Generalization, Model Selection, and Validation

Machine Learning Course - CS-433
Oct 10, 2023
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Generalization, validation?



What is the model selection problem?

- Ridge regression: $w_{\lambda} = \arg\min_{w} \frac{1}{2N} \sum_{n=1}^{N} (y_n x_n^{\mathsf{T}} w)^2 + \lambda \|w\|_2^2$ Hyperparameter
 - λ can be tuned to control the model complexity (to reduce overfitting)

 - Which λ should we use?
- Polynomial feature expansion: $(x_{(1)}, x_{(2)}) \xrightarrow{\phi} \frac{(x_{(1)}, x_{(2)}, x_{(1)}^2 + x_{(2)}^2)}{(x_{(1)}, x_{(2)}, 5x_{(1)}^2 + 2x_{(2)}^2, x_{(2)}^3 + 2x_{(1)}^2)}$
 - 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

Data Model:

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

$$S = \{(x_n, y_n)\}_{n=1}^N \sim \mathcal{D}$$
 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 model dependency

Generalization Error: how accurate is f at predicting?

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

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

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

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

This is the quantity we are fundamentally interested in

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Empirical Error: what we can compute

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

$$L_{S}(f) = \frac{1}{|S|} \sum_{(x_{n}, y_{n}) \in S} \mathcal{E}(y_{n}, f(x_{n})).$$

Also called: empirical risk/error/loss

 \triangle 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: $L_S(f) \to L_{\mathcal{D}}(f)$ but fluctuations! $|S| \to \infty$

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

Training error: what we are minimizing

 \triangle 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*:

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

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

<u>Problem:</u> 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

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

ightharpoonup Since $S_{ ext{test}}$ and $S_{ ext{train}}$ are independent: $L_{S_{ ext{test}}}(f_{S_{ ext{train}}}) pprox L_{2}(f_{S_{ ext{train}}})$

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\trace{\Delta} \text{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 $\ell(\,\cdot\,,\,\cdot\,) \in [a,b]$:

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

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

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

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

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

→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:
$$\frac{1}{N} \sum_{n=1}^{N} \Theta_n = \frac{1}{N} \sum_{n=1}^{N} \mathcal{E}(y_n, f(x_n)) = L_{Stest}(f)$$

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 $L_{\text{Stest}}(f)$ deviates from the true loss by more than a given constant?

→ classically addressed using concentration inequalities

Hoeffding inequality: a simple concentration bound

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

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^{N}\Theta_{n}-\mathbb{E}[\Theta]\right|\geq\varepsilon\right]\leq 2e^{-2N\varepsilon^{2}/(b-a)^{2}}\text{ for any }\varepsilon\geq0$$

Concentration bound: the empirical mean is concentrated around its mean

A. Use it with $\Theta_n = \mathcal{C}(y_n, f(x_n))$

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

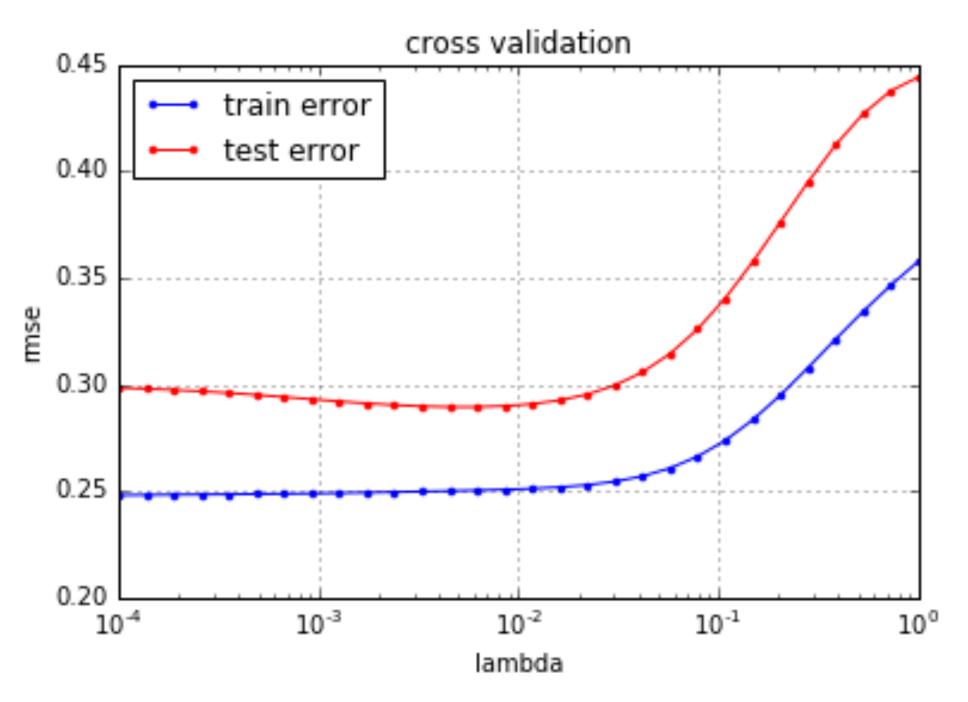
Model Selection: pick the best model

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

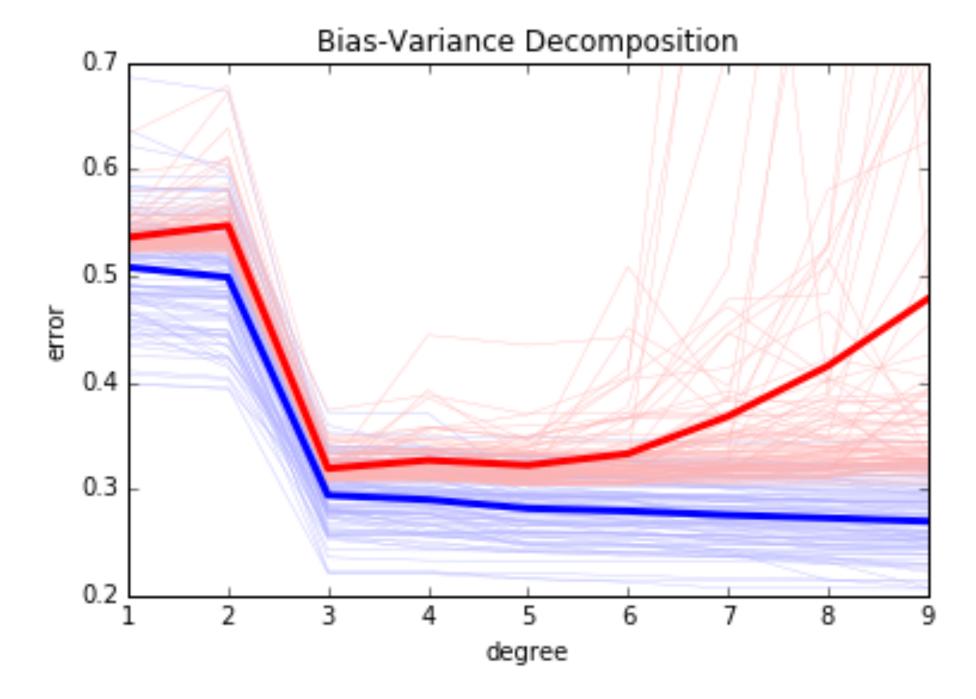
- 1. Split the data into $S = S_{\text{train}} \cup S_{\text{test}}$, generated independently from \mathscr{D}
- 2. Run the learning algorithm K times on the same training set S_{train} to compute the K prediction functions $f_{S_{\text{train}},\lambda_k}$
- 3. For each prediction function, compute the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

We then choose the value of the parameter λ 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 $f_{S_{train},\lambda}$ is a good approximation of the best model within our function class?
- How do we know that $L_{S ext{test}}(f_{S ext{train},\lambda_k}) \approx L_{\mathcal{D}}(f_{S ext{train},\lambda_k})$? 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 $L_{S}(f_k)$ from the true $L_{\mathcal{D}}(f_k)$?

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

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

- 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

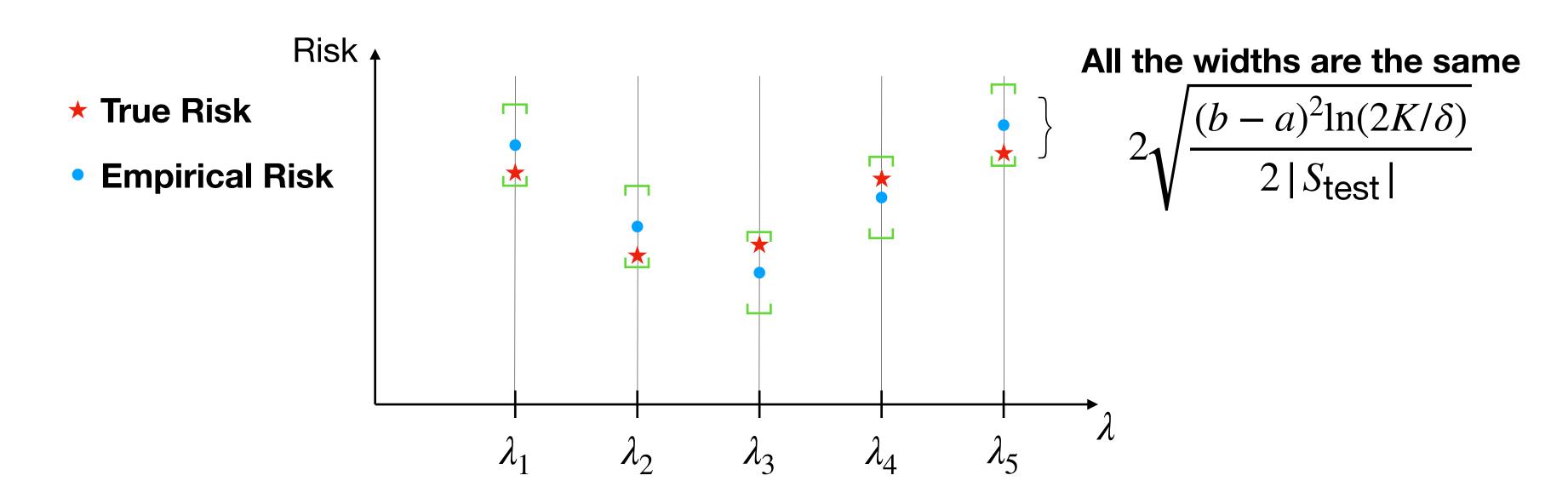
Proof: A simple union bound

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

$$\begin{split} \mathbb{P}\Big[\max_{k} \left| L_{\mathscr{D}}(f_{k}) - L_{S_{\mbox{test}}}(f_{k}) \right| &\geq \varepsilon \Big] &= \mathbb{P}\Big[\cup_{k} \left\{ \left| L_{\mathscr{D}}(f_{k}) - L_{S_{\mbox{test}}}(f_{k}) \right| \geq \varepsilon \right\} \Big] \\ & \text{UNION BOUND HERE } \leq \sum_{k} \mathbb{P}\Big[\left| L_{\mathscr{D}}(f_{k}) - L_{S_{\mbox{test}}}(f_{k}) \right| \geq \varepsilon \Big] \\ &\leq 2Ke^{-2N\varepsilon^{2}/(b-a)^{2}} \end{split}$$

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



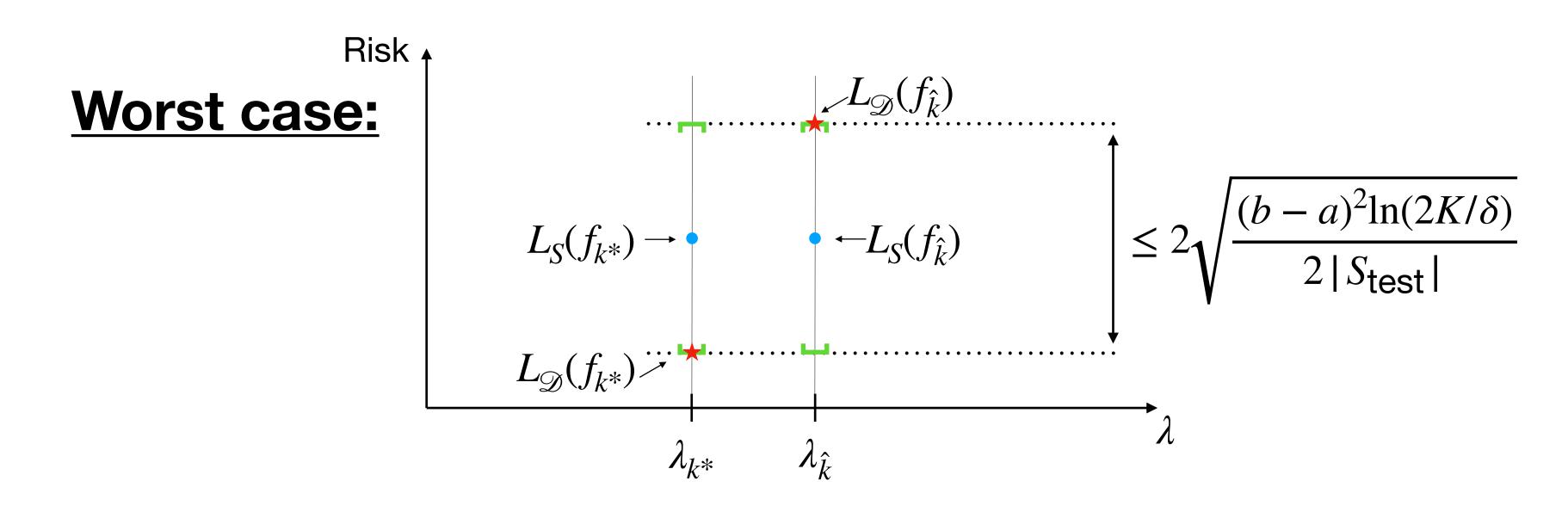
Let
$$k^* = \operatorname{argmin}_k L_{\mathcal{D}}(f_k)$$
 and $\hat{k} = \operatorname{argmin}_k L_{S_{\mbox{test}}}(f_k)$ then

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

Function with the smallest empirical risk

Function with the smallest true risk

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Let
$$k^* = \operatorname{argmin}_k L_{\mathcal{D}}(f_k)$$
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Function with the smallest true risk

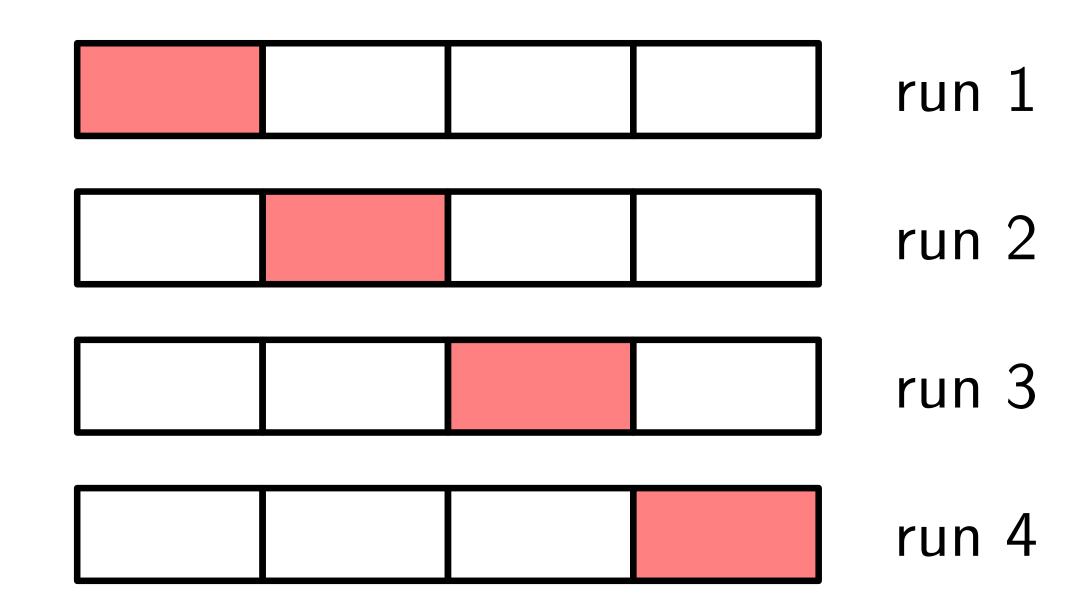
Cross-Validation



- 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 unbiased estimate of the generalizationerror and its variance

Do we still have some time?

Hoeffding's inequality:

Let Θ_1,\ldots,Θ_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
$$s \geq 0$$
,
$$\mathbb{P}\Big\{\frac{1}{N}\sum_{n=1}^N\Theta_n \geq \varepsilon\Big\} = \mathbb{P}\Big\{s\frac{1}{N}\sum_{n=1}^N\Theta_n \geq s\varepsilon\Big\}$$
$$= \mathbb{P}\Big\{e^{s\frac{1}{N}\sum_{n=1}^N\Theta_n} \geq e^{s\varepsilon}\Big\}$$
$$\leq \mathbb{E}[e^{s\frac{1}{N}\sum_{n=1}^N\Theta_n}]e^{-s\varepsilon} \qquad \text{(Markov inequality)}$$
$$= \prod_{n=1}^N \mathbb{E}[e^{\frac{s\Theta_n}{N}}]e^{-s\varepsilon} \qquad \text{(the r.v }\Theta_n \text{ are independent)}$$
$$= \mathbb{E}[e^{\frac{s\Theta}{N}}]^N e^{-s\varepsilon} \qquad \text{(the r.v }\Theta_n \text{ are i.d.)}$$
$$\leq e^{s^2(b-a)^2/(8N)}e^{-s\varepsilon} \qquad \text{(Hoeffding lemma)}$$

Proof (III)

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

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

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

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

Proof outline:

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

$$e^{SX} \le \frac{x - a}{b - a} e^{Sb} + \frac{b - x}{b - a} e^{Sa}$$

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

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