

ECEn 671: Mathematics of Signals and Systems

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Section 1

Gauss-Newton Optimization

Least Squares as a Gradient Descent Problem

Consider the least squares problem

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2$$

where $A \in \mathbb{R}^{m \times n}$ is tall. We know that the solution is

$$x^* = (A^\top A)^{-1} A^\top b.$$

Can we pose this as a gradient descent problem?

Least Squares as a Gradient Descent Problem

Define the residual as

$$\mathbf{r}(x) = \begin{pmatrix} r_1(x) \\ \vdots \\ r_m(x) \end{pmatrix} = Ax - b$$

and define the sum-of-squares error as

$$\begin{aligned} S(x) &= \frac{1}{2} \mathbf{r}^\top(x) \mathbf{r}(x) \\ &= \frac{1}{2} \sum_{j=1}^m r_j^2(x) \\ &= \frac{1}{2} (Ax - b)^\top (Ax - b) \\ &= \frac{1}{2} \|Ax - b\|_2^2. \end{aligned}$$

The least squares problem is to find x that minimizes $S(x)$.

Least Squares as a Gradient Descent Problem

The gradient of S is given by

$$\begin{aligned}\frac{\partial S}{\partial x} &= \frac{\partial \mathbf{r}^\top}{\partial x}(x) \mathbf{r}(x) \\ &= A^\top (Ax - b) = A^\top Ax - A^\top b.\end{aligned}$$

So the gradient descent algorithm gives

$$x^{[k+1]} = x^{[k]} - \alpha \left(A^\top Ax^{[k]} - A^\top b \right)$$

In general, we might allow $\alpha > 0$ to be a positive definite matrix $\mathcal{A} > 0$:

$$x^{[k+1]} = x^{[k]} - \mathcal{A} \left(A^\top Ax^{[k]} - A^\top b \right).$$

Least Squares as a Gradient Descent Problem

Selecting

$$\mathcal{A} = (A^\top A)^{-1}$$

gives

$$\begin{aligned}x^{[k+1]} &= x^{[k]} - (A^\top A)^{-1} \left(A^\top A x^{[k]} - A^\top b \right) \\&= x^{[k]} - (A^\top A)^{-1} (A^\top A) x^{[k]} + (A^\top A)^{-1} A^\top b \\&= (A^\top A)^{-1} A^\top b,\end{aligned}$$

which is the optimal solution.

Noting that $A = \frac{\partial \mathbf{r}}{\partial x}$, we have shown that the iteration

$$x^{[k+1]} = x^{[k]} - \left(\frac{\partial \mathbf{r}^\top}{\partial x}(x^{[k]}) \frac{\partial \mathbf{r}}{\partial x}(x^{[k]}) \right)^{-1} \frac{\partial \mathbf{r}^\top}{\partial x}(x^{[k]}) \mathbf{r}(x^{[k]})$$

converges to the optimal in one step when $\mathbf{r}(x) = Ax - b$.

Nonlinear Least Squares

Let $r_j(x)$, $j = 1, \dots, m$ be a general set of residual function to be minimized. In other words, suppose we wish to solve

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \mathbf{r}^\top(x) \mathbf{r}(x).$$

Let $\mathbf{J}(x) \triangleq \frac{\partial \mathbf{r}}{\partial x}(x)$. Then the Gauss-Newton (GN) iteration algorithm is given by

$$x^{[k+1]} = x^{[k]} - \left(\mathbf{J}^\top(x^{[k]}) \mathbf{J}(x^{[k]}) \right)^{-1} \mathbf{J}^\top(x^{[k]}) \mathbf{r}(x^{[k]})$$

We know that the GN method converges in one step for the linear least squares problem.