Overfitting & Generalisation

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Announcements

- Formula sheet will be given to you during exam, and will be available beforehand. See `exercises.pdf`.
- New exercises: Keep up-to-date, and discuss with TAs. Not enough of you are taking advantage.
- New coursework next Tuesday.

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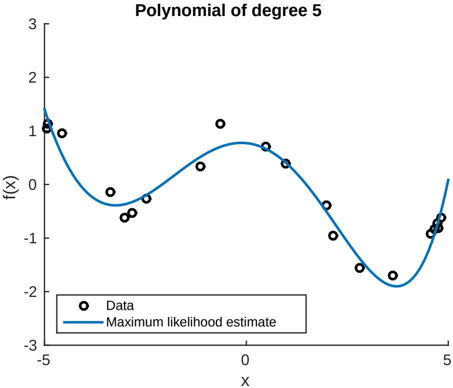
- You may already know the techniques we discuss today.
- But today, we let the mathematics **prove** why they work.

Curve fitting



- What we want: Find a curve that predicts well **even for unseen inputs**
- What we do: Minimise loss on **training points**:

$$L(\boldsymbol{\theta}) = \sum_n (f(\mathbf{x}_n; \boldsymbol{\theta}) - y_n)^2 \tag{1}$$

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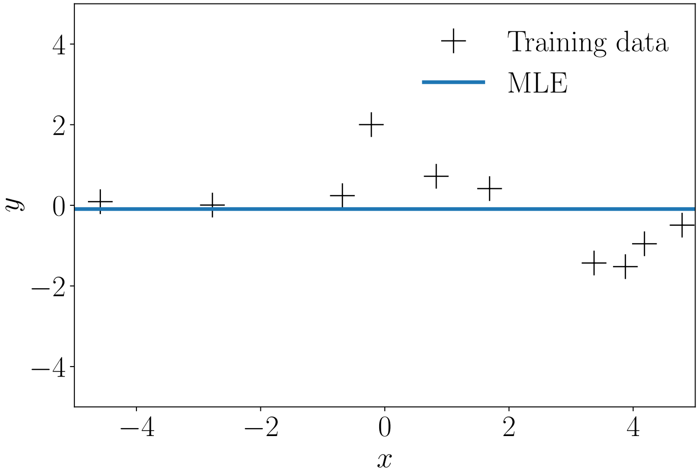
Two questions: As q increases,

- what will happen to the **training loss**?
- how good do you think the predictions will be?

Basis functions



$$\boldsymbol{\phi}(x) = [1]^{\mathsf{T}} \tag{3}$$

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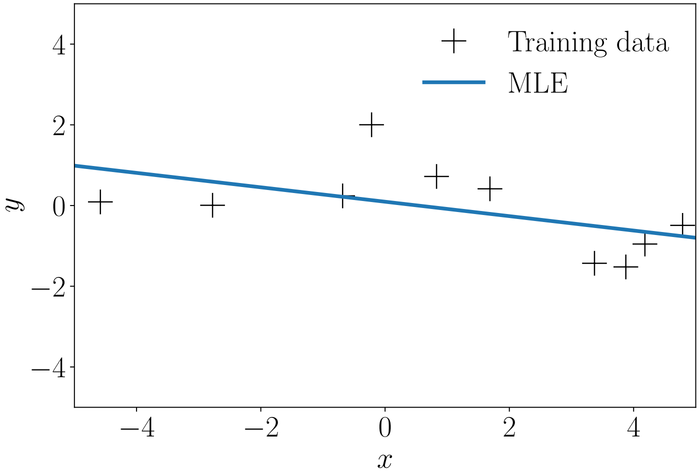

$$\boldsymbol{\phi}(x) = [1 \;\; x]^\top \tag{3}$$

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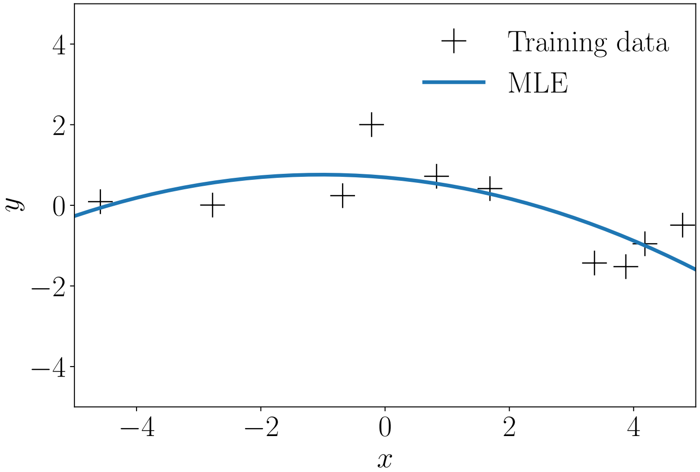

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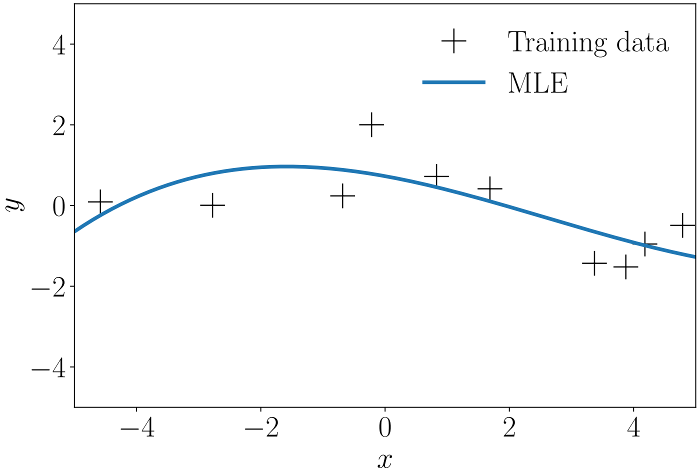

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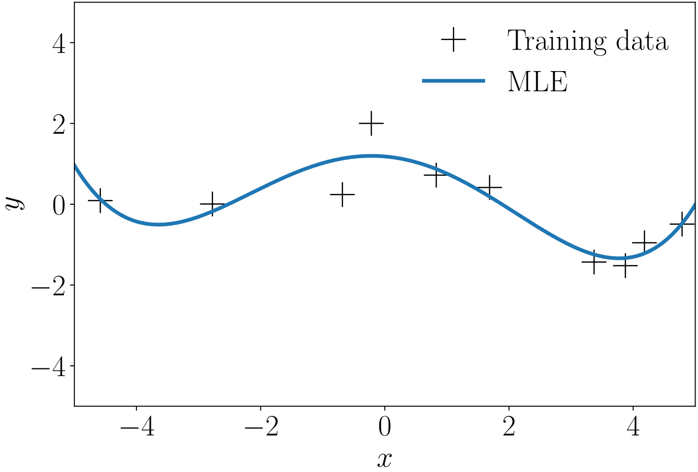

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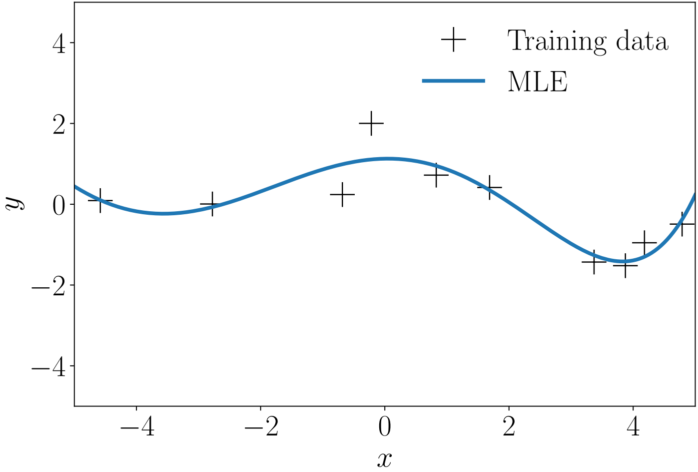

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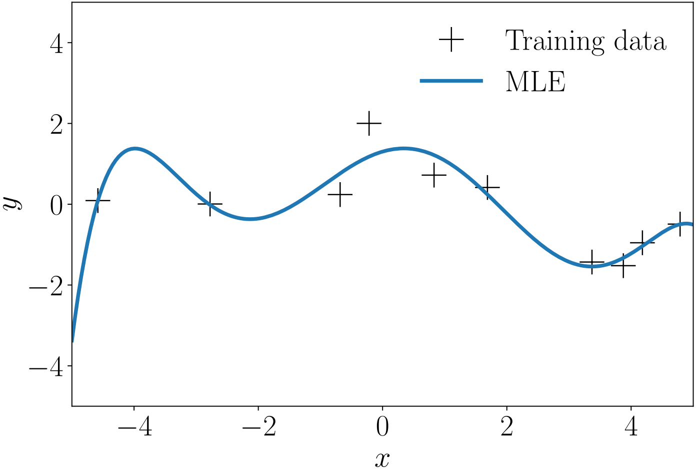

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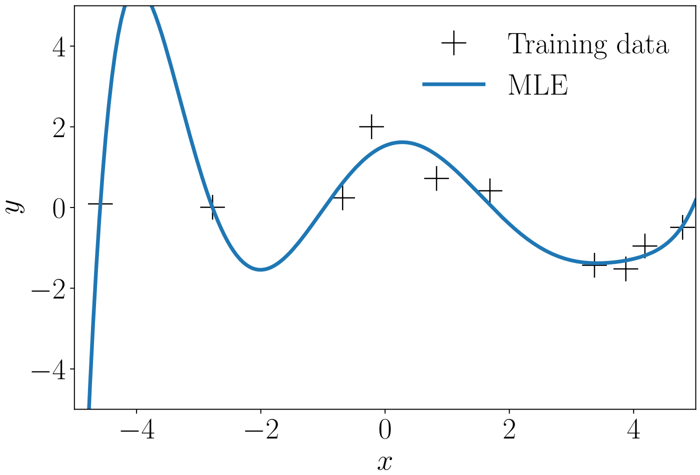

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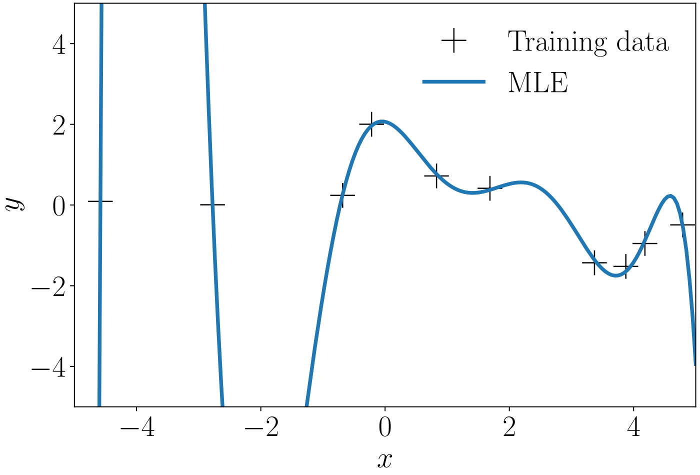

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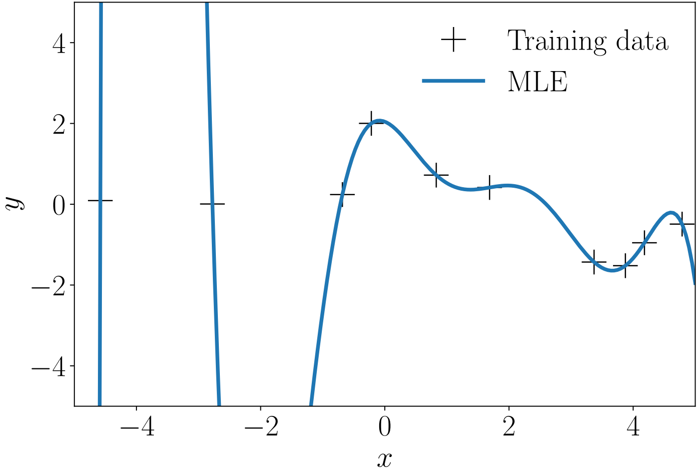

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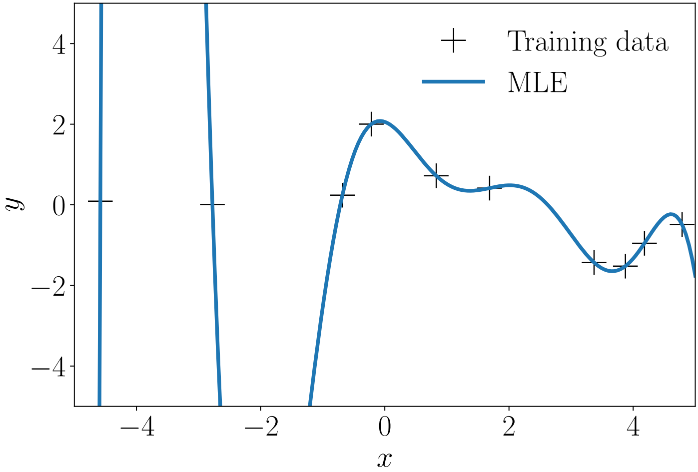

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Training loss

Q: How does the training loss change as M increases?

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But what about the predictions?

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- Only train on training set, and **measure** loss on the test set:

$$\boldsymbol{\theta}^* = \operatorname*{argmin}_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) \tag{6}$$

$$L_{\text{test}} = \frac{1}{N_{\text{test}}} \sum_{n=1}^{N_{\text{test}}} \ell(f(x_n; \boldsymbol{\theta}^*), y_n)\,, \qquad (x_n, y_n) \in \mathcal{S}_{\text{test}} \tag{7}$$

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Why does this work?

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Let's make the question precise by:

- Specifying one way for how we will use our predictions.
- Using the assumptions from lecture 1.

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- Does it even make sense? Is this quantity even well-defined?

Statistical View on the World

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We assume that the data we observe is the outcome of some random process. Each observation is one random variable. In this course, probabilities of the data generating process are denoted with $\mathbb{P}(\cdot)$, and which has distribution $\pi(\cdot)$.

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Example:

- We observe a dataset of 3 values $\{x_n\}_{n=1}^{3}$.
- This has density $\pi_{X_1,X_2,X_3}(x_1, x_2, x_3)$.

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Examples:

$$\pi_{X_1,X_2,X_3}(x_1,x_2,x_3) = \prod_{n=1}^{3} \pi(x_n)$$

$$\pi_{X_1,Y_1,X_2,Y_2,\ldots}(x_1,y_1,x_2,y_2,\ldots) = \pi_{X,Y}(\mathbf{x},\mathbf{y}) \qquad \mathbf{x},\mathbf{y} \in \mathbb{R}^N$$

$$= \prod_{n=1}^{N} \pi(x_n, y_n)$$

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- Let's use a **theorem** to prove this.

Weak Law of Large Numbers

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- for which will hold:

$$\lim_{N\to\infty} \mathbb{P}\left(|\overline{X}_n - \mu| < \epsilon\right) = 1 \tag{11}$$

Expected Loss

Deploy loss converging to expected loss:

- $x_n, y_n \stackrel{\text{iid}}{\sim} \pi_{X,Y} \implies \ell_n = \ell(f(x_n), y_n))$ is a RV, with density $\pi(\ell_n)$

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- With $\mu = \mathbb{E}_{\pi(\ell)}[\ell] = \mathbb{E}_{\pi(x,y)}[\ell(f(x, \boldsymbol{\theta}^*), y)]$ by LOTUS

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- Previous process in reverse $\implies$ **Monte Carlo** estimation

Monte Carlo Estimation

Want to find a difficult expectation / integral:

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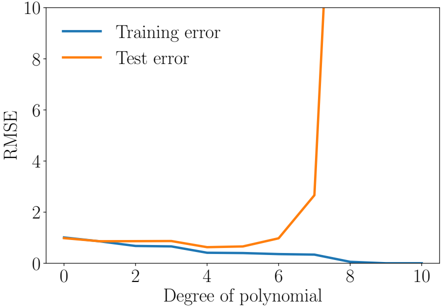
By considering it as a sum of independent RVs:

- Can show it to be **unbiased**, i.e. $\mathbb{E}_{p(x_1, x_2, \dots)}\left[\hat{I}\right] = I$ (board).
- Can show the variance reduces as c/N (board).
- Weak LLN implies $\lim_{N\to\infty} P(|\hat{I} - I| < \epsilon) = 1$ (relies on unbiasedness!)

Overfitting

Can use test loss estimator to **evaluate** various models:



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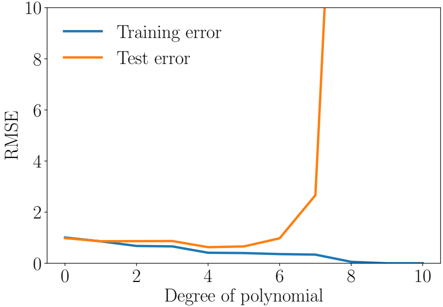

- We indeed see that training error continuously decreases.
- Test error only decreases with train error up to a point!
- When test error starts increasing $\implies$ overfitting.

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Summary

- Overfitting
- Assumptions behind test sets (many predictions + iid data generation)
- Law of Large Numbers (skill)
- Monte Carlo estimation (skill)