16. Gauss–Newton method

- definition and examples
- Gauss–Newton method
- Levenberg–Marquardt method
- separable nonlinear least squares

Nonlinear least squares

$$\text{minimize} \quad g(x) = \sum_{i=1}^{m} f_i(x)^2 = \|f(x)\|_2^2$$

- $f : \mathbf{R}^n \to \mathbf{R}^m$ is a differentiable function $f(x) = (f_1(x), \ldots, f_m(x))$ of n-vector x
- in general, a nonconvex optimization problem
- linear least squares is special case with $f(x) = Ax - b$

$$x^\star = A^+ b, \qquad g(x^\star) = \|(I - AA^+)b\|_2^2 = b^T(I - AA^+)b$$

  A^+ is the pseudo-inverse: $A^+ = (A^T A)^{-1} A^T$ if A has full column rank

- as in lecture 14 we denote the $m \times n$ Jacobian matrix of f by $f'(x)$:

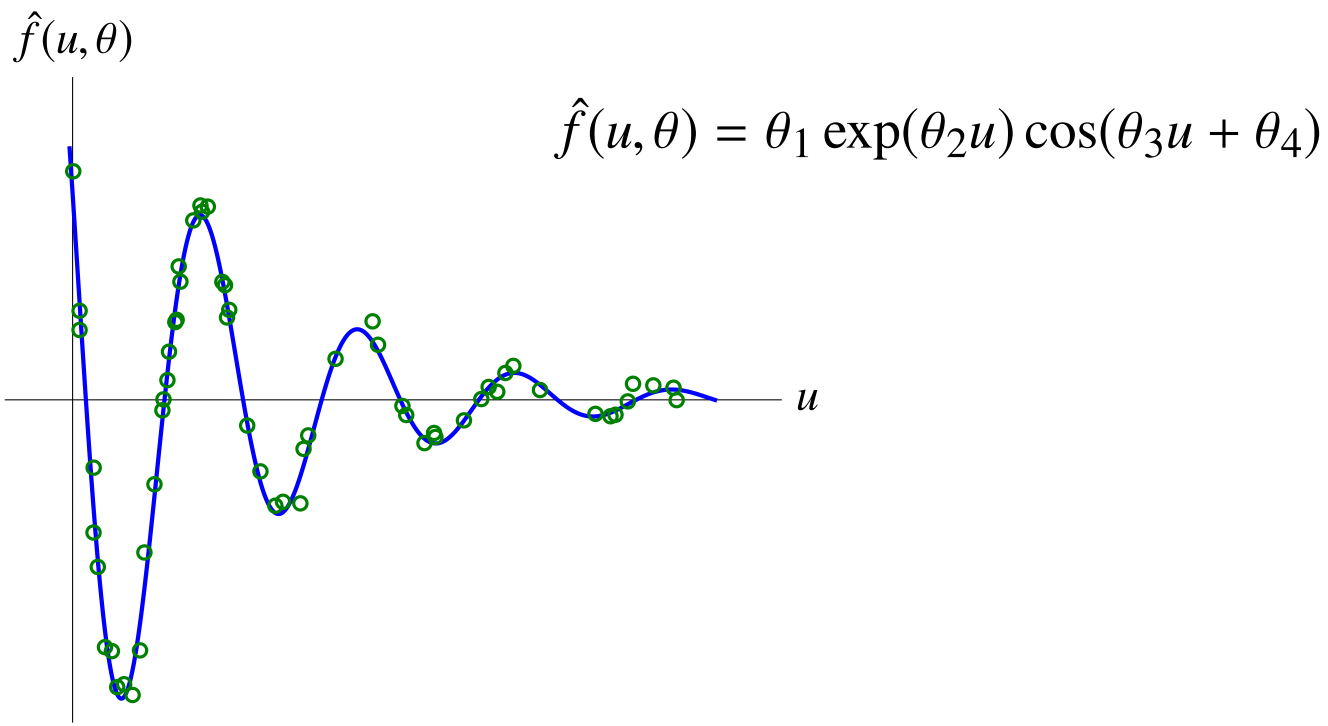
$$f'(x) = \begin{bmatrix} \nabla f_1(x)^T \\ \vdots \\ \nabla f_m(x)^T \end{bmatrix}$$

Model fitting

$$\text{minimize} \quad \sum_{i=1}^{N} (\hat{f}(u^{(i)}, \theta) - v^{(i)})^2$$

- model $\hat{f}(u, \theta)$ depends on model parameters $\theta_1, \ldots, \theta_p$
- $(u^{(1)}, v^{(1)}), \ldots, (u^{(N)}, v^{(N)})$ are data points
- the minimization is over the model parameters θ

Example

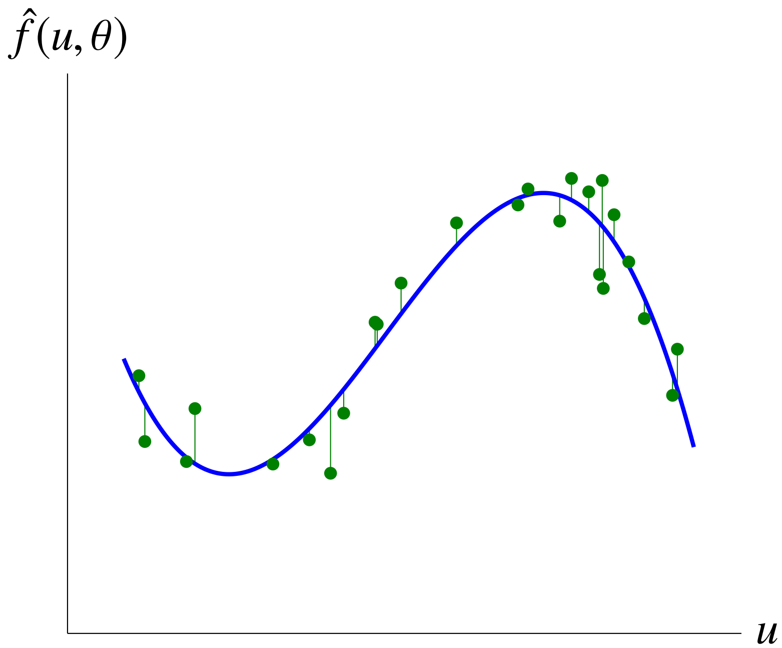


Orthogonal distance regression

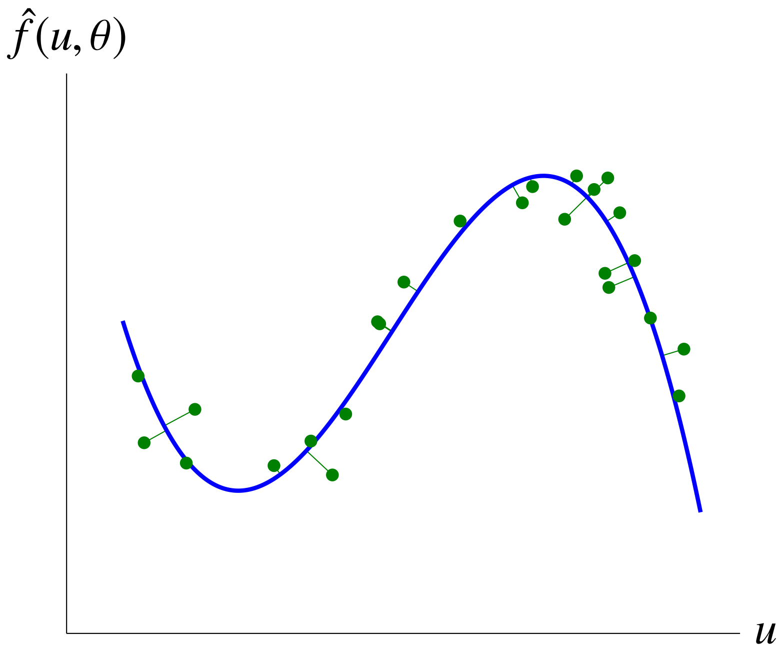
minimize the mean square distance of data points to graph of $\hat{f}(u,\theta)$

Example: orthogonal distance regression with cubic polynomial

$$\hat{f}(u,\theta) = \theta_1 + \theta_2 u + \theta_3 u^2 + \theta_4 u^3$$



standard least squares fit

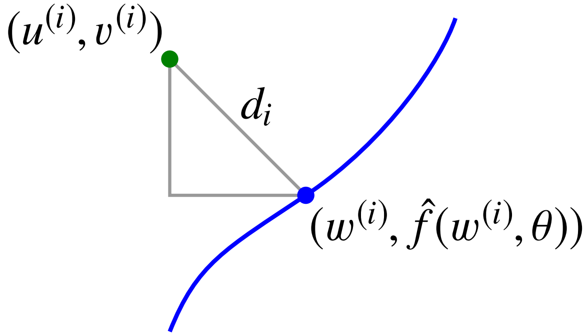


orthogonal distance fit

Nonlinear least squares formulation

$$\text{minimize} \quad \sum_{i=1}^{N} \left((\hat{f}(w^{(i)}, \theta) - v^{(i)})^2 + \|w^{(i)} - u^{(i)}\|_2^2 \right)$$

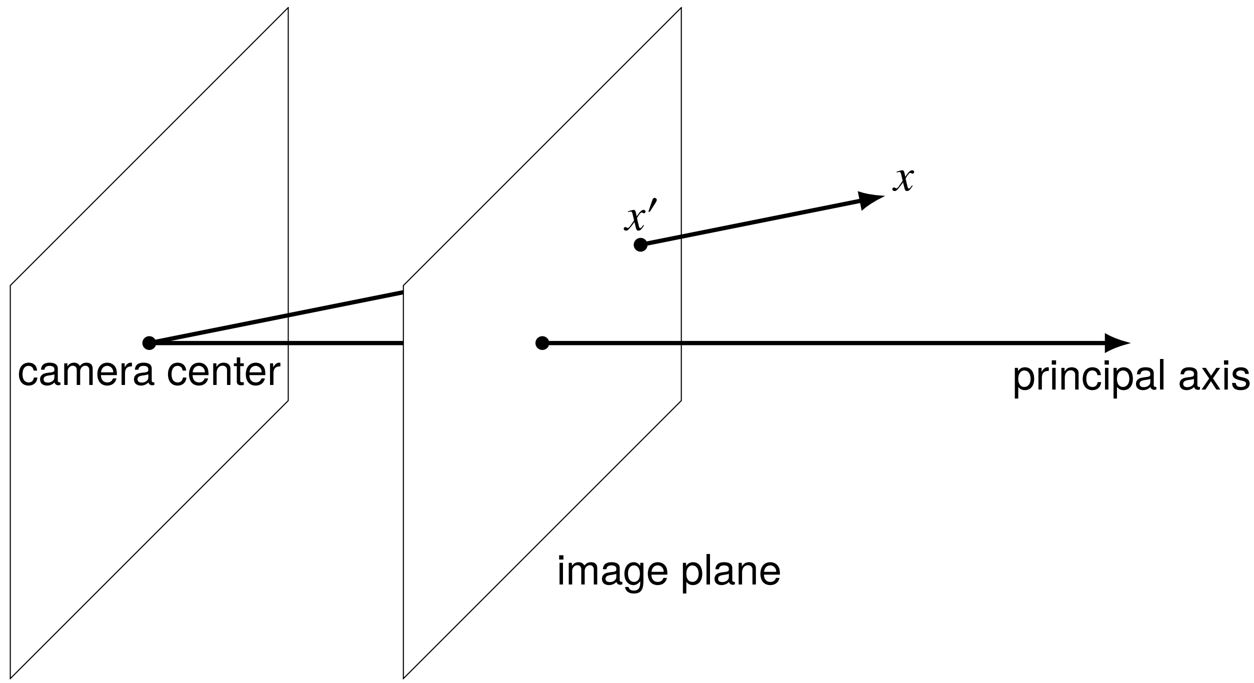
- optimization variables are model parameters θ and N points $w^{(i)}$
- ith term is squared distance of data point $(u^{(i)}, v^{(i)})$ to point $(w^{(i)}, \hat{f}(w^{(i)}, \theta))$



$$d_i^2 = (\hat{f}(w^{(i)}, \theta) - v^{(i)})^2 + \|w^{(i)} - u^{(i)}\|_2^2$$

- minimizing d_i^2 over $w^{(i)}$ gives squared distance of $(u^{(i)}, v^{(i)})$ to graph
- minimizing $\sum_i d_i^2$ over $w^{(1)}, \ldots, w^{(N)}$ and θ minimizes mean squared distance

Location from multiple camera views



Camera model: described by parameters $A \in \mathbf{R}^{2\times 3}$, $b \in \mathbf{R}^2$, $c \in \mathbf{R}^3$, $d \in \mathbf{R}$

- object at location $x \in \mathbf{R}^3$ creates image at location $x' \in \mathbf{R}^2$ in image plane

$$x' = \frac{1}{c^T x + d}(Ax + b)$$

  $c^T x + d > 0$ if object is in front of the camera

- A, b, c, d characterize the camera, and its position and orientation

Location from multiple camera views

- an object at location x_{ex} is viewed by l cameras (described by A_i, b_i, c_i, d_i)
- the image of the object in the image plane of camera i is at location

$$y_i = \frac{1}{c_i^T x_{\text{ex}} + d_i}(A_i x_{\text{ex}} + b_i) + v_i$$

- v_i is measurement or quantization error
- goal is to estimate 3-D location x_{ex} from the l observations $y_1, \ldots, y_l$

Nonlinear least squares estimate: compute estimate $\hat{x}$ by minimizing

$$\sum_{i=1}^{l} \left\| \frac{1}{c_i^T x + d_i}(A_i x + b_i) - y_i \right\|_2^2$$

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- **Gauss–Newton method**
- Levenberg–Marquardt method
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Gauss–Newton method

$$\text{minimize} \quad \|f(x)\|_2^2 = \sum_{i=1}^{m} f_i(x)^2$$

start at some initial guess x_0, and repeat for $k = 1, 2, \ldots$:

- linearize f around x_k:

$$f(x) \approx f(x_k) + f'(x_k)(x - x_k)$$

- substitute affine approximation for f in least squares problem:

$$\text{minimize} \quad \left\| f(x_k) + f'(x_k)(x - x_k) \right\|_2^2$$

- take the solution of this linear least squares problem as x_{k+1}

Gauss–Newton update

least squares problem solved in iteration k:

$$\text{minimize} \quad \|f'(x_k)(x - x_k) + f(x_k)\|_2^2$$

- if $f'(x_k)$ has full column rank, solution is given by

$$\begin{aligned} x_{k+1} &= x_k - (f'(x_k)^T f'(x_k))^{-1} f'(x_k)^T f(x_k) \\ &= x_k - f'(x_k)^+ f(x_k) \end{aligned}$$

- Gauss–Newton step $v_k = x_{k+1} - x_k$ is the solution of the linear LS problem

$$\text{minimize} \quad \|f'(x_k)v + f(x_k)\|_2^2$$

- to improve convergence, can add line search and update $x_{k+1} = x_k + t_k v_k$

Newton and Gauss–Newton steps

$$\text{minimize} \quad g(x) = \|f(x)\|_2^2 = \sum_{i=1}^{m} f_i(x)^2$$

Newton step at $x = x_k$:

$$\begin{aligned} v_{\text{nt}} &= -\nabla^2 g(x)^{-1} \nabla g(x) \\ &= -\left(f'(x)^T f'(x) + \sum_{i=1}^{m} f_i(x) \nabla^2 f_i(x) \right)^{-1} f'(x)^T f(x) \end{aligned}$$

Gauss–Newton step at $x = x_k$ (from previous page):

$$v_{\text{gn}} = -\left(f'(x)^T f'(x) \right)^{-1} f'(x)^T f(x)$$

- this can be written as $v_{\text{gn}} = -H^{-1} \nabla g(x)$ where $H = 2 f'(x)^T f'(x)$
- H is the Hessian without the terms $f_i(x) \nabla^2 f_i(x)$

Comparison

Newton step

- requires second derivatives of f
- not always a descent direction ($\nabla^2 g(x)$ is not necessarily positive definite)
- fast convergence near local minimum

Gauss–Newton step

- does not require second derivatives
- a descent direction: $H = 2f'(x)^T f'(x) \succ 0$ (if $f'(x)$ has full column rank)
- local convergence to $x^\star$ is similar to Newton method if

$$\sum_{i=1}^{m} f_i(x^\star)\nabla^2 f_i(x^\star)$$

is small (*e.g.*, $f(x^\star)$ is small, or f is nearly affine around $x^\star$)

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Levenberg–Marquardt method

addresses two difficulties in Gauss–Newton method:

- how to update x_k when columns of $f'(x_k)$ are linearly dependent
- what to do when the Gauss–Newton update does not reduce $\|f(x)\|_2^2$

Levenberg–Marquardt method

compute x_{k+1} by solving a *regularized* least squares problem

$$\text{minimize} \quad \|f'(x_k)(x - x_k) + f(x_k)\|_2^2 + \lambda_k \|x - x_k\|_2^2$$

- second term forces x to be close to x_k where local approximation is accurate
- with $\lambda_k > 0$, always has a unique solution (no rank condition on $f'(x_k)$)
- a proximal point update with convexified cost function

Levenberg–Marquardt update

regularized least squares problem solved in iteration k

$$\text{minimize} \quad \left\| f'(x_k)(x - x_k) + f(x_k) \right\|_2^2 + \lambda_k \left\| x - x_k \right\|_2^2$$

- solution is given by

$$x_{k+1} = x_k - \left(f'(x_k)^T f'(x_k) + \lambda_k I \right)^{-1} f'(x_k)^T f(x_k)$$

- Levenberg–Marquardt step $v_k = x_{k+1} - x_k$ is

$$\begin{aligned} v_k &= -\left(f'(x_k)^T f(x_k) + \lambda_k I \right)^{-1} f'(x_k)^T f(x_k) \\ &= -\frac{1}{2} \left(f'(x_k)^T f'(x_k) + \lambda_k I \right)^{-1} \nabla g(x_k) \end{aligned}$$

- for $\lambda_k = 0$ this is the Gauss–Newton step (if defined); for large λ_k,

$$v_k \approx -\frac{1}{2\lambda_k} \nabla g(x_k)$$

Regularization parameter

several strategies for adapting λ_k are possible; for example:

- at iteration k, compute the solution v of

$$\text{minimize} \quad \left\|f'(x_k)v + f(x_k)\right\|_2^2 + \lambda_k\|v\|_2^2$$

- if $\|f(x_k + v)\|_2^2 < \|f(x_k)\|_2^2$, take $x_{k+1} = x_k + v$ and decrease λ
- otherwise, do not update x (take $x_{k+1} = x_k$), but increase λ

Some variations

- compare actual cost reduction with reduction predicted by linearized problem
- solve a least squares problem with trust region

$$\begin{array}{ll}\text{minimize} & \|f'(x_k)v + f(x_k)\|_2^2 \\ \text{subject to} & \|v\|_2 \leq \gamma\end{array}$$

Summary: Levenberg–Marquardt method

choose x_0 and λ_0 and repeat for $k = 0, 1, \ldots$:

1. evaluate $f(x_k)$ and $A = f'(x_k)$
2. compute solution of regularized least squares problem:

$$\hat{x} = x_k - (A^T A + \lambda_k I)^{-1} A^T f(x_k)$$

3. define x_{k+1} and λ_{k+1} as follows:

$$\begin{cases} x_{k+1} = \hat{x} \text{ and } \lambda_{k+1} = \beta_1 \lambda_k & \text{if } \|f(\hat{x})\|_2^2 < \|f(x_k)\|_2^2 \\ x_{k+1} = x_k \text{ and } \lambda_{k+1} = \beta_2 \lambda_k & \text{otherwise} \end{cases}$$

- β_1, β_2 are constants with $0 < \beta_1 < 1 < \beta_2$
- terminate if $\nabla g(x_k) = 2A^T f(x_k)$ is sufficiently small

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Separable nonlinear least squares

$$\text{minimize} \quad \|A(y)x - b(y)\|_2^2$$

- $A : \mathbf{R}^p \to \mathbf{R}^{m \times n}$ and $b : \mathbf{R}^p \to \mathbf{R}^m$ are differentiable functions
- variables are $x \in \mathbf{R}^m$ and $y \in \mathbf{R}^p$
- reduces to linear least squares if $A(y)$ and $b(y)$ are constant

Example: the separable structure is common in model fitting problems

$$\text{minimize} \quad \sum_{i=1}^{N} \left(\hat{f}(u^{(i)}, \theta) - v^{(i)} \right)^2$$

- model $\hat{f}$ is linear combination of parameterized basis functions: $\theta = (x, y)$ and

$$\hat{f}(u, \theta) = x_1 h_1(u, y) + \cdots + x_p h_p(u, y)$$

- variables are coefficients $x_1, \ldots, x_p$ and parameters y

Derivative notation

$$f(x, y) = A(y)x - b(y)$$

- y is a p-vector, x is an n-vector, $A(y)$ is an $m \times n$ matrix
- we denote the rows of $A(y)$ by $a_i(y)^T$, with $a_i(y) \in \mathbf{R}^n$:

$$A(y) = \begin{bmatrix} a_1(y)^T \\ \vdots \\ a_m(y)^T \end{bmatrix}$$

- the Jacobian of $f(x, y)$ is the $m \times (n + p)$ matrix

$$f'(x, y) = \begin{bmatrix} A(y) & B(x, y) \end{bmatrix}, \qquad \text{where } B(x, y) = \begin{bmatrix} x^T a_1'(y) \\ \vdots \\ x^T a_m'(y) \end{bmatrix} - b'(y)$$

here $a_i'(y) \in \mathbf{R}^{n \times p}$ and $b'(y) \in \mathbf{R}^{m \times p}$ are the Jacobian matrices of a_i, b

Gauss–Newton algorithm

$$\text{minimize} \quad \|f(x,y)\|_2^2 = \|A(y)x - b(y)\|_2^2$$

- in the Gauss–Newton algorithm we choose for x_{k+1}, y_{k+1} the solution x, y of

$$\text{minimize} \quad \left\| \begin{bmatrix} A(y_k) & B(x_k, y_k) \end{bmatrix} \begin{bmatrix} x \\ y - y_k \end{bmatrix} - b(y_k) \right\|_2^2$$

- if we eliminate x in this problem, we compute y_{k+1} by solving

$$\text{minimize} \quad \left\| \left(I - A(y_k)A(y_k)^+\right) \left(B(x_k, y_k)(y - y_k) - b(y_k)\right) \right\|_2^2$$

from y_{k+1}, we then find

$$\begin{aligned} x_{k+1} &= A(y_k)^+ \left(b(y_k) - B(x_k, y_k)(y_{k+1} - y_k)\right) \\ &= \underset{x}{\operatorname{argmin}} \|A(y_k)x + B(x_k, y_k)(y_{k+1} - y_k) - b(y_k)\|_2^2 \end{aligned}$$

Variable projection algorithm (VARPRO)

$$\text{minimize} \quad \|f(x,y)\|_2^2 = \|A(y)x - b(y)\|_2^2$$

- we can also eliminate x in the original nonlinear LS problem, before linearizing
- substituting $x = A(y)^+ b(y)$ gives an equivalent nonlinear least squares problem

$$\text{minimize} \quad \left\|\left(I - A(y)A(y)^+\right) b(y)\right\|_2^2$$

- the Gauss–Newton applied to this problem is known as *variable projection*
- to improve convergence, we can add a step size or use Levenberg–Marquardt

Simplified variable projection

a further simplification results in the following iteration

1. compute $\hat{x} = A(y_k)^+ b(y_k)$, by solving the linear least squares problem

$$\text{minimize} \quad \|A(y_k)x - b(y_k)\|_2^2$$

2. compute y_{k+1} as the solution y of a second linear least squares problem

$$\text{minimize} \quad \left\| \left(I - A(y_k)A(y_k)^+\right) \left(B(\hat{x}, y_k)(y - y_k) - b(y_k)\right) \right\|_2^2$$

Interpretation

- step 2 is equivalent to solving the linear least squares problem

$$\text{minimize} \quad \left\| \begin{bmatrix} A(y_k) & B(\hat{x}, y_k) \end{bmatrix} \begin{bmatrix} x \\ y - y_k \end{bmatrix} - b(y_k) \right\|_2^2$$

  in the variables x, y, and using the solution y as y_{k+1}

- *cf.*, GN update of p. 16.18: we replace x_k in $B(x_k, y_k)$ with a better estimate $\hat{x}$

References

- Å. Björck, *Numerical Methods for Least Squares Problems* (1996), chapter 9.
- J. E. Dennis, Jr., and R. B. Schabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations* (1996), chapter 10.
- G. Golub and V. Pereyra, *Separable nonlinear least squares: the variable projection method and its applications*, Inverse Problems (2003).
- J. Nocedal and S. J. Wright, *Numerical Optimization* (2006), chapter 10.