13. Nonlinear least squares

- nonlinear least squares
- Gauss-Newton method
- Levenberg-Marquardt method
- nonlinear data fitting

Nonlinear least squares

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

- x is variable, $f_1(x), \ldots, f_m(x)$ are *residuals*
- $f : \mathbb{R}^n \to \mathbb{R}^m$ is vector residual with components $f_i(x)$:

$$f(x) = (f_1(x), f_2(x), \ldots, f_m(x))$$

- objective function is $\|f(x)\|^2$
- problem reduces to (linear) least squares if $f(x) = Ax - b$
- solution approximate or solves the set of nonlinear equations $f(x) = 0$

Example: Location from range measurements

- 3-vector x is position in 3-D, which we will estimate
- range measurements give (noisy) distance to known locations

$$\rho_i = \|x - a_i\| + v_i, \quad i = 1, \ldots, m$$

  a_i are known locations, v_i are noises

- least squares location estimation: choose $\hat{x}$ that minimizes

$$\sum_{i=1}^{m} \left(\|x - a_i\| - \rho_i\right)^2$$

- GPS works like this

Gradient of nonlinear least squares cost

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

- first derivative of g with respect to x_j:

$$\frac{\partial g}{\partial x_j}(z) = 2\sum_{i=1}^{m} f_i(z)\frac{\partial f_i}{\partial x_j}(z)$$

- gradient of g at z:

$$\nabla g(z) = \begin{bmatrix} \frac{\partial g}{\partial x_1}(z) \\ \vdots \\ \frac{\partial g}{\partial x_n}(z) \end{bmatrix} = 2\sum_{i=1}^{m} f_i(z)\nabla f_i(z) = 2Df(z)^T f(z)$$

Optimality condition

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

necessary condition for optimality: if x minimizes $g(x)$ then it must satisfy

$$\nabla g(x) = 2Df(x)^T f(x) = 0$$

- this generalizes the normal equations: if $f(x) = Ax - b$, then $Df(x) = A$ and

$$\nabla g(x) = 2A^T(Ax - b)$$

- for general f, the condition $\nabla g(x) = 0$ is not sufficient for optimality

Outline

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- **Gauss-Newton method**
- Levenberg-Marquardt method
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Linear least square approximation at each iteration

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

- $x^{(k)}$ is estimate of a solution at time k
- $\hat{f}(x; x^{(k)})$ is first order Taylor approximation of f around $x^{(k)}$:

$$\hat{f}(x; x^{(k)}) = f(x^{(k)}) + Df(x^{(k)})(x - x^{(k)})$$

  this is a good approximation if x near $x^{(k)}$ ($\|x - x^{(k)}\|$ is small)

- Gauss-Newton method produces new estimate $x^{(k+1)}$ that solves the problem

$$\text{minimize} \quad \|\hat{f}(x; x^{(k)})\|^2 = \|f(x^{(k)}) + Df(x^{(k)})(x - x^{(k)})\|^2$$

- the above problem is a linear least-squares problem with

$$A = Df(x^{(k)}), \quad b = Df(x^{(k)})x^{(k)} - f(x^{(k)})$$

Gauss-Newton method

setting $x^{(k+1)}$ to be the solution of the previous problem, we have

$$\begin{aligned} x^{(k+1)} &= (A^TA)^{-1}A^Tb \\ &= \left(Df(x^{(k)})^TDf(x^{(k)})\right)^{-1}Df(x^{(k)})^T\left(Df(x^{(k)})x^{(k)} - f(x^{(k)})\right) \\ &= x^{(k)} - \left(Df(x^{(k)})^TDf(x^{(k)})\right)^{-1}Df(x^{(k)})^Tf(x^{(k)}) \end{aligned}$$

- assumes that $A = Df(x^{(k)})$ has linearly independent columns
- if converged (*i.e.*, $x^{(k+1)} = x^{(k)}$) then

$$Df(x^{(k)})^Tf(x^{(k)}) = 0$$

  hence $x^{(k)}$ satisfies the optimality condition since gradient is $2Df(x)^Tf(x)$

Gauss-Newton algorithm

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given a starting point $x^{(1)}$ and solution tolerance ϵ

repeat for $k \geq 0$**:**

1. evaluate $Df(x^{(k)}) = (\nabla f_1(x^{(k)})^T, \ldots, \nabla f_m(x^{(k)})^T)$
2. set

$$x^{(k+1)} = x^{(k)} - \left(Df(x^{(k)})^T Df(x^{(k)})\right)^{-1} Df(x^{(k)})^T f(x^{(k)})$$

if stopping criteria holds, stop and output $x^{(k+1)}$

Stopping criteria

$$\|f(x^{(k)})\|^2 \leq \epsilon, \quad \|Df(x^{(k)})^T f(x^{(k)})\| \leq \epsilon, \quad \|x^{(k+1)} - x^{(k)}\| \leq \epsilon$$

- if $x^{(k+1)} = x^{(k)}$, then $x^{(k)}$ satisfies the optimality condition
- this does not mean that $x^{(k)}$ is a good solution
- it is common to run the algorithm from different starting points and choose the best solution of these multiple runs

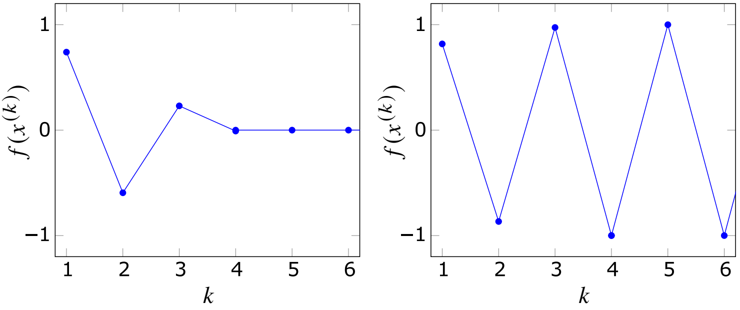
Issues with Gauss-Newton method

- approximation $\|f(x)\|^2 \approx \|\hat{f}(x; x^{(k)})\|^2$ holds when x near $x^{(k)}$
- when $x^{(k+1)}$ is not near $x^{(k)}$, the affine approximation will not be accurate
- so the algorithm may fail or diverge ($\|f(x^{(k+1)})\| > \|f(x^{(k)})\|$)
- a second major issue is that columns of the matrix $Df(x^{(k)})$ may not always be linearly independent; in this case, the next iterate is not defined

Example

$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

- starting point $x^{(1)} = 0.9$: converges very rapidly to $x^\star = 0$
- starting point $x^{(1)} = 1.1$: does not converge



Relation to Newton method for nonlinear equations

- Gauss-Newton update

$$x^{(k+1)} = x^{(k)} - \left(Df(x^{(k)})^T Df(x^{(k)})\right)^{-1} Df(x^{(k)})^T f(x^{(k)})$$

- if $m = n$, then $Df(x)$ is square and this is the Newton update

$$x^{(k+1)} = x^{(k)} - Df(x^{(k)})^{-1} f(x^{(k)})$$

Relation to Newton method for unconstrained minimization

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

- gradient:

$$\nabla g(x) = 2\sum_{i=1}^{m} f_i(x)\nabla f_i(x) = 2Df(x)^T f(x)$$

- second derivatives:

$$\frac{\partial^2 g}{\partial x_j \partial x_k}(x) = 2\sum_{i=1}^{m}\left(\frac{\partial f_i}{\partial x_j}(x)\frac{\partial f_i}{\partial x_k}(x) + f_i(x)\frac{\partial^2 f_i}{\partial x_j \partial x_k}(x)\right)$$

- Hessian

$$\nabla^2 g(x) = 2Df(x)^T Df(x) + 2\sum_{i=1}^{m} f_i(x)\nabla^2 f_i(x)$$

Newton and Gauss-Newton steps

(Undamped) Newton step at $x = x^{(k)}$:

$$\begin{aligned} v_{\mathrm{nt}} &= -\nabla^2 g(x)^{-1} \nabla g(x) \\ &= -\left(Df(x)^T Df(x) + \sum_{i=1}^{m} f_i(x) \nabla^2 f_i(x) \right)^{-1} Df(x)^T f(x) \end{aligned}$$

Gauss-Newton step at $x = x^{(k)}$:

$$v_{\mathrm{gn}} = -\left(Df(x)^T Df(x) \right)^{-1} Df(x)^T f(x)$$

- can be written as $v_{\mathrm{gn}} = -H_{\mathrm{gn}}^{-1} \nabla g(x)$ where $H_{\mathrm{gn}} = Df(x)^T Df(x)$
- H_{gn} is the Hessian without the term $\sum_i f_i(x) \nabla^2 f_i(x)$

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

- Gauss-Newton iteration is cheaper (does not require second derivatives)
- a descent direction (if columns of $Df(x)$ are linearly independent):

$$\nabla g(x)^T v_{\mathrm{gn}} = -2 v_{\mathrm{gn}}^T Df(x)^T Df(x) v_{\mathrm{gn}} < 0 \quad \text{if } v_{\mathrm{gn}} \neq 0$$

- 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 (for each i, $f_i(x^\star)$ is small or f_i is nearly affine around $x^\star$)

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Regularized approximate problem

ensure x is close to $x^{(k)}$ by regularization

$$\text{minimize} \quad \|f(x^{(k)}) + Df(x^{(k)})(x - x^{(k)})\|^2 + \lambda^{(k)}\|x - x^{(k)}\|^2$$

- regularization parameter $\lambda^{(k)}$ controls how close $x^{(k+1)}$ is to $x^{(k)}$
- regularization fixes invertibility issue of Gauss-Newton (no condition on $Df(x)$)
- the above problem can be rewritten as

$$\text{minimize} \quad \left\| \begin{bmatrix} Df(x^{(k)}) \\ \sqrt{\lambda^{(k)}} I \end{bmatrix} x - \begin{bmatrix} Df(x^{(k)})x^{(k)} - f(x^{(k)}) \\ \sqrt{\lambda^{(k)}} x^{(k)} \end{bmatrix} \right\|^2$$

this is just a least-squares problem with objective $\|Ax - b\|^2$ where

$$A = \begin{bmatrix} Df(x^{(k)}) \\ \sqrt{\lambda^{(k)}} I \end{bmatrix}, \quad b = \begin{bmatrix} Df(x^{(k)})x^{(k)} - f(x^{(k)}) \\ \sqrt{\lambda^{(k)}} x^{(k)} \end{bmatrix}$$

the solution is

$$x^{(k+1)} = x^{(k)} - \left(Df(x^{(k)})^T Df(x^{(k)}) + \lambda^{(k)} I\right)^{-1} Df(x^{(k)})^T f(x^{(k)})$$

we see $x^{(k+1)} = x^{(k)}$ only if optimality condition hold $Df(x^{(k)})^T f(x^{(k)})$

Updating $\lambda^{(k)}$

- if $\lambda^{(k)}$ is very small, then $x^{(k+1)}$ can be far from $x^{(k)}$, and the method may fail
- if $\lambda^{(k)}$ is large enough, then $x^{(k+1)}$ becomes close to $x^{(k)}$ and the affine approximation will be accurate enough
- a simple way to update $\lambda^{(k)}$ is to check whether

$$\|f(x^{(k+1)})\|^2 < \|f(x^{(k)})\|^2$$

  if so, then we can decrease $\lambda^{(k+1)}$; otherwise, we increase $\lambda^{(k+1)}$

Levenberg-Marquardt algorithm

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given a starting point $x^{(1)}$, solution tolerance ϵ, and $\lambda^{(1)} > 0$

repeat for $k \geq 0$

1. evaluate $Df(x^{(k)}) = \left(\nabla f_1(x^{(k)})^T, \ldots, \nabla f_m(x^{(k)})^T\right)$
2. update

$$x^{(k+1)} = x^{(k)} - \left(Df(x^{(k)})^T Df(x^{(k)}) + \lambda^{(k)} I\right)^{-1} Df(x^{(k)})^T f(x^{(k)})$$

   if stopping criteria holds, stop and output $x^{(k+1)}$

3. if $\|f(x^{(k+1)})\|^2 < \|f(x^{(k)})\|^2$, then decrease $\lambda^{(k+1)}$ (*e.g.*, $\lambda^{(k+1)} = 0.8\lambda^{(k)}$); otherwise, increase $\lambda^{(k+1)}$ (*e.g.*, $\lambda^{(k+1)} = 2\lambda^{(k)}$) and keep $x^{(k)} = x^{(k+1)}$

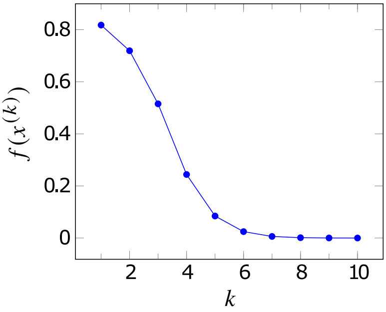
Stopping criteria

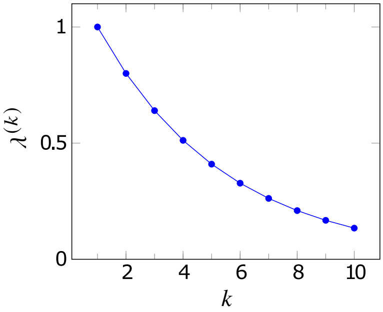
$$\|f(x^{(k)})\|^2 \leq \epsilon, \quad \|Df(x^{(k)})^T f(x^{(k)})\| \leq \epsilon, \quad \|x^{(k+1)} - x^{(k)}\| \leq \epsilon$$

Example

$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

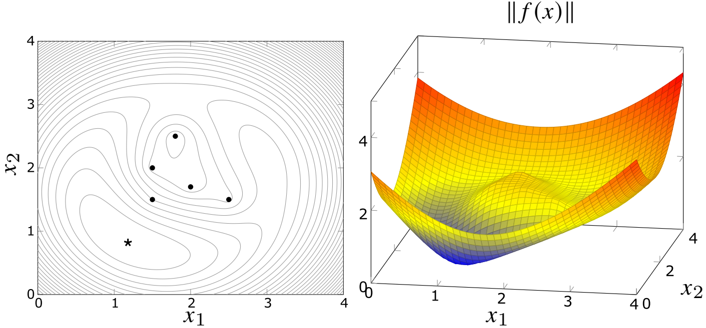
- we saw Gauss-Newton does not converge starting at $x^{(1)} = 1.1$
- for Levenberg-Marquardt starting at $x^{(1)} = 1.1$ and $\lambda^{(1)} = 1$ converges



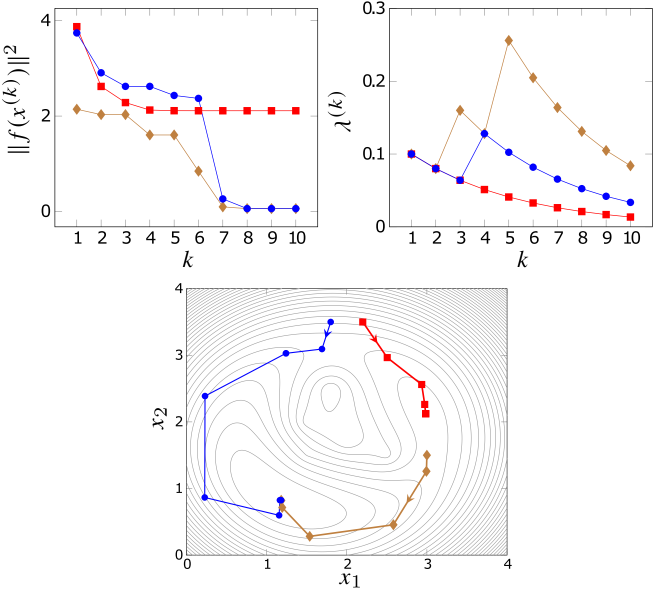


Example: Location from range measurements

- range to 5 points (blue circles)
- red square shows $\hat{x}$



Levenberg-Marquardt from three initial points



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- **nonlinear data fitting**

Nonlinear model fitting

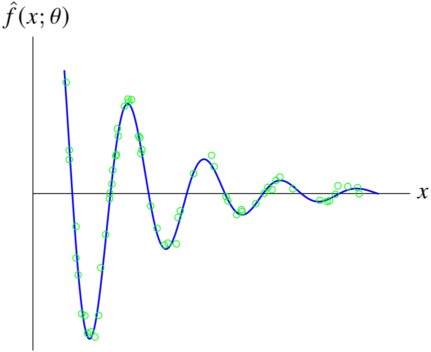
$$\text{minimize} \quad \sum_{i=1}^{N} \left(\hat{f}(x^{(i)};\theta) - y^{(i)}\right)^2$$

- $x^{(1)}, \ldots, x^{(N)}$ are feature vectors and $y^{(1)}, \ldots, y^{(N)}$ are associated outcomes
- model $\hat{f}(x;\theta)$ is parameterized by parameters $\theta_1, \ldots, \theta_p$
- this generalizes the linear in parameters model

$$\hat{f}(x;\theta) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$$

- here we allow $\hat{f}(x,\theta)$ to be a nonlinear function of θ
- the minimization is over the model parameters θ

Example

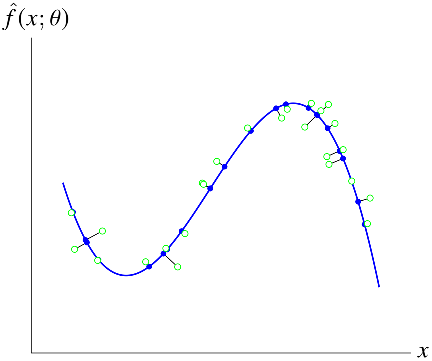


a nonlinear least squares problem with four variables $\theta_1, \theta_2, \theta_3, \theta_4$:

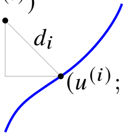
$$\text{minimize} \quad \sum_{i=1}^{N} \left(\theta_1 e^{\theta_2 x^{(i)}} \cos(\theta_3 x^{(i)} + \theta_4) - y^{(i)} \right)^2$$

Orthogonal distance regression

- to fit model, minimize sum square distance of data points to graph
- example: orthogonal distance regression to cubic polynomial



Nonlinear least squares formulation



$$d_i^2 = (\hat{f}(u^{(i)}, \theta) - y^{(i)})^2 + \|u^{(i)} - x^{(i)}\|^2$$

- linear in parameters model: $\hat{f}(x;\theta) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$
- minimizing over $(u^{(i)}, \theta)$ gives squared distance of $(x^{(i)}, y^{(i)})$ to graph $\hat{f}$

Orthogonal distance regression

$$\text{minimize} \quad \sum_{i=1}^{N} \left((\hat{f}(u^{(i)};\theta) - y^{(i)})^2 + \|u^{(i)} - x^{(i)}\|^2 \right)$$

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

Classification

Linear least squares classifier

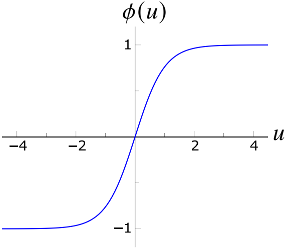
- data points $(x^{(i)}, y^{(i)})$ where $y^{(i)} \in \{-1, 1\}$
- classifier is $\hat{f}(x) = \mathrm{sign}(\tilde{f}(x))$ where $\tilde{f}(x) = \theta_1 f_1(x) + \cdots + \theta_p f_p(x)$
- θ is chosen by minimizing $\sum_{i=1}^N (\tilde{f}(x_i) - y_i)^2$ (plus optionally regularization)

Nonlinear least squares classifier

- choose θ to minimize $\sum_{i=1}^N (\mathrm{sign}(\tilde{f}(x^{(i)})) - y^{(i)})^2$
- replace sign function with smooth approximation ϕ, *e.g.*, sigmoid function

$$\text{minimize} \quad \sum_{i=1}^{N} \left(\phi(\tilde{f}(x^{(i)})) - y^{(i)}\right)^2$$

$$\phi(u) = \frac{e^u - e^{-u}}{e^u + e^{-u}}$$



References and further readings

- S. Boyd and L. Vandenberghe. *Introduction to Applied Linear Algebra: Vectors, Matrices, and Least Squares,* Cambridge University Press, 2018.

- L. Vandenberghe. *EE133A lecture notes,* Univ. of California, Los Angeles. (`http://www.seas.ucla.edu/~vandenbe/ee133a.html`)