Statistical Learning II

Lecture 4 - Least squares

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Summary of ERM

Let $\mathscr{D} = \{(x_i, y_i) \in \mathscr{X} \times \mathscr{Y} : i = 1,\ldots,n\}$ denote training data sampled i.i.d. from p.

Given a choice of:

- Parametric hypothesis class $\mathscr{H} = \{f_\theta : \mathscr{X} \to \mathscr{Y} : \theta \in \Theta\}$
- Loss function $\ell : \mathscr{X} \times \mathscr{Y} \to \mathbb{R}_+$

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Key questions

- What optimisation procedure to choose?

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- What properties of the data distribution p makes the problem easier / harder?

Least-squares regression

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Ordinary least-squares (OLS) regression is defined as:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^d} \hat{\mathscr{R}}_n(\boldsymbol{\theta}) := \frac{1}{2n} \sum_{i=1}^{n} \left(y_i - \langle \boldsymbol{\theta}, \boldsymbol{x}_i \rangle \right)^2$$

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Where we have defined the data matrix $\boldsymbol{X} \in \mathbb{R}^{n \times d}$ and label vector $\boldsymbol{y} \in \mathbb{R}^n$:

$$\boldsymbol{X} = \begin{bmatrix} - & \boldsymbol{x}_1 & - \\ - & \boldsymbol{x}_2 & - \\ & \vdots & \\ - & \boldsymbol{x}_n & - \end{bmatrix} \in \mathbb{R}^{n \times d} \qquad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Bayes risk for OLS

Remarks:

- This corresponds to an ERM problem on the class of linear functions:

$$\mathscr{H} = \{f_\theta(\boldsymbol{x}) = \langle \boldsymbol{\theta}, \boldsymbol{x} \rangle : \boldsymbol{\theta} \in \mathbb{R}^d\}$$

with the square loss functions:

$$\ell(y, f_\theta(\boldsymbol{x})) = \frac{1}{2}\left(y - f_\theta(\boldsymbol{x})\right)^2$$

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- The Bayes predictor and risk are given by:

$$f_\star(\boldsymbol{x}) = \mathbb{E}[y \,|\, \boldsymbol{x}] \qquad \mathscr{R}_\star = \mathbb{E}\left[\frac{1}{2}(y - \mathbb{E}[y \,|\, \boldsymbol{x}])^2\right]$$

Exercise: show this.

Intercept

Remarks:

- Without loss of generality, can add an intercept:

$$f_\theta(\boldsymbol{x}) = \langle \boldsymbol{\theta}, \boldsymbol{x} \rangle + b$$

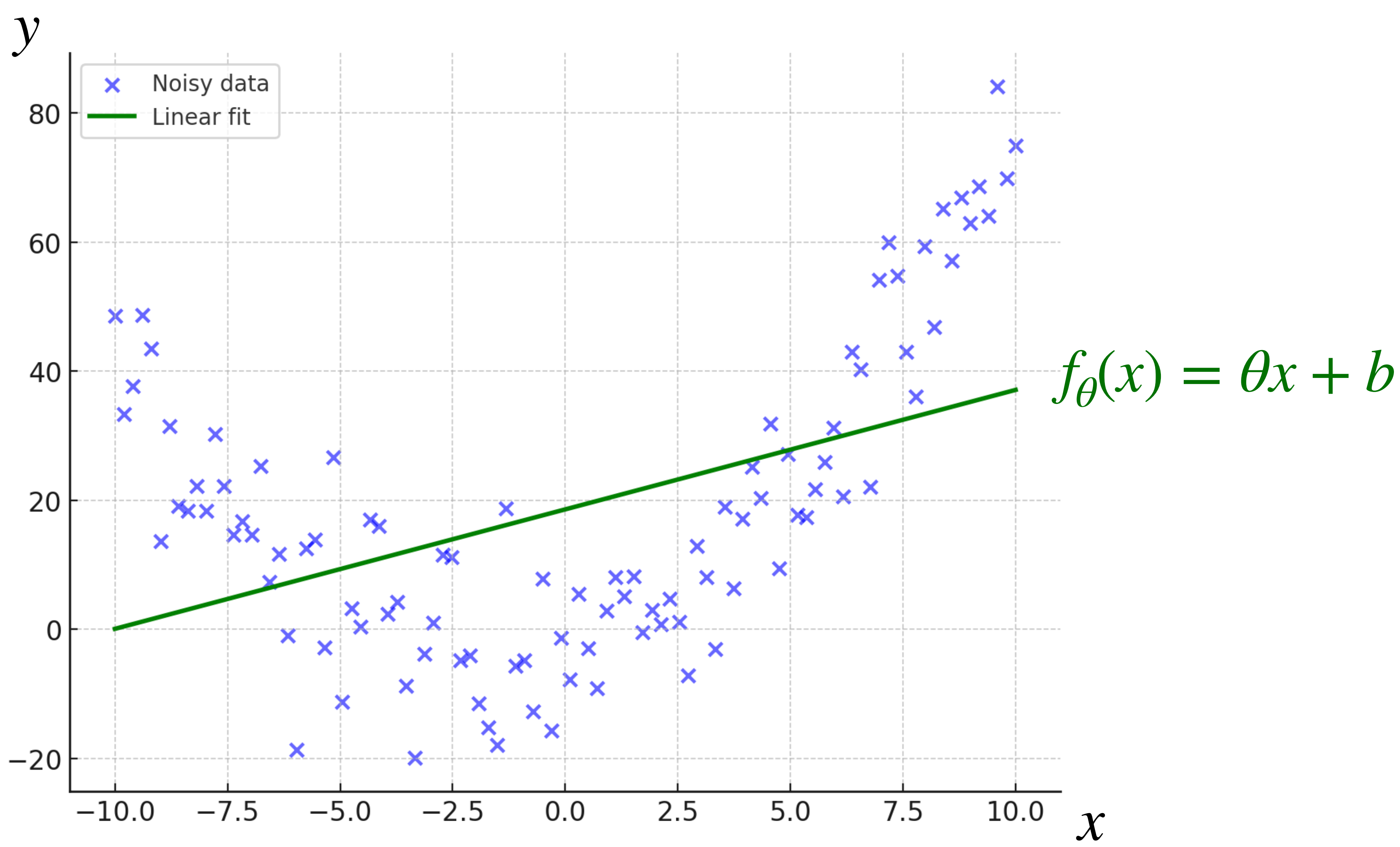
By redefining:

$$\tilde{\boldsymbol{X}} = \begin{bmatrix} - & \boldsymbol{x}_1 & - & 1 \\ - & \boldsymbol{x}_2 & - & 1 \\ & \vdots & & \\ - & \boldsymbol{x}_n & - & 1 \end{bmatrix} \in \mathbb{R}^{n \times (d+1)}$$

Inductive bias of OLS

Remarks:

- Inductive bias: can only fit affine functions of $\boldsymbol{x} \in \mathbb{R}^d$



Convexity of OLS

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For $n \geq d$, $\hat{\mathscr{R}}_n$ is strictly convex if and only if $\operatorname{rank}(\boldsymbol{X}^\top \boldsymbol{X}) = d$. This implies that $\hat{\mathscr{R}}_n$ can have at most one global minimum.

Closed-form solution

- Gradient: $$\nabla_{\boldsymbol{\theta}} \hat{\mathscr{R}}_n = -\frac{1}{n} \boldsymbol{X}^\top (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) \in \mathbb{R}^d$$

If it exists, a minima must satisfy:

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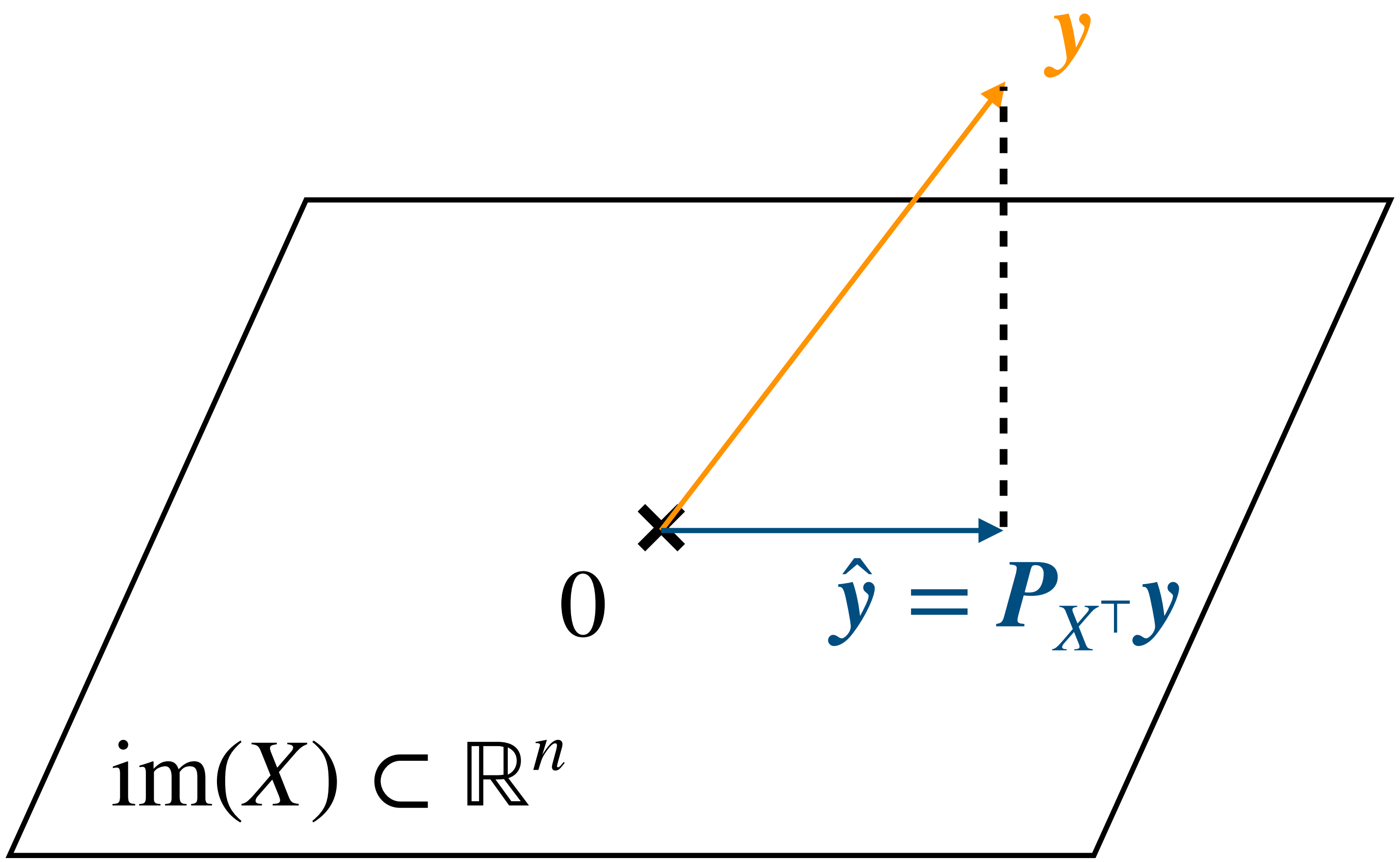
If $\mathrm{rank}(X) = \min(n, d)$: $$\hat{\boldsymbol{\theta}}_{OLS} = \begin{cases} (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y} & \text{if } n \geq d \\ \boldsymbol{X}^\top (\boldsymbol{X}\boldsymbol{X}^\top)^{-1} \boldsymbol{y} & \text{if } n < d \end{cases}$$

Geometrical interpretation

This gives a natural interpretation of the OLS predictor as an orthogonal projection of the labels in the row space of $\boldsymbol{X}$:

$$\hat{\boldsymbol{\theta}}_{OLS} = \boldsymbol{X}^{+}\boldsymbol{y} \quad \Rightarrow \quad \hat{\boldsymbol{y}}_{OLS} = \boldsymbol{X}\hat{\boldsymbol{\theta}}_{OLS} = \boldsymbol{X}\boldsymbol{X}^{+}\boldsymbol{y}$$

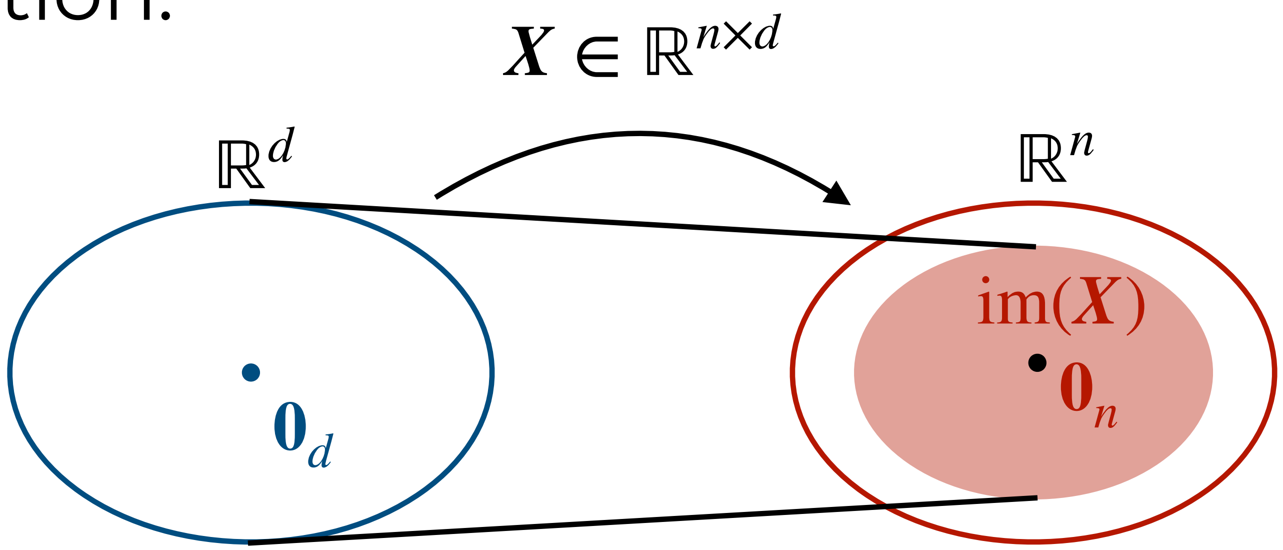


$$\min_{z \in \mathrm{im}(X)} ||\boldsymbol{y} - \boldsymbol{z}||_2^2$$

Two scenarios

From now on, let's assume $\boldsymbol{X}$ is full-rank.

- For $n \geq d$: more equations than variables. $\boldsymbol{X}\boldsymbol{\theta} = \boldsymbol{y}$ admits an unique solution.



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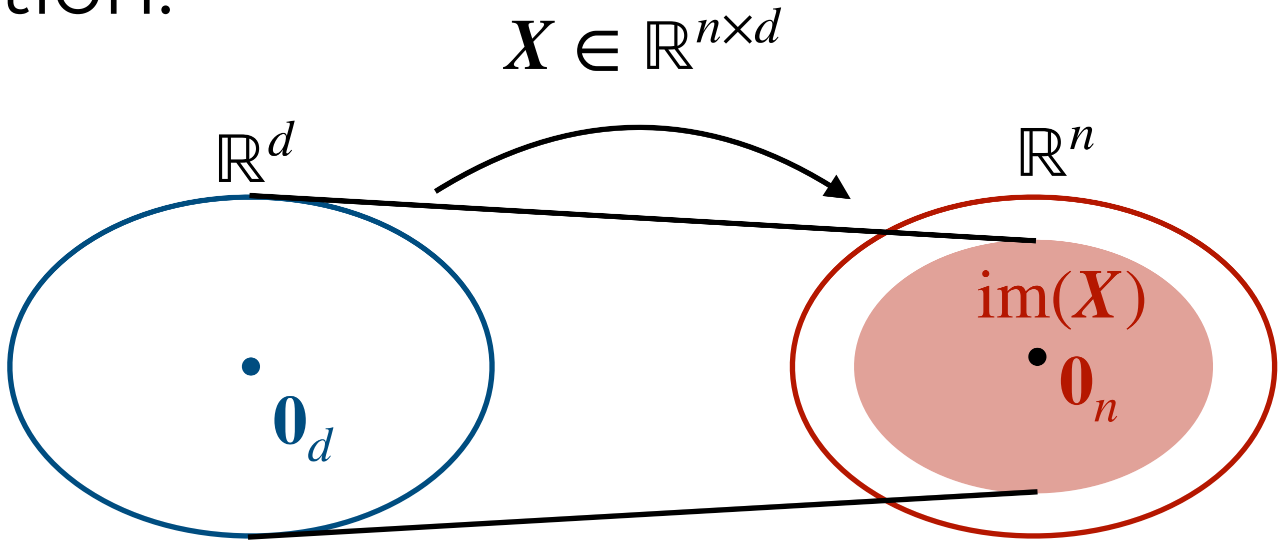
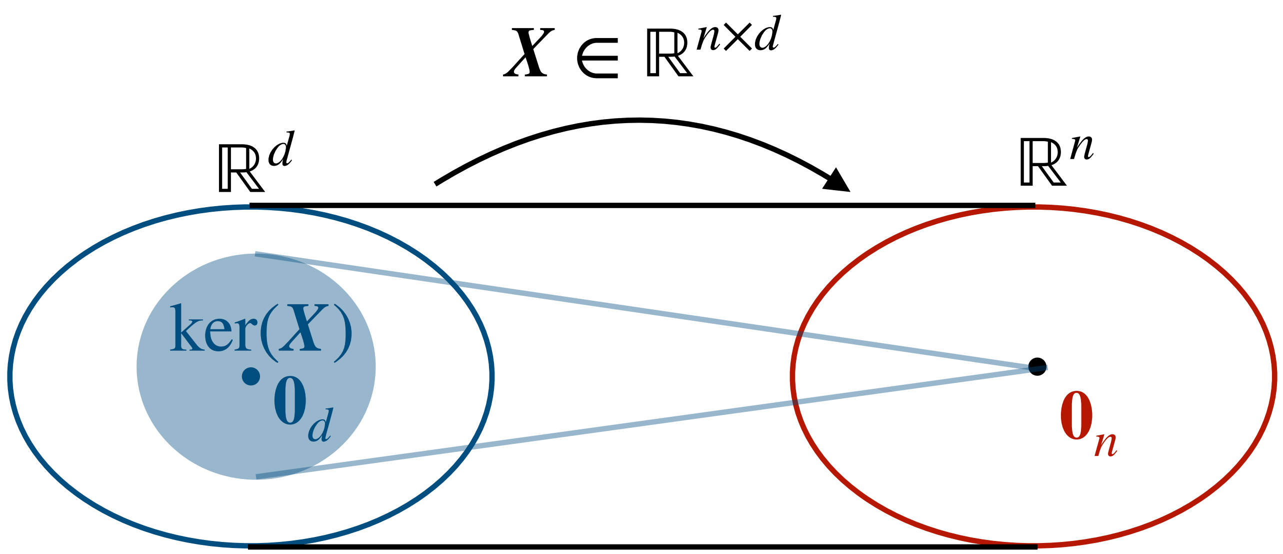


- For $n < d$: more variables than equations. $\boldsymbol{X\theta} = \boldsymbol{y}$ admits several solutions.



OLS as least norm solution

Assume $\mathrm{rank}(\boldsymbol{X}) = n < d$. Then, OLS admits the following interpretation as the minimum ℓ_2-norm solution:

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