# Generalization, Model Selection, and Validation

Machine Learning Course - CS-433
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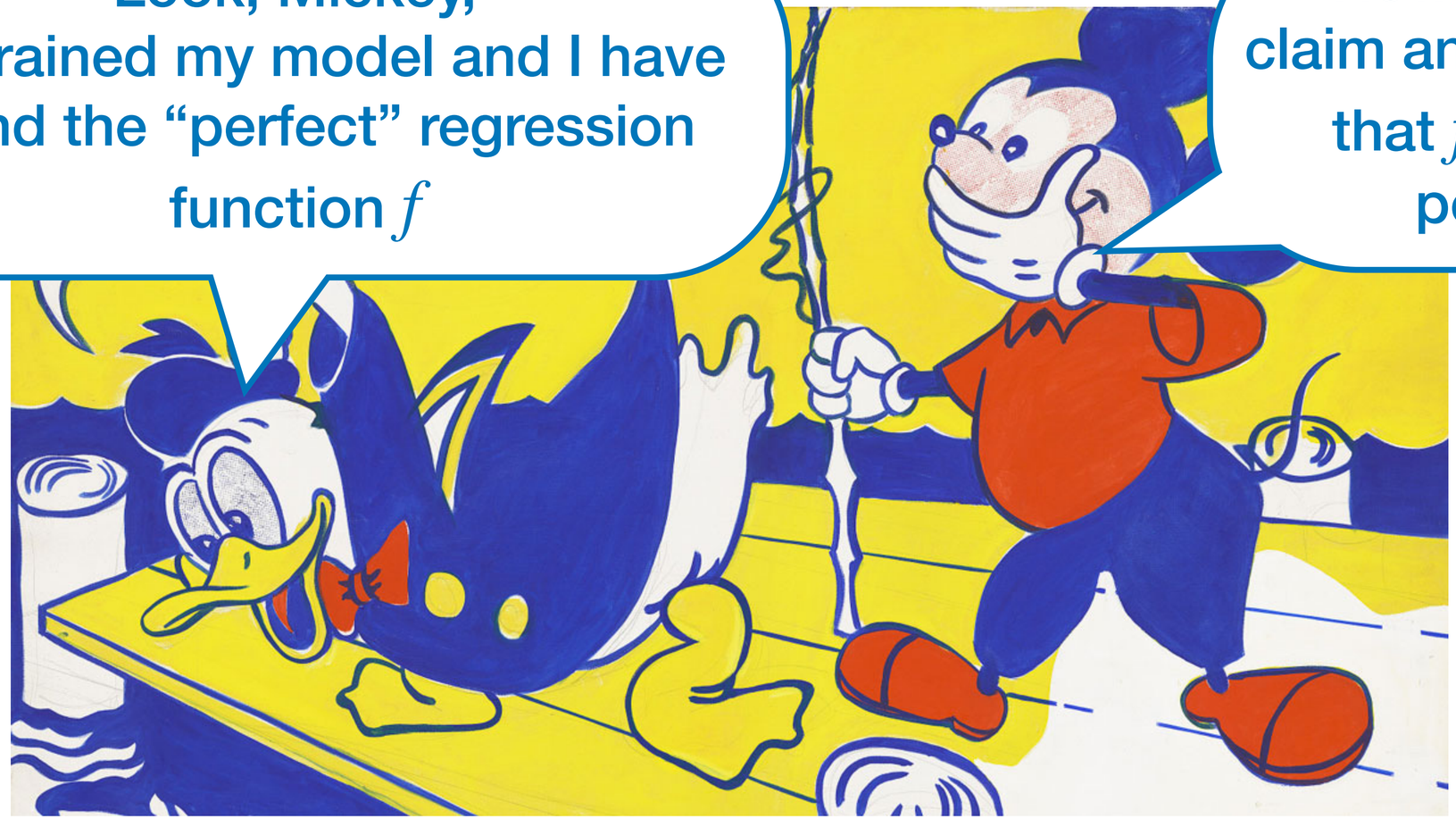
# Generalization, validation?

Look, Mickey,
I've trained my model and I have found the "perfect" regression function $f$

How can I verify this claim and have confidence that $f$ will have good performance?



# What is the model selection problem?

- Ridge regression: $w_\lambda = \arg\min_w \frac{1}{2N}\sum_{n=1}^{N}(y_n - x_n^\top w)^2 + \lambda\|w\|_2^2$

  Hyperparameter

  - $\lambda$ can be tuned to control the model complexity (to reduce overfitting)
  - In practice: $(\lambda_1, \cdots, \lambda_k) \longrightarrow$ Algorithm $\longrightarrow (w_1, \cdots, w_k)$
  - Which $\lambda$ should we use?

- Polynomial feature expansion: $(x_{(1)}, x_{(2)}) \xrightarrow{\phi} (x_{(1)}, x_{(2)}, x_{(1)}^2 + x_{(2)}^2)$

  $(x_{(1)}, x_{(2)}, 5x_{(1)}^2 + 2x_{(2)}^2, x_{(2)}^3 + 2x_{(1)})$

  - Enrich the model complexity, by augmenting the feature vector $x$.
  - Here the degree d is the hyperparameter

We are facing the same problem: **how do we choose these hyperparameters?**

# Model selection for neural networks

**Algorithms?**

SGD
Adam
Which step-size?
Which batch-size?
Which momentum?

**Architectures?**

FullyConnected
ConvNet
ResNet
Transformer
Which width?
Which depth?
Batch normalization?

**Regularizations?**

Weight decay?
Early stopping?
Data augmentations?

# Probabilistic Setup

Data Model:

Unknown distribution $\mathscr{D}$ with range $\mathscr{X} \times \mathscr{Y}$
We see a dataset $S$ of independent samples from $\mathscr{D}$:

$$S = \{(x_n, y_n)\}_{n=1}^{N} \sim \mathscr{D} \quad \text{i.i.d.}$$

Learning Algorithm:

$$\mathscr{A}(S) = f_S$$

Input Output

Ridge regression: gradient descent or least-squares estimator

Can add a subscript $f_{S,\lambda}$ to indicate the hyper parameter dependency

# Generalization Error: how accurate is $f$ at predicting?

We compute the ***expected error*** over all samples drawn from distribution $\mathscr{D}$:

$$L_{\mathscr{D}}(f) = \mathbb{E}_{(x,y)\sim\mathscr{D}}[\ell(y, f(x))]$$

where $\ell(\,\cdot\,,\cdot\,)$ is the loss function

- Ex: $\ell(y, y') = \frac{1}{2}(y - y')^2$, logistic loss, hinge loss

The quantity $L_{\mathscr{D}}(f)$ has many names: **True / Expected / Generalization** **Risk / Error / Loss**

This is the quantity we are fundamentally interested in

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Problem: $\mathscr{D}$ is unknown

# Empirical Error: what we can compute

We can approximate the true error by **averaging the loss function over the dataset**

$$L_S(f) = \frac{1}{|S|} \sum_{(x_n,y_n)\in S} \ell(y_n, f(x_n)) \,.$$

Also called: **empirical risk/error/loss**

⚠ The samples are random thus $L_S(f)$ is a random variable

It is an unbiased estimator of the true error

Law of large number: $L_S(f) \underset{|S|\to\infty}{\to} L_{\mathcal{D}}(f)$ but fluctuations!

**Generalization gap**: $|L_{\mathcal{D}}(f) - L_S(f)|$

# Training error: what we are minimizing

⚠ the prediction function $f_S$ is itself a function of the data S

When the model has been trained on the same data it is applied to, the empirical error is called the ***training error:***

$$L_S(f_S) = \frac{1}{|S|} \sum_{(x_n, y_n) \in S} \ell(y_n, f_S(x_n))$$

This is the objective function you are minimizing to find the predictor

It might not be representative of the error we see on “fresh” samples

The reason that $L_S(f_S)$ might not be close to $L_{\mathcal{D}}(f_S)$ is of course overfitting

# Splitting the data

*Problem:* Validating model on the same data we trained it on
Fix: **Split the data** into an independent *training and test set:*

$$S = S_{\text{train}} \cup S_{\text{test}}$$

1. We **learn** the function $f_{S_{\text{train}}}$ using the **train set**
2. We **validate** it computing the error on the **test set**

$$L_{S_{\text{test}}}(f_{S_{\text{train}}}) = \frac{1}{|S_{\text{test}}|} \sum_{(y_n, x_n) \in S_{\text{test}}} \ell(y_n, f_{S_{\text{train}}}(x_n))$$

➡ Since $S_{\text{test}}$ and $S_{\text{train}}$ are independent: $L_{S_{\text{test}}}(f_{S_{\text{train}}}) \approx L_{\mathcal{D}}(f_{S_{\text{train}}})$

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⚠ We have less data both for the learning and the validation tasks (tradeoff)

# Generalization gap:
# How far is the test from the true error?

Claim: given a model $f$ and a test set $S_{\text{test}} \sim \mathscr{D}$ i.i.d. (not used to learn $f$) and a loss $\ell(\cdot, \cdot) \in [a, b]$:

$$\mathbb{P}\left[ \left| \underbrace{L_{\mathscr{D}}(f) - L_{S_{\text{test}}}(f)}_{\text{Generalization Gap}} \right| \geq \sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2\,|S_{\text{test}}|}} \right] \leq \delta$$

The error decreases as $\mathcal{O}(1/\sqrt{|S_{\text{test}}|})$ with the number of test points

High probability bound: $\delta$ is only in the $\ln$

➡The more data points we have, the more confident we are that the empirical loss we measure is close to the true loss

# Why do you care?

- Given a predictor $f$ and a dataset $S$ you can control the expected risk:

$$\mathbb{P}\Bigg( \underbrace{L_{\mathscr{D}}(f)}_{\text{not computable}} \geq \underbrace{L_S(f)}_{\text{Computable}} + \underbrace{\sqrt{\frac{(a-b)^2 \ln(2/\delta)}{2\,|S_{test}|}}}_{\text{deviation}} \Bigg) \leq \delta$$

- Given a dataset $S$
  1. Split: $S = S_{\text{train}} \cup S_{\text{test}}$
  2. Train: $\mathscr{A}(S_{\text{train}}) = f_{S_{\text{train}}}$
  3. Validate:

$$\mathbb{P}\left( L_{\mathscr{D}}(f_{S_{\text{train}}}) \geq L_{S_{\text{test}}}(f_{S_{\text{train}}}) + \sqrt{\frac{(a-b)^2 \ln(2/\delta)}{2\,|S_{test}|}} \right) \leq \delta$$

➡We can obtain a probabilistic upper bound on the expected risk

# The proof relies only on concentration inequalities

Since $(x_n, y_n) \in S_{\text{test}}$ are chosen independently, the associated losses $\Theta_n = \ell(y_n, f(x_n)) \in [a, b]$ given a fixed model $f$, are also i.i.d. random variables

Empirical loss: $\frac{1}{N}\sum_{n=1}^{N} \Theta_n = \frac{1}{N}\sum_{n=1}^{N} \ell(y_n, f(x_n)) = L_{S_{\text{test}}}(f)$

True loss: $\mathbb{E}[\Theta_n] = \mathbb{E}[\ell(y_n, f(x_n))] = L_{\mathcal{D}}(f)$

What is the chance that the empirical loss $L_{S_{\text{test}}}(f)$ deviates from the true loss by more than a given constant?

➡ classically addressed using **concentration inequalities**

# Hoeffding inequality: a simple concentration bound

Claim: Let $\Theta_1, \ldots, \Theta_N$ be a sequence of i.i.d. random variables with mean $\mathbb{E}[\Theta]$ and range $[a, b]$

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^{N}\Theta_n - \mathbb{E}[\Theta]\right| \geq \varepsilon\right] \leq 2e^{-2N\varepsilon^2/(b-a)^2} \text{ for any } \varepsilon \geq 0$$

Concentration bound: the empirical mean is concentrated around its mean

A. Use it with $\Theta_n = \ell(y_n, f(x_n))$

B. Equating $\delta = 2e^{-2|S_{\text{test}}|\varepsilon^2/(b-a)^2}$ we get $\varepsilon = \sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2|S_{\text{test}}|}}$ □

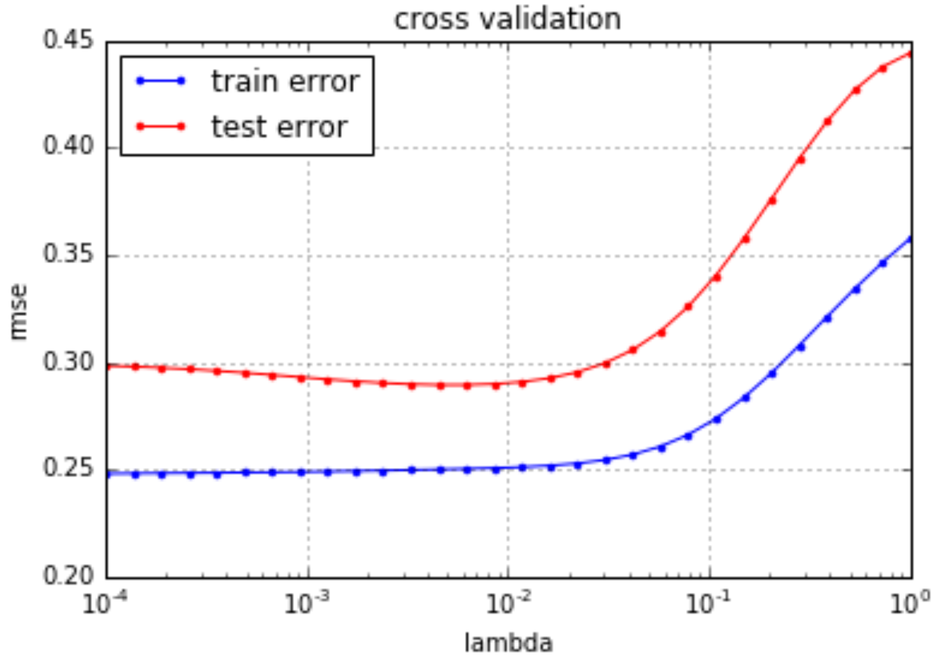
# Model Selection: pick the best model

Goal: select the hyperparameters of our model ($\lambda$ for ex. in ridge regression)
We have a set of candidate values $\{\lambda_k\}_{k=1}^{K}$. Which one should we choose?

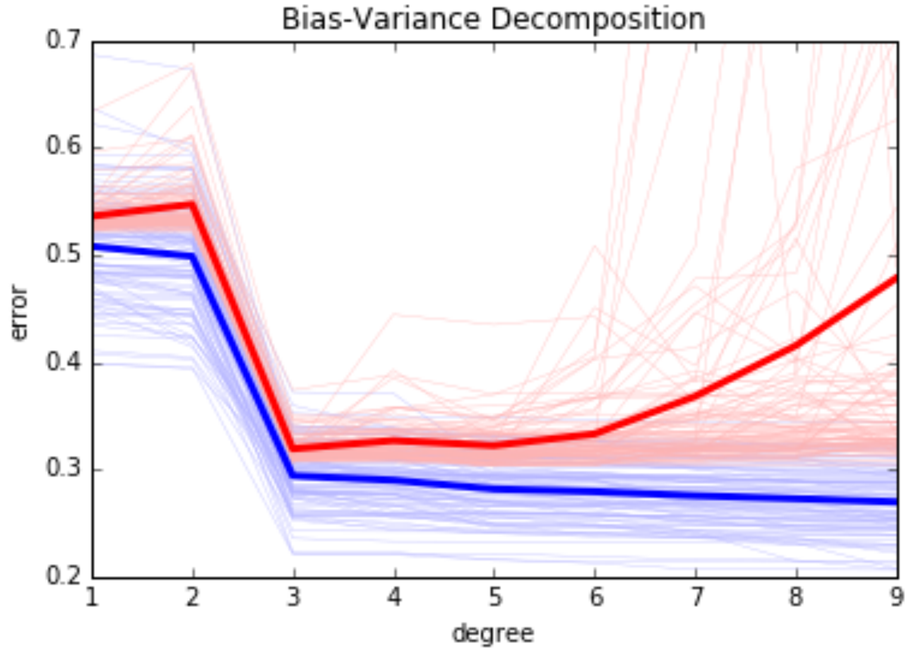
1. Split the data into $S = S_{\text{train}} \cup S_{\text{test}}$, generated independently from $\mathscr{D}$
2. Run the learning algorithm $K$ times on the same training set $S_{\text{train}}$ to compute the $K$ prediction functions $f_{S_{\text{train}},\lambda_k}$
3. For each prediction function, compute the test error $L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k})$

We then choose the value of the parameter $\lambda$ giving the smallest test error

# Examples




Ridge regression




Degree in case of a polynomial feature expansion

# Does model selection work?

Two questions:

- How do we know that the best function $f_{S_{\text{train}},\lambda}$ is a good approximation of the best model within our function class?

- How do we know that $L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k}) \approx L_{\mathcal{D}}(f_{S_{\text{train}},\lambda_k})$?

  We have discussed it for a single model
  What about several models?
  I.e., what is the justification that the min is actually good?

## How far is each of the $K$ test errors $L_{S_{\text{test}}}(f_k)$ from the true $L_{\mathcal{D}}(f_k)$?

Claim: we can bound the maximum deviation for all $K$ candidates, by

$$\mathbb{P}\left[ \max_k \left| L_{\mathcal{D}}(f_k) - L_{S_{\text{test}}}(f_k) \right| \geq \sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2\,|S_{\text{test}}|}} \right] \leq \delta$$

- The error decreases as $\mathcal{O}(1/\sqrt{|S_{\text{test}}|})$ with the number test points
- When testing $K$ hyper-parameters, the error only goes up by $\sqrt{\ln(K)}$

➡So we can test many different models without incurring a large penalty

- It can be extended to infinitely many models

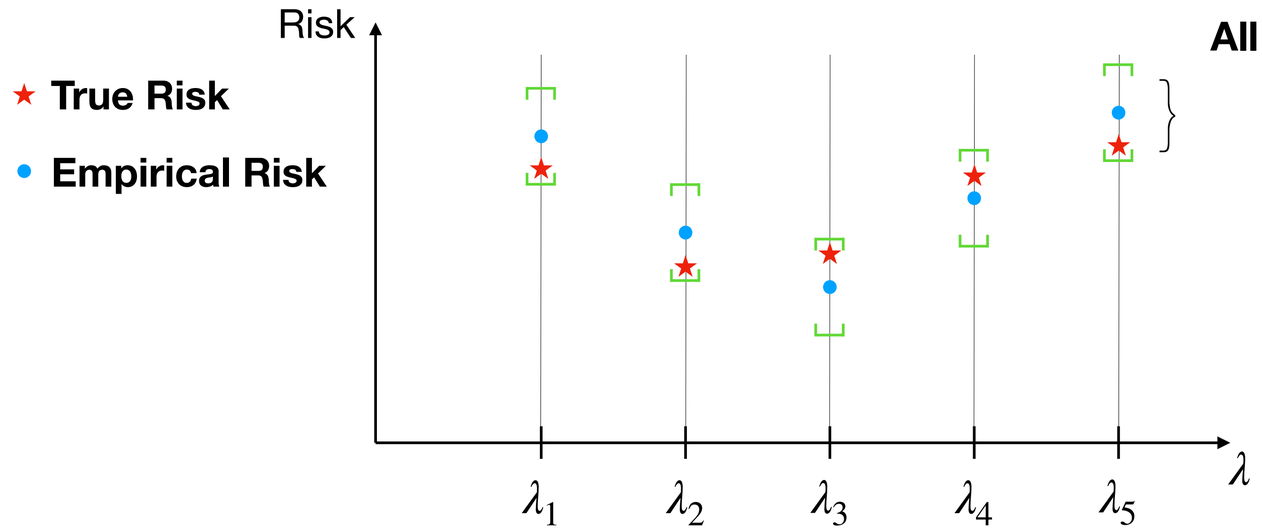
# Proof: A simple union bound

The proof of this statement follows the proof of the special case $K = 1$

$$\begin{aligned}
\mathbb{P}\left[\ \max_k \left| L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k) \right| \geq \varepsilon \right] &= \mathbb{P}\left[\ \cup_k \left\{ \left| L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k) \right| \geq \varepsilon \right\} \right] \\
&\leq \sum_k \mathbb{P}\left[ \left| L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k) \right| \geq \varepsilon \right] \\
&\leq 2Ke^{-2N\varepsilon^2/(b-a)^2}
\end{aligned}$$

Hence, equating $\delta = 2Ke^{-2N\varepsilon^2/(b-a)^2}$ , we get $\varepsilon = \sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2N}}$ as stated

# If we choose the “best” function according to the empirical risk then its true risk is not too far away from the true risk of the optimal choice




**All the widths are the same**

$$2\sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2\,|S_{\text{test}}|}}$$

Let $k^* = \text{argmin}_k L_{\mathcal{D}}(f_k)$ and $\hat{k} = \text{argmin}_k L_{S_{\text{test}}}(f_k)$ then

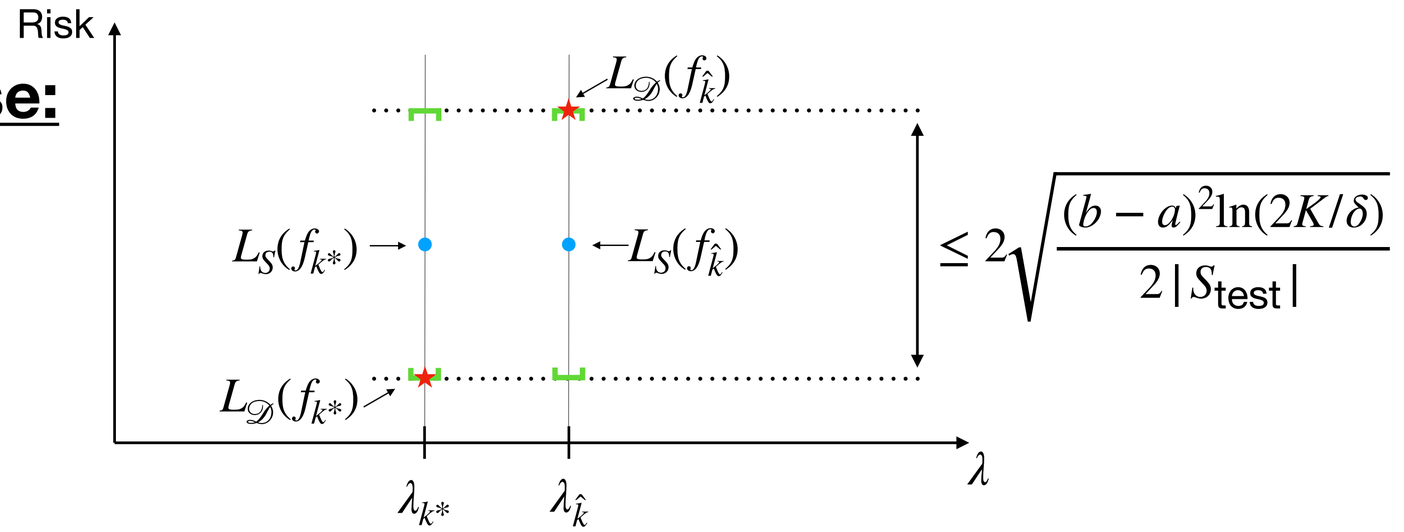
$$\mathbb{P}\left[\; L_{\mathcal{D}}(f_{\hat{k}}) \geq L_{\mathcal{D}}(f_{k^*}) + 2\sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2\,|S_{\text{test}}|}} \;\right] \leq \delta$$

**Function with the smallest empirical risk**

**Function with the smallest true risk**

# If we choose the “best” function according to the empirical risk then its true risk is not too far away from the true risk of the optimal choice

**Worst case:**




Let $k^* = \text{argmin}_k L_{\mathcal{D}}(f_k)$ and $\hat{k} = \text{argmin}_k L_{S_{\text{test}}}(f_k)$ then

$$\mathbb{P}\left[ L_{\mathcal{D}}(f_{\hat{k}}) \geq L_{\mathcal{D}}(f_{k*}) + 2\sqrt{\frac{(b-a)^2\ln(2K/\delta)}{2|S_{\text{test}}|}} \right] \leq \delta$$

**Function with the smallest empirical risk**

**Function with the smallest true risk**

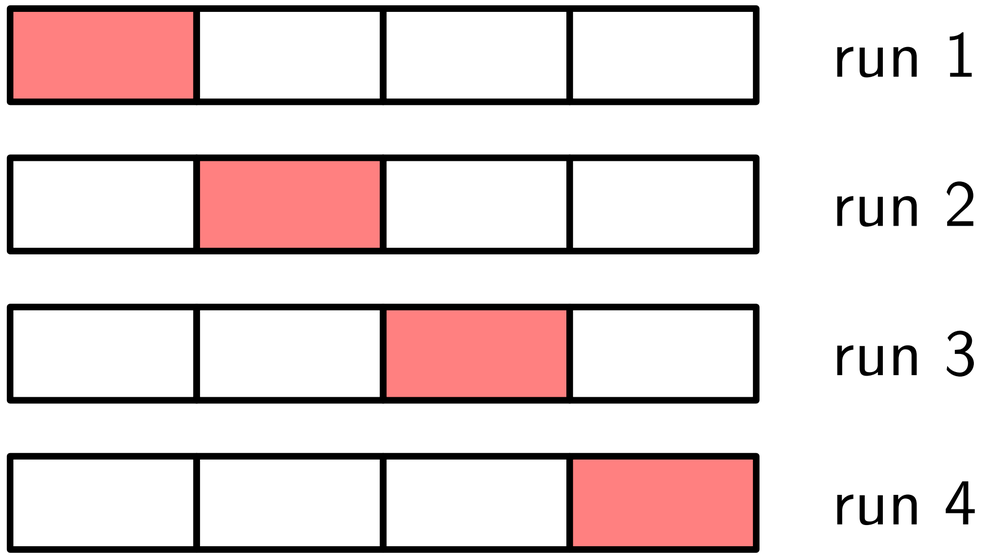
# Cross-Validation


- Splitting the data once into two parts (one for training and one for testing) is not the most efficient way to use the data

- Cross-validation is a better way

# K-fold Cross-Validation

1. Randomly partition the data into $K$ groups
2. Train $K$ times. Each time leave out exactly one of the $K$ groups for testing and use the remaining $K-1$ groups for training.
3. Average the $K$ results




- We have used all data for training, and all data for testing, and used each data point the same number of times
- Cross-validation returns an estimate of the *generalization-error* and its variance

# Do we still have some time?

**Hoeffding's inequality:**

Let $\Theta_1, \ldots, \Theta_N$ be a sequence of i.i.d. random variables with mean $\mathbb{E}[\Theta]$ and range $[a, b]$. Then, for any $\varepsilon > 0$

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^{N}\Theta_n - \mathbb{E}[\Theta]\right| \geq \varepsilon\right] \leq 2e^{-2N\varepsilon^2/(b-a)^2}$$

# Proof (I)

- We equivalently assume that $\mathbb{E}[\Theta] = 0$ and that $\Theta_n \in [a, b]$
- We will only show that

$$\mathbb{P}\left\{ \frac{1}{N} \sum_{n=1}^{N} \Theta_n \geq \varepsilon \right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$$

This, together with the equivalent bound

$$\mathbb{P}\left\{ \frac{1}{N} \sum_{n=1}^{N} \Theta_n \leq -\varepsilon \right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$$

will prove the claim

# Proof (II)

For any $s \geq 0$,

$$\mathbb{P}\left\{ \frac{1}{N} \sum_{n=1}^{N} \Theta_n \geq \varepsilon \right\} = \mathbb{P}\left\{ s\frac{1}{N} \sum_{n=1}^{N} \Theta_n \geq s\varepsilon \right\}$$

$$= \mathbb{P}\left\{ e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n} \geq e^{s\varepsilon} \right\}$$

$$\leq \mathbb{E}[e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n}]e^{-s\varepsilon} \qquad \text{(Markov inequality)}$$

$$= \prod_{n=1}^{N} \mathbb{E}[e^{\frac{s\Theta_n}{N}}]e^{-s\varepsilon} \qquad \text{(the r.v } \Theta_n \text{ are independent)}$$

$$= \mathbb{E}[e^{\frac{s\Theta}{N}}]^N e^{-s\varepsilon} \qquad \text{(the r.v } \Theta_n \text{ are i.d.)}$$

$$\leq e^{s^2(b-a)^2/(8N)}e^{-s\varepsilon} \qquad \text{(Hoeffding lemma)}$$

# Proof (III)

What do we do now? We have for any $s \geq 0$

$$\mathbb{P}\left\{ \frac{1}{N} \sum_{n=1}^{N} \Theta_n \geq \varepsilon \right\} \leq e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon}$$

In particular for the minimum value obtained for $s = \frac{4N\varepsilon}{(b-a)^2}$

$$\mathbb{P}\left\{ \frac{1}{N} \sum_{n=1}^{N} \Theta_n \geq \varepsilon \right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$$

# Hoeffding lemma

For any random variable $X$, with $\mathbb{E}[X] = 0$ and $X \in [a, b]$ we have

$$\mathbb{E}[e^{sX}] \leq e^{\frac{1}{8}s^2(b-a)^2} \text{ for any } s \geq 0$$

Proof outline:

Consider the convex function $s \mapsto e^{sx}$. In the range $[a, b]$ it is upper bounded by the chord

$$e^{sx} \leq \frac{x-a}{b-a}e^{sb} + \frac{b-x}{b-a}e^{sa}$$

Taking the expectation and recalling that $\mathbb{E}[X] = 0$, we get

$$\mathbb{E}[e^{sX}] \leq \frac{b}{b-a}e^{sa} - \frac{a}{b-a}e^{sb} \leq e^{s^2(b-a)^2/8}$$