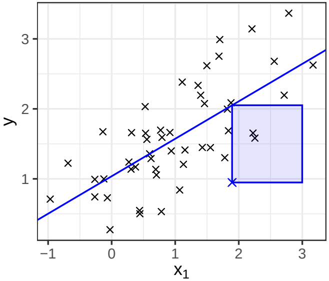
Introduction to Machine Learning

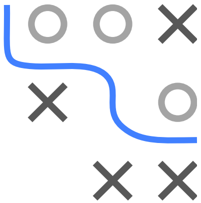
Supervised Regression
Deep Dive: Proof OLS Regression



Learning goals

- Understand analytical derivation of OLS estimator for LM

ANALYTICAL OPTIMIZATION



- Special property of LM with *L*2 loss: **analytical solution** available

$$\hat{\boldsymbol{\theta}} \in \arg\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2$$
$$= \arg\min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2$$

- Find via **normal equations**

$$\frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 0$$

- Solution: **ordinary-least-squares (OLS)** estimator

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

ANALYTICAL OPTIMIZATION – PROOF

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \Big(\underbrace{y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}}_{=:\epsilon_i} \Big)^2 = \| \underbrace{\mathbf{y} - \mathbf{X}\boldsymbol{\theta}}_{=:\boldsymbol{\epsilon}} \|_2^2; \quad \boldsymbol{\theta} \in \mathbb{R}^{\tilde{p}} \text{ with } \tilde{p} := p + 1$$

$$\begin{aligned}
0 &= \frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \quad \text{(sum notation)} \\
0 &= \frac{\partial}{\partial \boldsymbol{\theta}} \sum_{i=1}^{n} \epsilon_i^2 \quad \Big| \text{ sum \& chain rule} \\
0 &= \sum_{i=1}^{n} \frac{\partial \epsilon_i^2}{\partial \epsilon_i} \frac{\partial \epsilon_i}{\partial \boldsymbol{\theta}} \\
0 &= \sum_{i=1}^{n} 2\epsilon_i (-1) (\mathbf{x}^{(i)})^\top \\
0 &= \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}) (\mathbf{x}^{(i)})^\top \\
\boldsymbol{\theta}^\top \sum_{i=1}^{n} \mathbf{x}^{(i)} (\mathbf{x}^{(i)})^\top &= \sum_{i=1}^{n} y^{(i)} (\mathbf{x}^{(i)})^\top \quad \Big| \text{ transpose} \\
\left(\sum_{i=1}^{n} \underbrace{\mathbf{x}^{(i)} (\mathbf{x}^{(i)})^\top}_{\tilde{p} \times \tilde{p}} \right) \boldsymbol{\theta} &= \sum_{i=1}^{n} \mathbf{x}^{(i)} y^{(i)} \\
(\mathbf{X}^\top \mathbf{X}) \boldsymbol{\theta} &= \mathbf{X}^\top \mathbf{y}
\end{aligned}$$

NB: $\sum_{i=1}^{n} \mathbf{x}^{(i)} (\mathbf{x}^{(i)})^\top = \mathbf{X}^\top \mathbf{X}$ is easy to show (try it!) – and good to remember (this is basically the estimation of Cov(X))

$$\begin{aligned}
0 &= \frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \quad \text{(matrix notation)} \\
0 &= \frac{\partial \|\boldsymbol{\epsilon}\|_2^2}{\partial \boldsymbol{\theta}} \\
0 &= \frac{\partial \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}}{\partial \boldsymbol{\theta}} \quad \Big| \text{ chain rule} \\
0 &= \frac{\partial \boldsymbol{\epsilon}^\top \boldsymbol{\epsilon}}{\partial \boldsymbol{\epsilon}} \cdot \frac{\partial \boldsymbol{\epsilon}}{\partial \boldsymbol{\theta}} \\
0 &= 2\boldsymbol{\epsilon}^\top \cdot (-1 \cdot \mathbf{X}) \\
0 &= (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top \mathbf{X} \\
0 &= \mathbf{y}^\top \mathbf{X} - \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X} \\
\boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X} &= \mathbf{y}^\top \mathbf{X} \quad \Big| \text{ transpose} \\
\mathbf{X}^\top \mathbf{X} \boldsymbol{\theta} &= \mathbf{X}^\top \mathbf{y} \\
\boldsymbol{\theta} &= \underbrace{\underbrace{(\mathbf{X}^\top \mathbf{X})^{-1}}_{\tilde{p} \times \tilde{p}} \underbrace{\mathbf{X}^\top}_{\tilde{p} \times n} \underbrace{\mathbf{y}}_{n \times 1}}_{\tilde{p} \times 1}
\end{aligned}$$