Solving the Least-Squares Problem Using Gradients

Objectives

- Introduce gradients of linear and quadratic functions of $\underline{w}$
- Use gradients to solve least-squares problem
- Show solution is a minimizer
- Introduce projection matrices

The Least-Squares Problem

$$\min_{\underline{w}} \|\underline{A}\,\underline{w} - \underline{d}\|_2^2$$

$\underline{A}$: N features; $\underline{w}$: P model parameters; $\underline{d}$: N labels

Note: $\|\underline{z}\|_2^2 = \underline{z}^T\underline{z}$

$(\underline{A}\underline{B})^T = \underline{B}^T\underline{A}^T$

$$(\underline{A}\underline{w} - \underline{d})^T(\underline{A}\underline{w} - \underline{d}) \Rightarrow$$

$$\min_{\underline{w}} \underbrace{\underline{w}^T\underline{A}^T\underline{A}\underline{w} - \underline{w}^T\underline{A}^T\underline{d} - \underline{d}^T\underline{A}\underline{w} + \underline{d}^T\underline{d}}_{f(\underline{w})}$$

$f(\underline{w})$: quadratic in $\underline{w}$

Scalar problem: $\min_w \underbrace{a^2w^2 - 2\beta w + \gamma^2}_{g(w)}$ set $\frac{d}{dw}g(w) = 0$

$2a^2w - 2\beta = 0 \Rightarrow w = a^{-2}\beta$ $\quad a^2 > 0 \Rightarrow$ concave up, min

★ Gradients: differentiate $f(\underline{w})$ with respect to vector $\underline{w}$

$$\frac{\partial}{\partial \underline{w}} f(\underline{w}) = \underline{0}$$

L_2 Norm is $\|z\|_2$

On the previous page it is $\|z\|_2^2 = z_1^2 + z_2^2 + \cdots + z_n^2$

$$z^T z = \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} \begin{bmatrix} z_1 & \cdots & z_n \end{bmatrix} = z_1^2 + \cdots + z_n^2$$

$$\therefore z^T z = \|z\|_2^2$$

Gradients

$$\nabla_{\underline{w}} f(\underline{w}) = \left[\frac{\partial}{\partial w_1} f(\underline{w}) \quad \frac{\partial}{\partial w_2} f(\underline{w}) \cdots \frac{\partial}{\partial w_p} f(\underline{w}) \right]^T$$

3 (goal: 2)

① Linear case

Suppose $f(\underline{w}) = \underline{w}^T \underline{h} = \underline{h}^T \underline{w} = \sum_{i=1}^{p} w_i h_i \rightarrow \frac{\partial}{\partial w_j} f(\underline{w}) = h_j$

$$\nabla_{\underline{w}} f(\underline{w}) = [h_1 \; h_2 \cdots h_p]^T = \underline{h}$$

The gradients are just the h (coefficients of each w_i)

② Quadratic case

Suppose $f(\underline{w}) = \underline{w}^T \underline{Q} \underline{w}$ Can show $\nabla_{\underline{w}} f(\underline{w}) = \underline{Q}^T \underline{w} + \underline{Q} \underline{w}$

Symmetric case: $\underline{Q} = \underline{Q}^T \Rightarrow \nabla_{\underline{w}} f(\underline{w}) = 2\underline{Q}\underline{w}$

If $\underline{Q} = \underline{A}^T \underline{A} \Rightarrow (\underline{A}^T \underline{A})^T = \underline{A}^T \underline{A}$ symmetric

Solution: $\nabla_{\underline{w}} (\underline{w}^T \underline{A}^T \underline{A} \underline{w} - \underline{w}^T \underline{A}^T \underline{d} - \underline{d}^T \underline{A} \underline{w} + \underline{d}^T \underline{d}) = \underline{0}$

$$2\underline{A}^T \underline{A} \underline{w} - \underline{A}^T \underline{d} - \underline{A}^T \underline{d} = \underline{0} \Rightarrow \underline{w} = (\underline{A}^T \underline{A})^{-1} \underline{A}^T \underline{d}$$

Solution Attributes

$\underline{w} = (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$ $\quad \underline{A}: N \times P,\ P \le N,\ \text{rank}\,\underline{A} = P \Rightarrow (\underline{A}^T\underline{A})^{-1}$ exists

Minimizer ?

$$f(\underline{w}) = \underline{w}^T\underline{A}^T\underline{A}\underline{w} - \underline{w}^T\underline{A}^T\underline{d} - \underline{d}^T\underline{A}\underline{w} + \underline{d}^T\underline{d}$$

$$f(\underline{w}) = (\underline{w} - (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d})^T\underline{A}^T\underline{A}(\underline{w} - (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}) + \underline{d}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$

$$= \underline{w}^T\underline{A}^T\underline{A}\underline{w} - \underline{w}^T\underline{A}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{A}\underline{w} + \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^T\underline{A}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$

$\underline{w}_0$

$$+ \underline{d}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$

$$= \underline{w}^T\underline{A}^T\underline{A}\underline{w} - \underline{w}^T\underline{A}^T\underline{d} - \underline{d}^T\underline{A}\underline{w} + \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d} + \underline{d}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$

So $\quad f(\underline{w}) = \underline{z}^T(\underline{w})\,\underline{A}^T\underline{A}\,\underline{z}(\underline{w}) + \underline{d}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$

$\underline{z}(\underline{w}) = \underline{w} - \underline{w}_0\ ;\ \underline{w}_0 = (\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$

$\underline{A}^T\underline{A} > 0 \Rightarrow \min_{\underline{w}} f(\underline{w})$ when $\underline{w} = \underline{w}_0$

$$\min_{\underline{w}} f(\underline{w}) = \underline{d}^T\underline{d} - \underline{d}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d}$$

So why are we doing this?

Completing the square : $f(w) = (w - w_0)^T A^T A (w - w_0) + \text{Constant}$

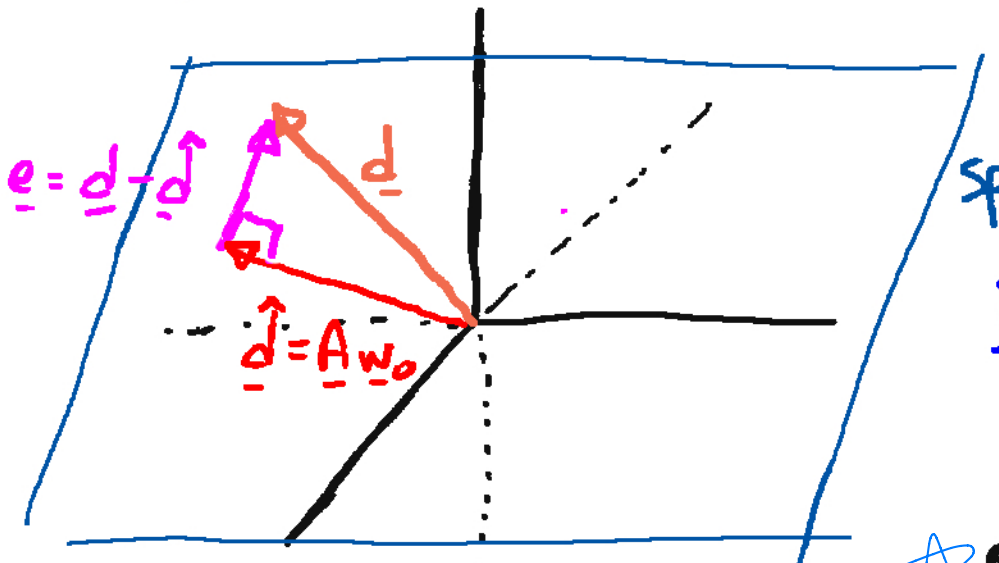
When $w = w_0$ → minimum and that is 0

$$\therefore \min f(w) = d^T d - \underbrace{b^T A (A^T A)^{-1} A^T d}_{\hat{d}}$$

$$= d^T d - d^T \hat{d}$$

$\left(w_0 = (A^T A)^{-1} A^T d \quad \text{is the best solution} \right)$

Projection and the Pythagorean Theorem



Right triangle

$$\|\underline{d}\|_2^2 = \|\underline{e}\|_2^2 + \|\hat{\underline{d}}\|_2^2$$

$$\Rightarrow \|\underline{e}\|_2^2 = \|\underline{d}\|_2^2 - \|\hat{\underline{d}}\|_2^2$$

$$= \underline{d}^T\underline{d} - \underline{d}^T\underline{P}_A\underline{d}$$

$$= \underline{d}^T(\underline{I} - \underline{P}_A)\underline{d}$$

$$\hat{\underline{d}} = \underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{d} = \underline{P}_A\underline{d}$$

(w_0)

$$\underline{P}_A = \underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T$$ "projection matrix"

$\underline{P}_A$ projects $\underline{d}$ onto span$\{\underline{A}\}$

$$\underline{P}_A^2 = \underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T\underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T = \underline{A}(\underline{A}^T\underline{A})^{-1}\underline{A}^T$$

$$= \underline{P}_A$$ (No matter what power, always P_A for projection)

$$\underline{e} = \underline{d} - \hat{\underline{d}} = (\underline{I} - \underline{P}_A)\underline{d} = \underline{P}_{A\perp}\underline{d}$$

$\underline{P}_{A\perp} = \underline{I} - \underline{P}_A$ projects onto space $\perp$ to span$\{\underline{A}\}$

$$\underline{P}_{A\perp}^2 = (\underline{I} - \underline{P}_A)(\underline{I} - \underline{P}_A) = \underline{I} - 2\underline{P}_A + \underline{P}_A^2$$

$$= \underline{I} - \underline{P}_A = \underline{P}_{A\perp}$$

($d^T d P_A^2 = d^T d P_A$)

P_A perpendicular: same as above, no matter how many power raised to it. It'll always be $P_{A\perp}$

(This is also a projection matrix)