with α_k that satisfies the Wolfe conditions, has

$$\lim_{k\to\infty} J_k^T R_k = 0$$

Levenberg-Marquardt method

- Gauss-Newton + trust region
- The problem becomes

$$\min_p \frac{1}{2}\|Jp + R\|^2 \quad \text{subject to } \|p\| \le \Delta_k$$

- Optimal condition: (recall that in chap 4)

$$\begin{aligned}(J^T J + \lambda I)p &= -J^T R \\ \lambda(\Delta - \|p\|) &= 0\end{aligned}$$

- Equivalent linear least-square problem

$$\min_p \frac{1}{2}\left\|\begin{pmatrix} J \\ \sqrt{\lambda} I \end{pmatrix} p + \begin{pmatrix} R \\ 0 \end{pmatrix}\right\|^2$$

Convergence of Levenberg-Marquardt

- Suppose $\mathcal{L}=\{x \mid f(x) \leq f(x_0)\}$ is bounded and each r_j is Lipschitz continuously differentiable in a neighborhood $\mathcal{N}$ of $\mathcal{L}$. Assume for each k, the approximation solution p_k of the Levenberg-Marquardt method satisfies the inequality

$$m_k(0) - m_k(p_k) \geq c_1 \|J_k^T r_k\| \min\left(\Delta_k, \frac{\|J_k^T r_k\|}{\|J_k^T J_k\|}\right)$$

for some constant $c_1>0$, and $\|p_k\| \leq \gamma \Delta_k$ for some $\gamma>1$. Then $\lim_{k \to \infty} J_k^T R_k = 0$

Large residual problem

$$\nabla^2 f(x) = J(x)^T J(x) + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)^T$$

- When the second term of the Hessian is large
  - Use quasi-Newton to approximate the second term
  - The secant equation of $\nabla^2 r_j(x)$ is

$$(B_j)(x_{k+1} - x_k) = \nabla r_j(x_{k+1}) - \nabla r_j(x_k)$$

  - The secant equation of the second term and the update formula (next slide)

$$\begin{aligned} S_{k+1}(x_{k+1}-x_k) &= \sum_{j=1}^{m} r_j(x_{k+1})(B_j)_{k+1}(x_{k+1}-x_k) \\ &= \sum_{j=1}^{m} r_j(x_{k+1})[\nabla r_j(x_{k+1}) - \nabla r_j(x_k)] \\ &= J_{k+1}^T R_{k+1} - J_k^T R_{k+1} \end{aligned}$$

Dennis, Gay, Welsch update formula.

$$S_{k+1} = S_k + \frac{(z - S_k s)y^T + y(z - S_k s)^T}{y^T s} - \frac{(z - S_k s)^T s}{(y^T s)^2} y y^T$$

$$\begin{aligned} s &= x_{k+1} - x_k \\ y &= J_{k+1}^T r_{k+1} - J_k^T r_k \\ z &= J_{k+1}^T r_{k+1} - J_k^T r_{k+1} \end{aligned}$$