Statistical Learning II

Lecture 8 - Bias-Variance decomposition (Continued)

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Risk of OLS

Therefore, we have the following final result for the excess risk of OLS

$$\mathbb{E}_{\boldsymbol{\varepsilon}}\left[\mathscr{R}(\hat{\boldsymbol{\theta}}_{OLS})\right] - \sigma^2 = \sigma^2 \frac{d}{n}$$

Remarks:

- Excess risk is proportional to the noise level $\mathbb{E}[\varepsilon^2] = \sigma^2$.
- Excess risk is proportional to the data dimension.
- To achieve excess risk $\Delta\mathscr{R} < \delta$, need:

$$n > \frac{\sigma^2 d}{\delta}$$

samples.

Bias-variance decomposition

Generally, if we have a data generative model for the training data $\mathscr{D} = \{(\boldsymbol{x}_i, y_i) \in \mathbb{R}^{d+1} : i = 1, \ldots, n\}$:

$$y_i = f_\star(\boldsymbol{x}) + \varepsilon_i = \text{signal} + \text{noise}$$

With $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{E}[\varepsilon^2] = \sigma^2$

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$$\mathbb{E}_{\boldsymbol{\varepsilon}}[\mathcal{R}(\hat{\boldsymbol{\theta}})] - \sigma^2 = \mathbb{E}\left[(f_\star(\boldsymbol{x}) - f_{\hat{\theta}}(\boldsymbol{x}))^2\right]$$

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&= \mathbb{E}\left[(f_\star(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{\varepsilon}}[f_{\hat{\theta}}(x)])^2\right] + \mathbb{E}\left[(\mathbb{E}_{\boldsymbol{\varepsilon}}[f_{\hat{\theta}}(\boldsymbol{x})] - f_{\hat{\theta}}(\boldsymbol{x}))^2\right]
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\end{aligned}$$

$$= \text{bias}^2 + \text{variance}$$

Bias-variance decomposition

$$\mathbb{E}_{\boldsymbol{\varepsilon}}[\mathscr{R}(\hat{\boldsymbol{\theta}})] - \sigma^2 = \mathscr{B} + \mathscr{V}$$

$$\mathscr{B} = \mathbb{E}\left[(f_\star(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{\varepsilon}}[f_{\hat{\theta}}(\boldsymbol{x})])^2\right]$$

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Recall the the approximation + estimation decomposition from lecture 3:

$$\mathscr{R}(\theta) - \mathscr{R}_\star = \left(\mathscr{R}(\theta) - \inf_{\theta' \in \Theta} \mathscr{R}(\theta')\right) + \left(\inf_{\theta' \in \Theta} \mathscr{R}(\theta') - \mathscr{R}_\star\right)$$

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For the OLS setting from before ($\mathrm{rank}(X) = d < n$):

$$\mathbb{E}[f_{\hat{\theta}}(\boldsymbol{x})] = \langle \boldsymbol{\theta}_\star, \boldsymbol{x} \rangle = f_\star(\boldsymbol{x}) \quad \Rightarrow \quad \mathscr{B} = 0 \qquad \mathscr{V} = \sigma^2 \frac{d}{n}$$

Marvels and pitfalls of OLS

To summarise, the OLS estimator $\hat{\boldsymbol{\theta}}_{\mathrm{OLS}}(\boldsymbol{X}, y) = \boldsymbol{X}^{+}\boldsymbol{y}$:

- Can only fit linear functions.
- For $n > d$, has low bias $\mathscr{B} = 0$
- When, $n \gg d$, has low variance $\mathscr{V} = \sigma^2 \dfrac{d}{n}$

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But what about $n \approx d$? Consider for instance $n = d$.

$\boldsymbol{X} \in \mathbb{R}^{d \times d}$ is invertible $\Rightarrow$ $\boldsymbol{y} = \boldsymbol{X}\hat{\boldsymbol{\theta}}_{\mathrm{OLS}}$ interpolates the training data.

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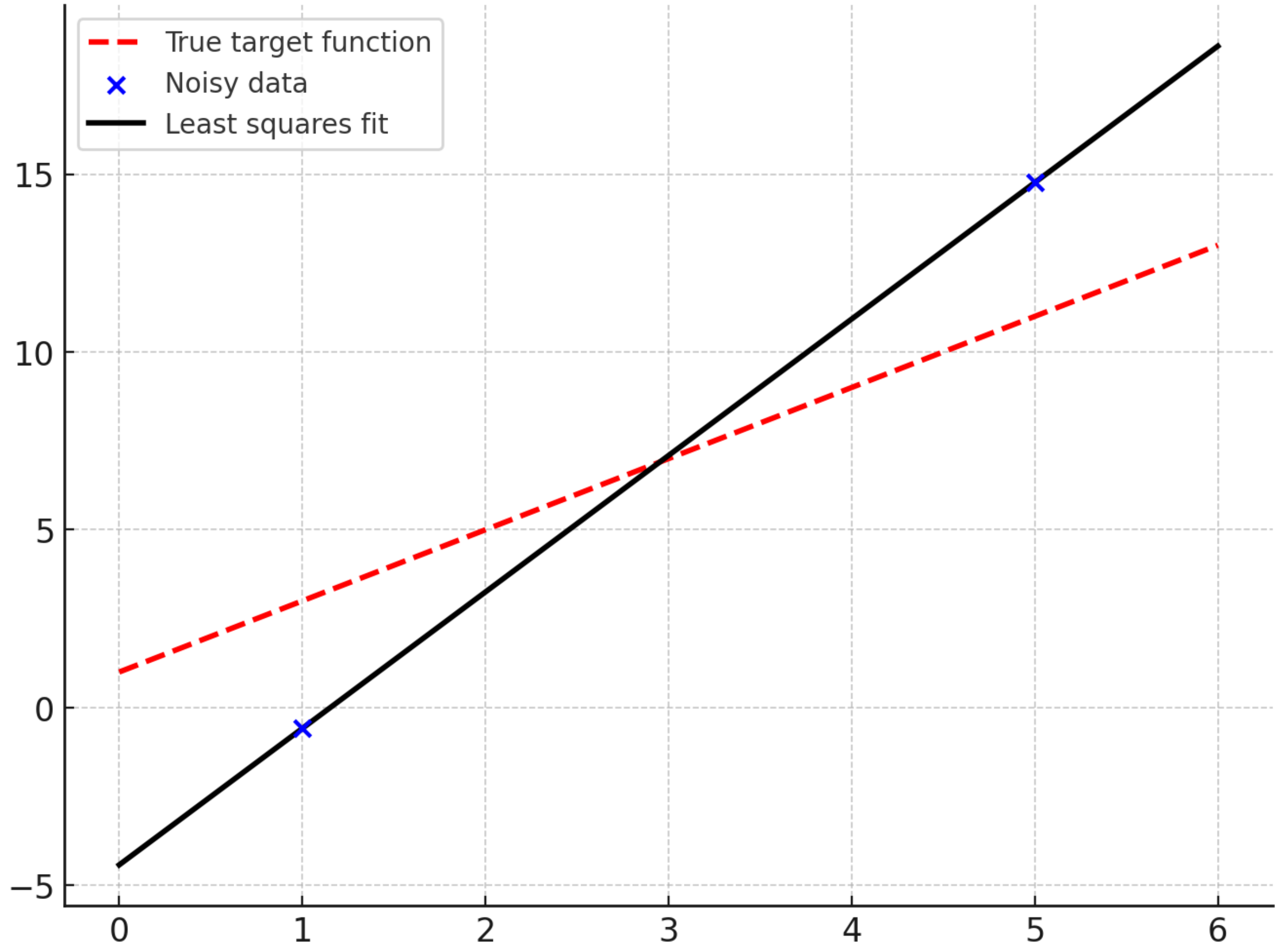

$$\mathbb{E}_{\boldsymbol{\varepsilon}}[\mathcal{R}(\hat{\boldsymbol{\theta}}_{\mathrm{OLS}})] = 2\sigma^2$$

$$\hat{\mathcal{R}}_n(\hat{\boldsymbol{\theta}}_{\mathrm{OLS}}) = 0$$

The test error above is valid for the fixed design.

Marvels and pitfalls of OLS

Recall that:

$$\hat{\boldsymbol{\theta}}_{OLS}(\boldsymbol{X}, \boldsymbol{y}) = \boldsymbol{\theta}_\star + \frac{1}{n}\hat{\boldsymbol{\Sigma}}_n^{-1}\boldsymbol{X}^\top \boldsymbol{\varepsilon}$$

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Marvels and pitfalls of OLS

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$$= \boldsymbol{\theta}_\star + \sum_{j=1}^{d} \frac{1}{\sigma_j}\langle \boldsymbol{u}_j, \boldsymbol{\varepsilon}\rangle \boldsymbol{v}_j$$

Hence:
- signal is stronger in directions with larger s.v.
- noise dominates directions with smaller s.v.

OLS has larger variance for data with small "effective dimension".

What to do?

Classical strategies to mitigate variance:

- Dimensionality reduction: PCA, random projections (sketching), etc.
- Variable subset selection: Stepwise selection, best Subset Selection, etc.
- Regularisation: ridge, LASSO, etc.

Ridge regression

Ridge regression

Note the averaged norm of the OLS is given by:

$$\mathbb{E}_{\boldsymbol{\varepsilon}}\left[||\hat{\boldsymbol{\theta}}_{OLS}||_2^2\right] = ||\boldsymbol{\theta}_\star||_2^2 + \sigma^2 \sum_{j=1}^{d} \frac{1}{\sigma_j^2}$$

Therefore, small s.v.s lead to larger expected norm.

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💡 <u>Key idea</u>: penalise the norm.

$$\min_{\boldsymbol{\theta}\in\mathbb{R}^d} \frac{1}{2n}||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}||_2^2 + \frac{\lambda}{2}||\boldsymbol{\theta}||_2^2$$

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Least squares empirical risk

Regularisation or “ridge” penalty

Ridge regression

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \frac{1}{2n} ||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}||_2^2 + \frac{\lambda}{2} ||\boldsymbol{\theta}||_2^2$$

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$$\min_{\boldsymbol{\theta}\in\mathbb{R}^d} \hat{\mathscr{R}}_n^{\lambda}(\boldsymbol{\theta}) := \frac{1}{2n}||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}||_2^2 + \frac{\lambda}{2}||\boldsymbol{\theta}||_2^2$$

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Remarks:

- The regularised empirical risk is a strongly convex function of $\boldsymbol{\theta} \in \mathbb{R}^d$

$$\nabla_{\boldsymbol{\theta}} \hat{\mathscr{R}}_n^{\lambda}(\boldsymbol{\theta}) = -\frac{1}{n}\boldsymbol{X}^\top\left(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\right) + \lambda\boldsymbol{\theta}$$

$$\nabla_{\boldsymbol{\theta}}^2 \hat{\mathscr{R}}_n^{\lambda}(\boldsymbol{\theta}) = \frac{1}{n}\boldsymbol{X}^\top\boldsymbol{X} + \lambda\boldsymbol{I}_d \succ 0$$

$$(= \hat{\boldsymbol{\Sigma}}_n + \lambda\boldsymbol{I}_n)$$

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In other words, minimiser always exist and is unique.

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$$\Updownarrow$$

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The unique solution is given by:

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For $\lambda \to 0^+$, $\hat{\boldsymbol{\theta}}_{\lambda} \to \hat{\boldsymbol{\theta}}_{\mathrm{OLS}}$

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Remarks:

- As before, consider s.v.d. of $\boldsymbol{X} = \sum_{j=1}^{\mathrm{rank}(\boldsymbol{X})} \sigma_j \boldsymbol{u}_j \boldsymbol{v}_j^\top$

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Ridge performs shrinkage: small s.v.s are suppressed!