

# Generalization, Model Selection, and Validation

Machine Learning- CS-433

30 Sep 2025

Robert West

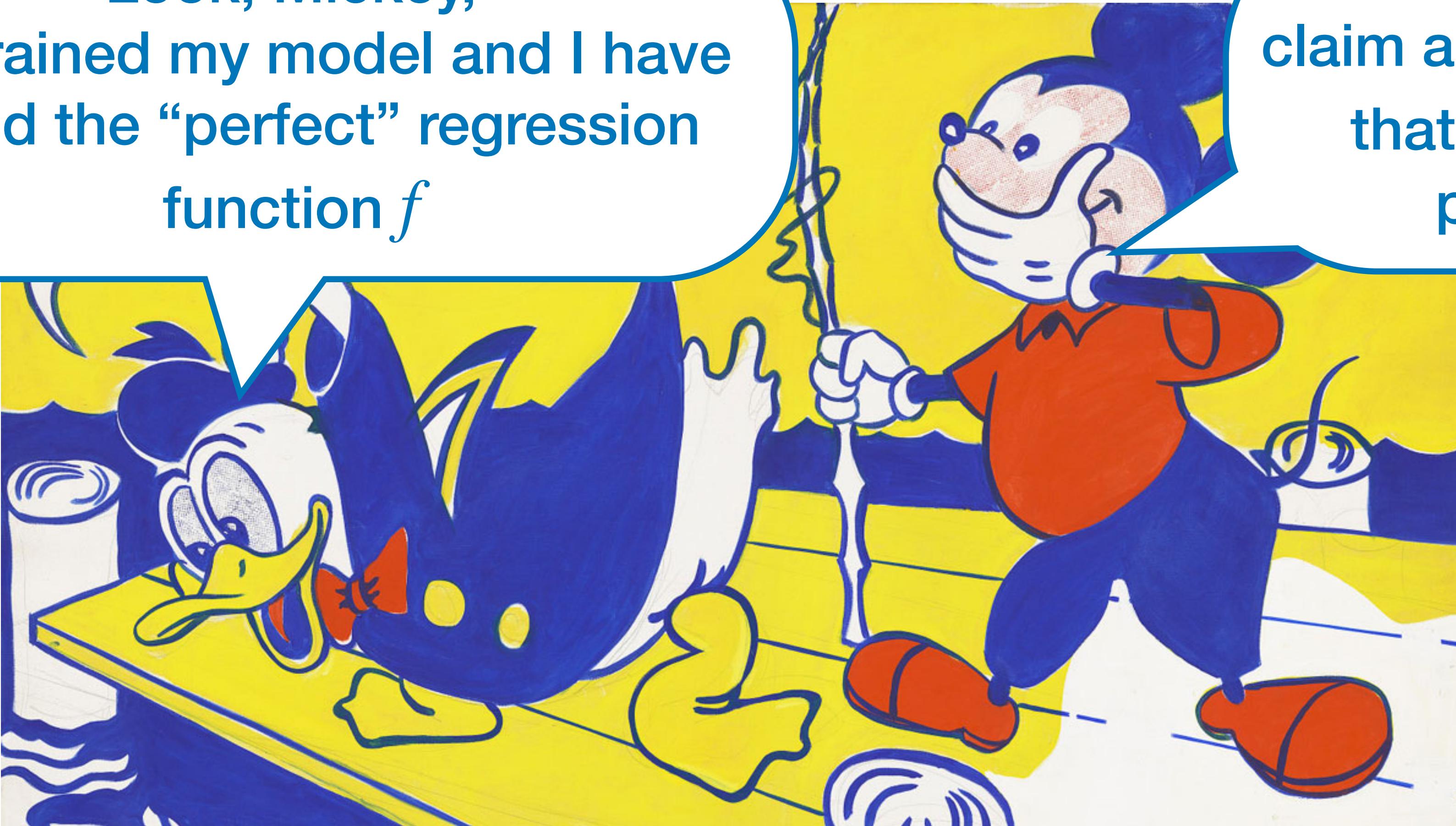
(Slide credit: Martin Jaggi & Nicolas Flammarion)



# 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:**  $w_\lambda = \arg \min_w \frac{1}{2N} \sum_{n=1}^N (y_n - x_n^\top w)^2 + \lambda \|w\|_2^2$   $w \in \mathbb{R}^D$ 
  - $\lambda$  can be tuned to control the model complexity (to reduce overfitting)
  - In practice:  $(\lambda_1, \dots, \lambda_k) \rightarrow \text{Algorithm} \rightarrow (w_1, \dots, w_k)$
  - Which  $\lambda$  should we use?
- **Polynomial feature expansion:**  $\phi(x) = (x, x^2, x^3, \dots)$   
 $(x_{(1)}, x_{(2)}) \xrightarrow{\phi} (x_{(1)}, x_{(2)}, x_{(1)}^2 + x_{(2)}^2)$   
 $(x_{(1)}, x_{(2)}, 5x_{(1)}^2 + 2x_{(2)}^2, x_{(2)}^3 + 2x_{(1)}^2)$ 
  - 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

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

input      desired output

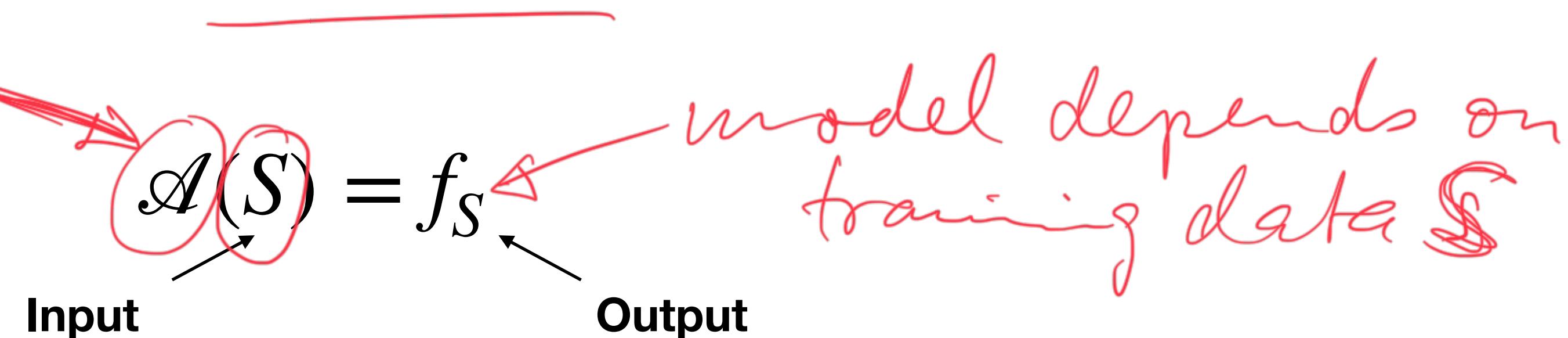
## Data Model:

Unknown distribution  $\mathcal{D}$  with range  $\mathcal{X} \times \mathcal{Y}$

We see a dataset  $S$  of independent samples from  $\mathcal{D}$ .

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

## Learning Algorithm:



$A$ : 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  $\mathcal{D}$ :

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

what you do predict

what you should predict

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

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

The quantity  $L_{\mathcal{D}}(f)$  has many names:

{ True  
Expected  
Generalization }

{ Risk  
Error  
Loss }

This is the quantity we are fundamentally interested in

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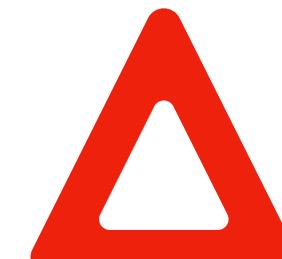
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--	---

This is the quantity we are fundamentally interested in



Problem:  $\mathcal{D}$  is unknown

# Empirical Error: what we can compute

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

Law of large numbers:  
 ~~$\mathcal{D} \rightarrow E$~~

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

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

LLN

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

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

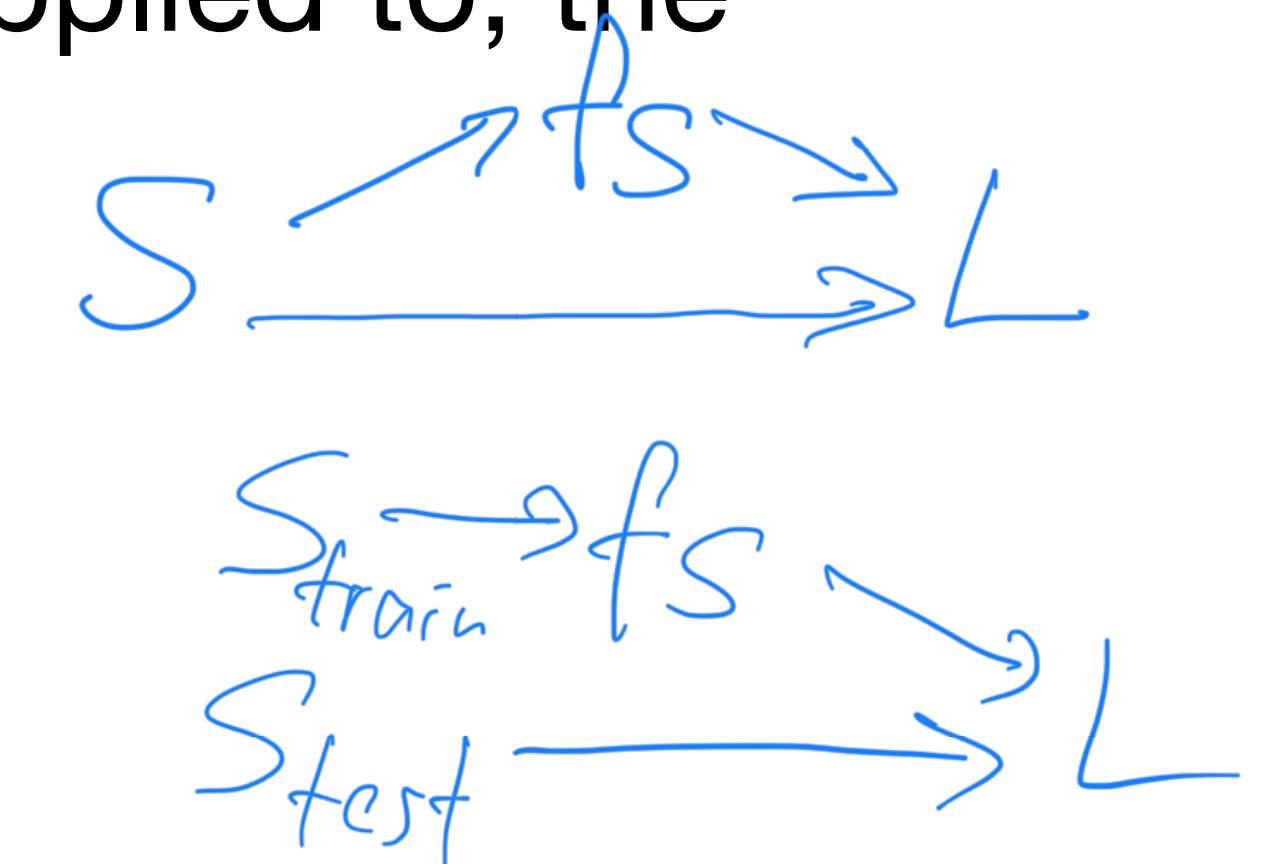
$$\begin{aligned} E(x, y) &\approx [g(x, y)] \\ &= \sum_{(x, y)} \Pr_{\mathcal{D}}(x, y) g(x, y) \end{aligned}$$

# 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 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:

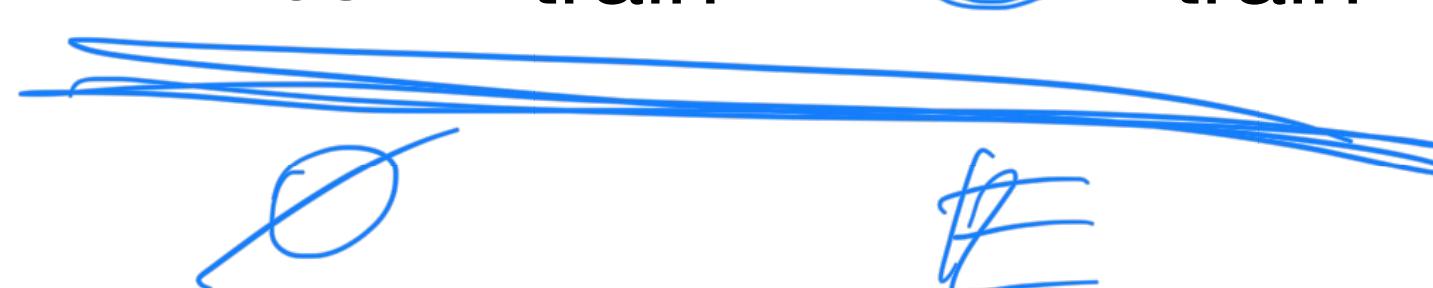
$$S = S_{\text{train}} \cup S_{\text{test}}$$

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:  $L_{S_{\text{test}}}(f_{S_{\text{train}}}) \approx L_{\mathcal{D}}(f_{S_{\text{train}}})$

*N samples  
from  $\mathcal{D}$  i.i.d.*



# 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:

*disjointly*

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

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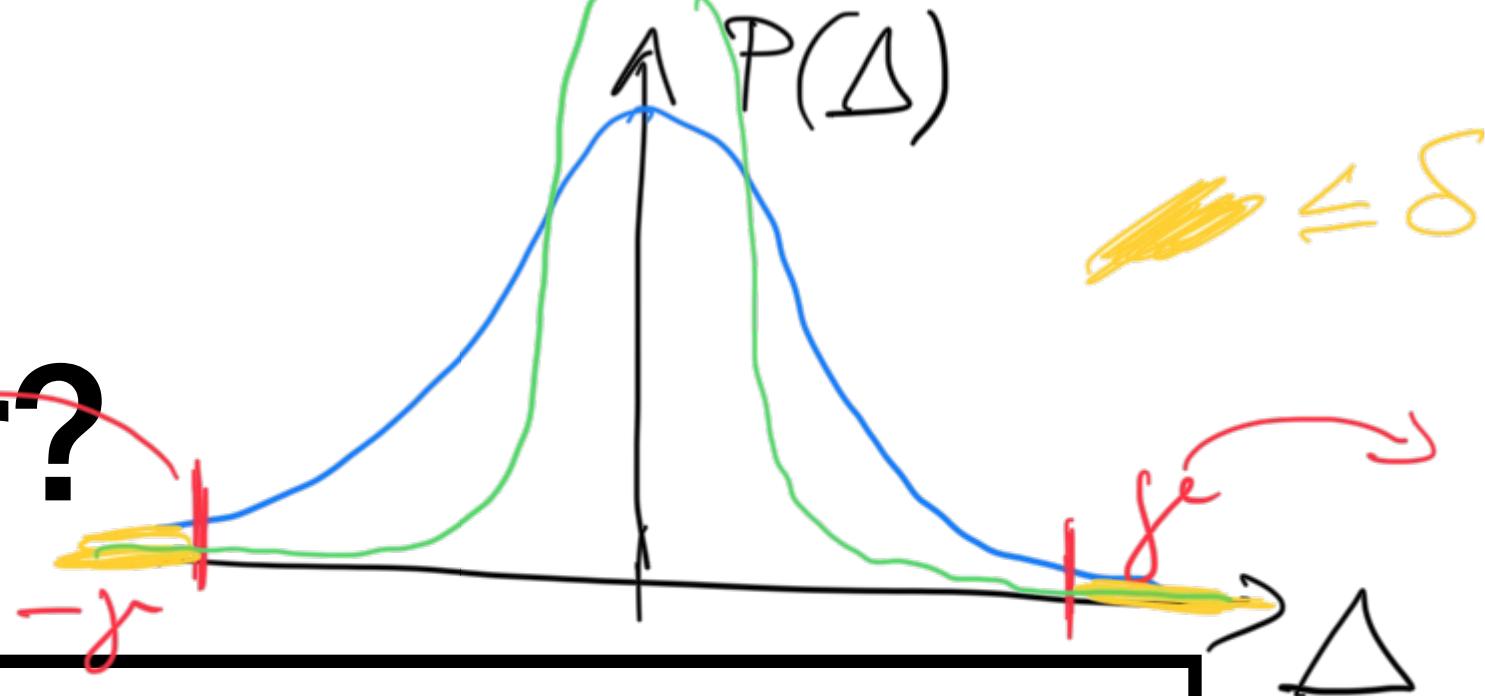
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We have less data both for the learning and the validation tasks (tradeoff)

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



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

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

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:

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

- Given a dataset  $S$

1. Split:  $S = S_{\text{train}} \cup S_{\text{test}}$
2. Train:  $\mathcal{A}(S_{\text{train}}) = f_{S_{\text{train}}}$
3. Use:

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

→ 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  $\Theta_1, \dots, \Theta_N$  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  $\varepsilon = \sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2|S_{\text{test}}|}}$   $\square$

# Model Selection: pick the best model

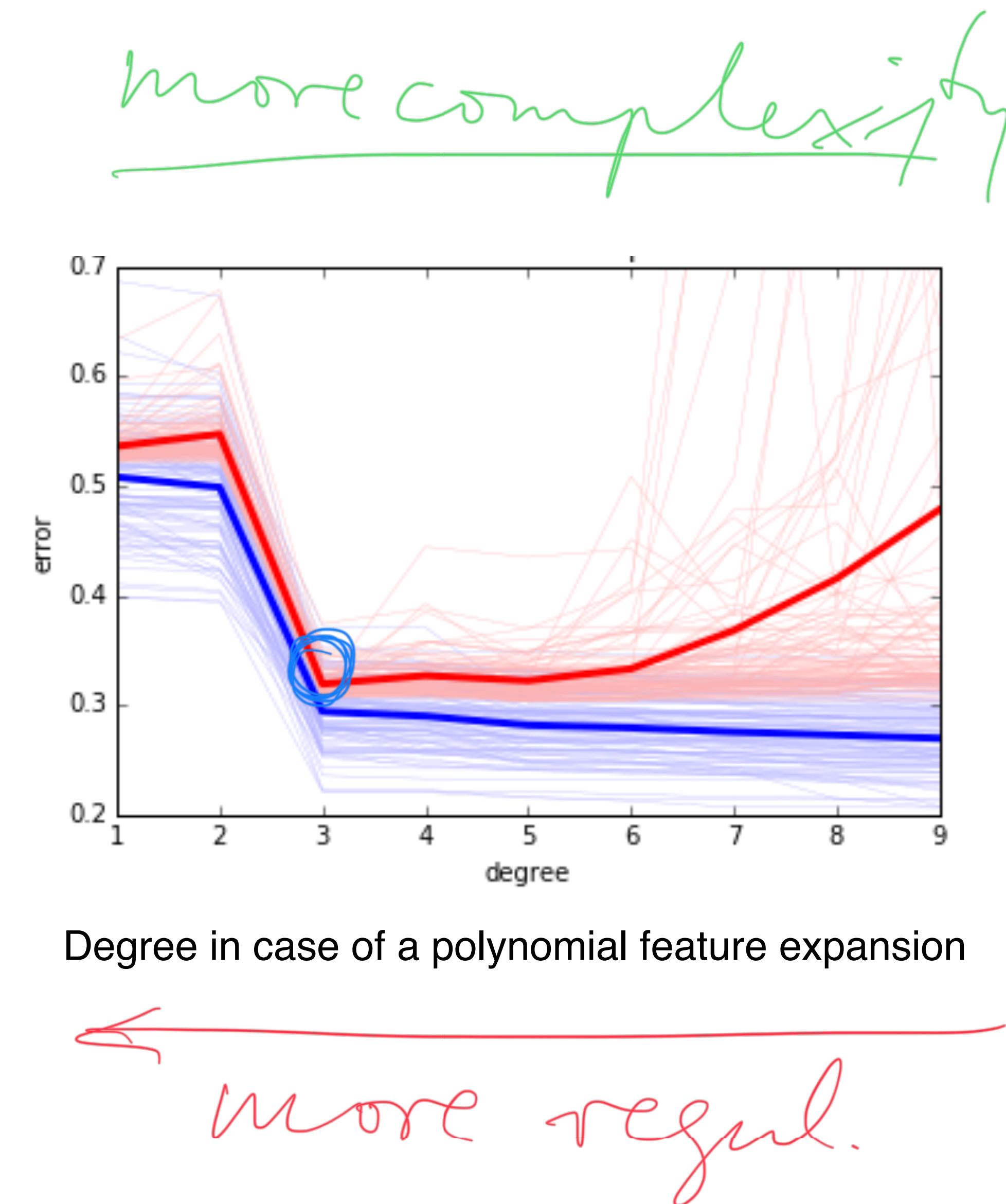
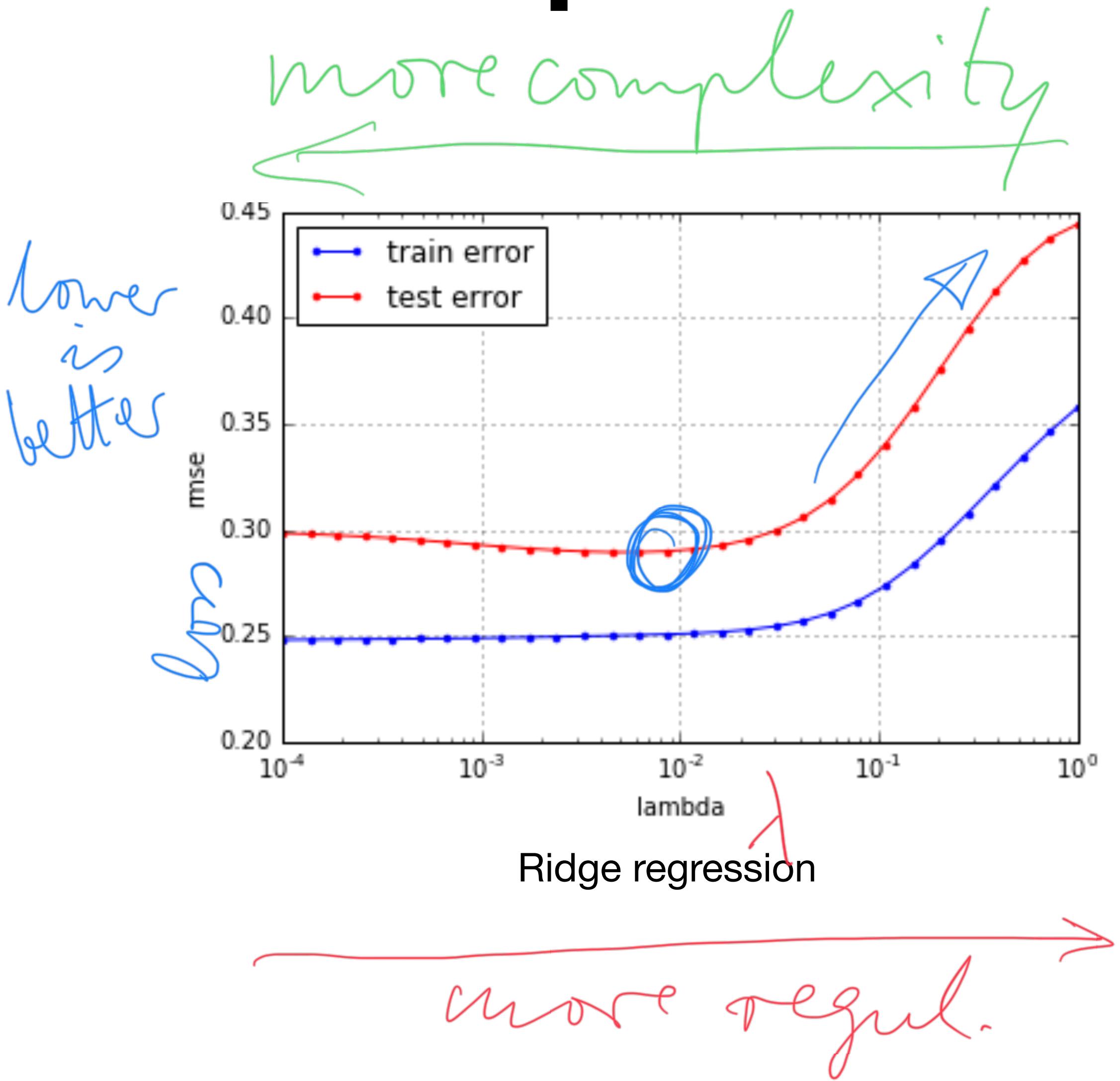
Goal: select the hyperparameters of our model ( $\lambda$  for ex. in ridge regression)

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  $\mathcal{D}$
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



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

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

- 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

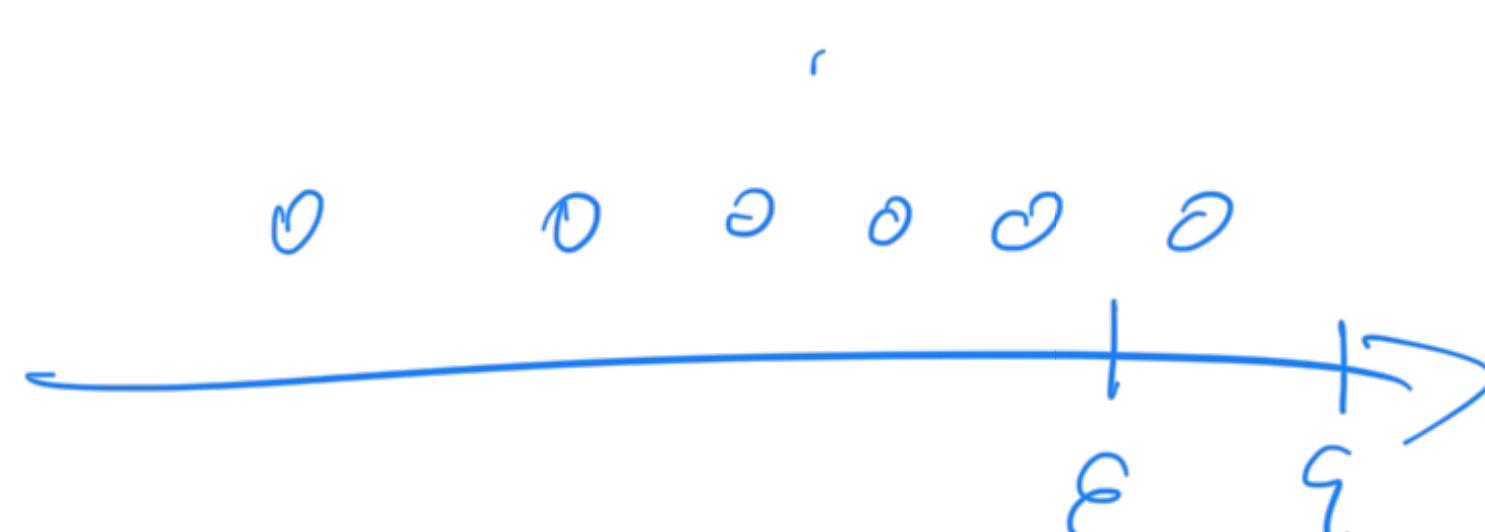
# Proof: A simple union bound



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

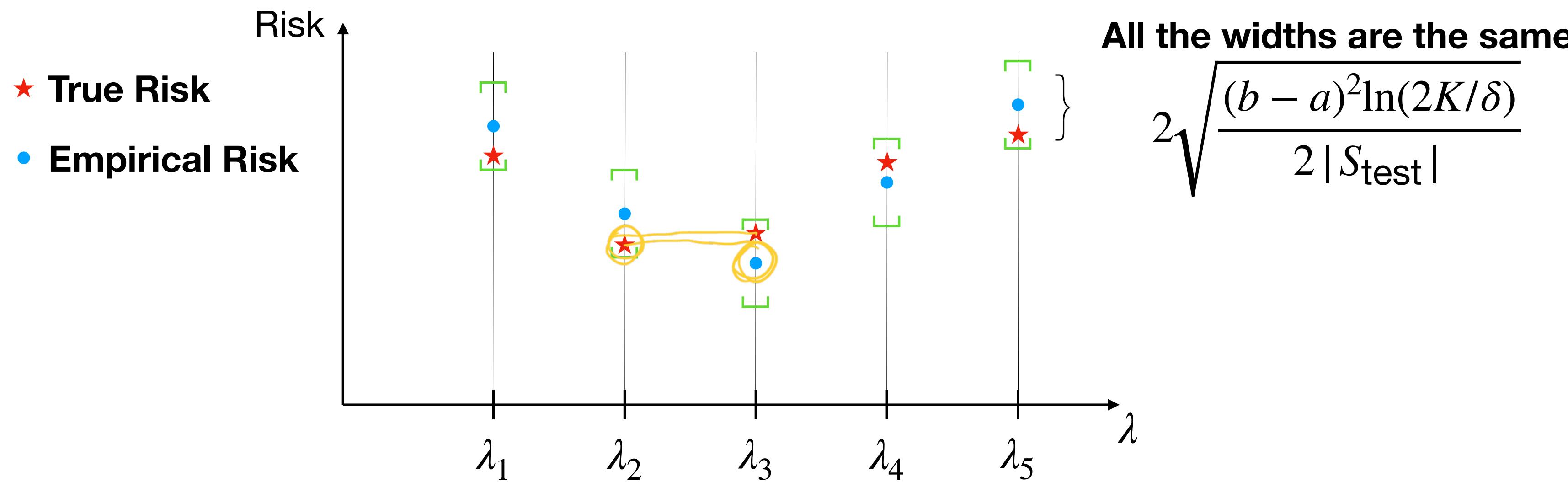
$$\begin{aligned} P(A \cup B) \\ P(A) + P(B) \end{aligned}$$

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



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



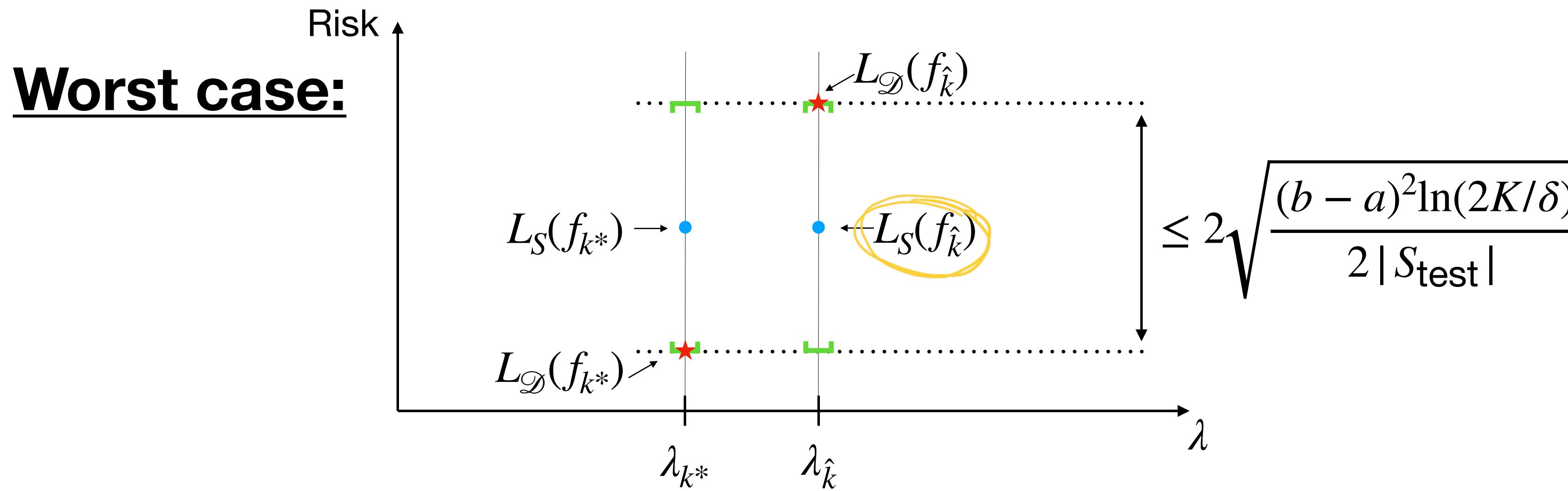
Let  $k^* = \operatorname{argmin}_k L_{\mathcal{D}}(f_k)$  and  $\hat{k} = \operatorname{argmin}_k L_{S_{\text{test}}}(f_k)$  then

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

Function with  
the smallest empirical risk

Function with  
the smallest true risk

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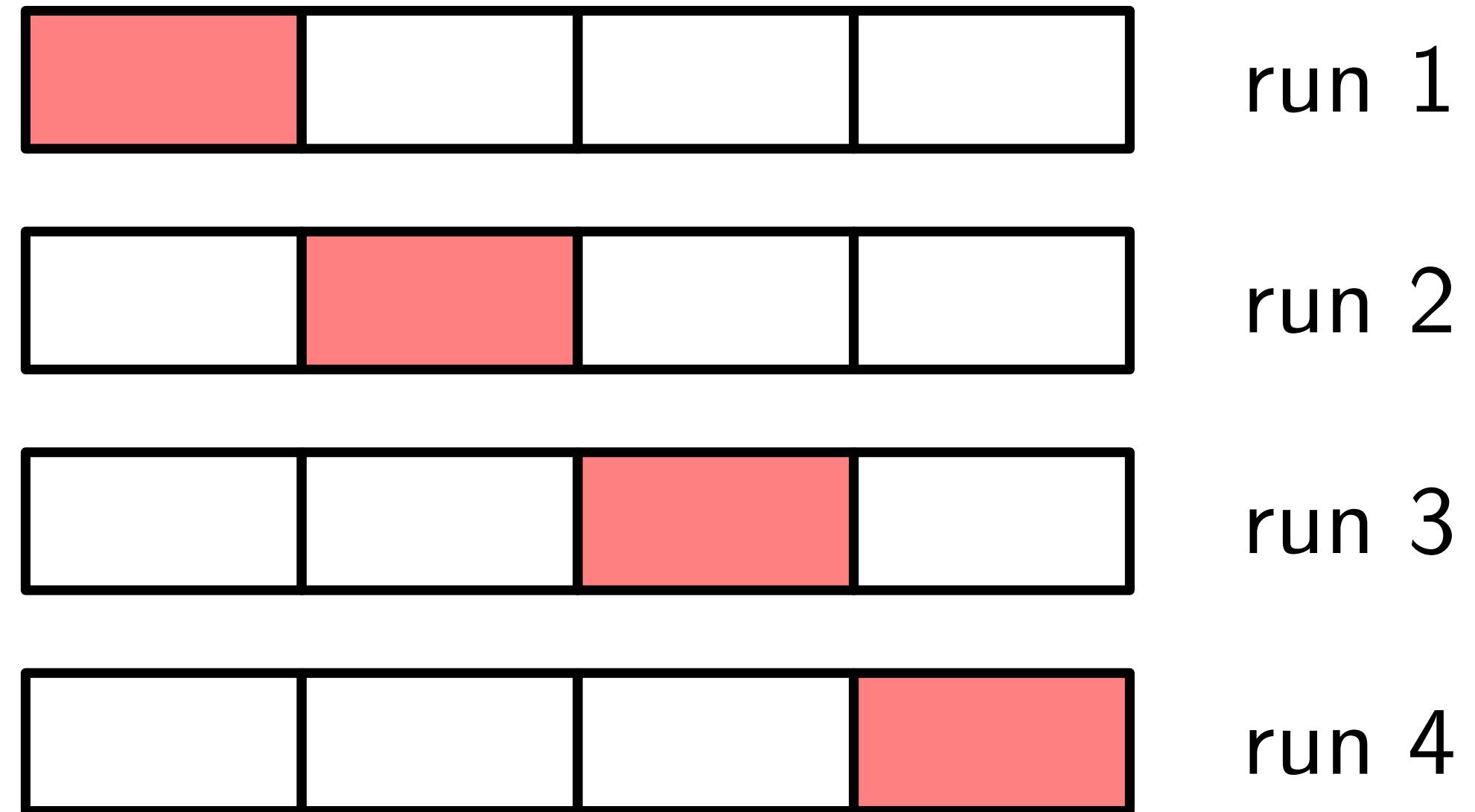
# Cross-Validation



- 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

# M-fold Cross-Validation\*

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

\* Usually called “K-fold”, but that would clash with K as used before (# values tried for hyperparam)...

# Do we still have some time?

**Hoeffding's inequality:**

Let  $\Theta_1, \dots, \Theta_N$  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)

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For any  $s \geq 0$ ,  $\mathbb{P}\left\{\frac{1}{N} \sum_{n=1}^N \Theta_n \geq \varepsilon\right\} = \mathbb{P}\left\{s \frac{1}{N} \sum_{n=1}^N \Theta_n \geq s\varepsilon\right\}$

# Proof (II)

$$\begin{aligned} \text{For any } s \geq 0, \quad \mathbb{P}\left\{\frac{1}{N} \sum_{n=1}^N \Theta_n \geq \varepsilon\right\} &= \mathbb{P}\left\{s \frac{1}{N} \sum_{n=1}^N \Theta_n \geq s\varepsilon\right\} \\ &= \mathbb{P}\left\{e^{s \frac{1}{N} \sum_{n=1}^N \Theta_n} \geq e^{s\varepsilon}\right\} \end{aligned}$$

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 & = \mathbb{E}[e^{\frac{s\Theta}{N}}]^N e^{-s\varepsilon} \quad (\text{the r.v } \Theta_n \text{ are i.d.}) \\
 & \leq e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon} \quad (\text{Hoeffding lemma})
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# Hoeffding lemma

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

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

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Proof outline:

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

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

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

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

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