Generalization, Model Selection, and Validation

Machine Learning Course - CS-433
Oct 10, 2023
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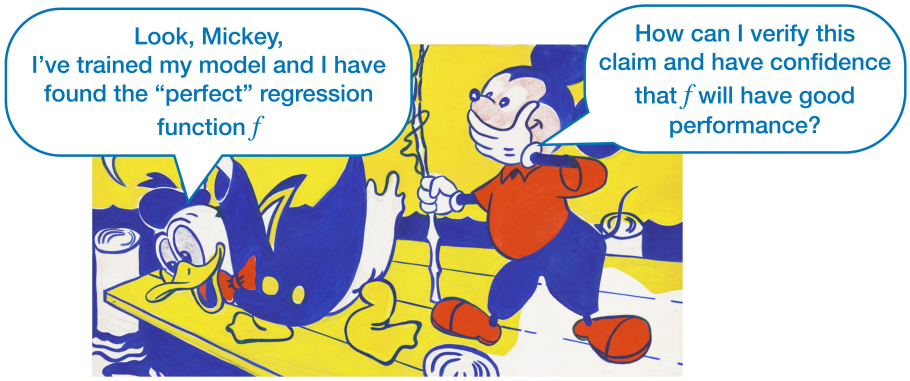
EPFL

Generalization, validation?



What is the model selection problem?

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

Hyperparameter

- In practice: $(\lambda_1, \cdots, \lambda_k) \longrightarrow$ Algorithm $\longrightarrow (w_1, \cdots, w_k)$
- Which λ should we use?
- Polynomial feature expansion: $(x_{(1)}, x_{(2)}) \xrightarrow{\phi} \begin{pmatrix} \left(x_{(1)}, x_{(2)}, x_{(1)}^2 + x_{(2)}^2\right) \\ \left(x_{(1)}, x_{(2)}, 5x_{(1)}^2 + 2x_{(2)}^2, x_{(2)}^3 + 2x_{(1)}\right) \end{pmatrix}$
- 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

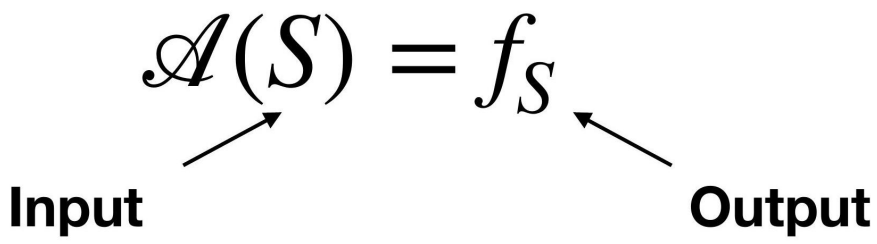
Data Model:

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:



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 $\mathscr{D}$:

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

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: $\left\{\begin{array}{l}\text{True}\\ \text{Expected}\\ \text{Generalization}\end{array}\right.$ $\left\{\begin{array}{l}\text{Risk}\\ \text{Error}\\ \text{Loss}\end{array}\right.$
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

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

Also called: empirical risk/error/loss

Δ 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: $L_S(f) \underset{|S|\to\infty}{\to} L_{\mathscr{D}}(f)$ but fluctuations!

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

Training error: what we are minimizing

Δ 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:

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

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 $L_S\left(f_S\right)$ might not be close to $L_{\mathscr{D}}\left(f_S\right)$ 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

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

$\Rightarrow$ Since S_{test} and S_{train} are independent: $L_{S_{\text{test}}}\left(f_{S_{\text{train}}}\right) \approx L_{\mathscr{D}}\left(f_{\text{train}}\right)$

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Δ 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 $\ell(\cdot, \cdot) \in [a, b]$:

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

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

$\rightarrow$ 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:

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

- Given a dataset S

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

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

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

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

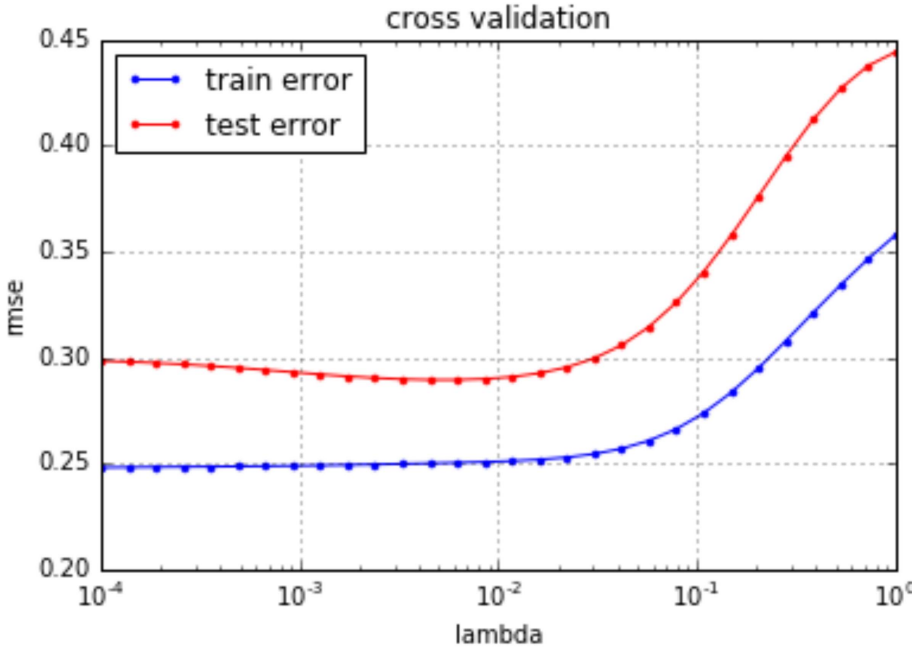
Model Selection: pick the best model

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?

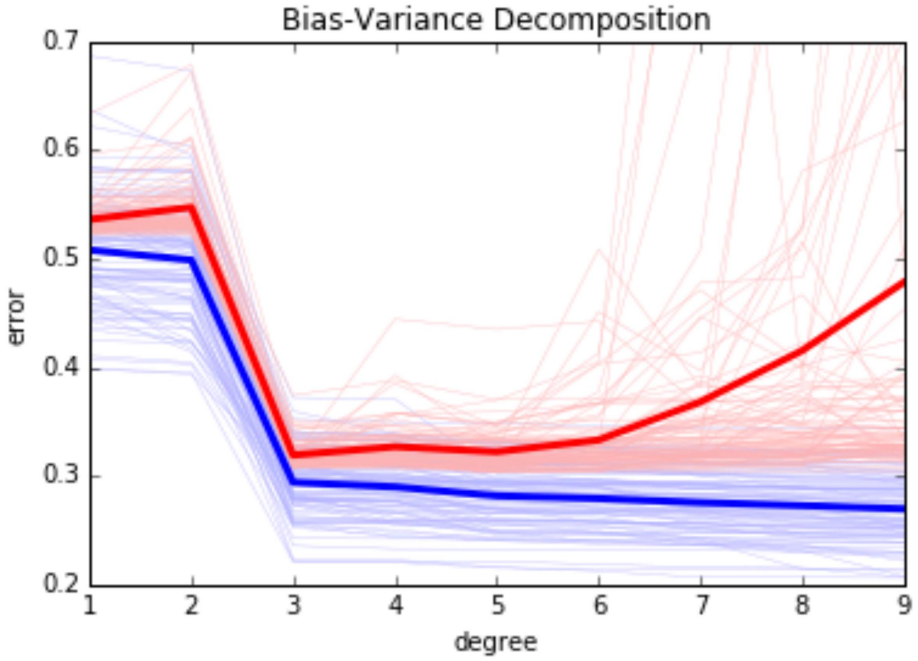
1. Split the data into $S = S_{\text{train}} \cup S_{\text{test}}$, generated independently from $\mathscr{D}$
2. Run the learning algorithm K times on the same training set S_{train} to compute the K prediction functions $f_{S_{\text{train}},\lambda_k}$
3. For each prediction function, compute the test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

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 $f_{S_{\text{train},\lambda}}$ is a good approximation of the best model within our function class?
- How do we know that $L_{S_{\text{test}}}\ (f_{S_{\text{train}},\lambda_k}) \approx L_{\mathscr{D}}\left(f_{S_{\text{train}},\lambda_k}\right)$?

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 $L_{S_{\mathbf{test}}}\ (f_k)$ from the true $L_{\mathscr{D}}\left(f_k\right)$?

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

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

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

- When testing K hyper-parameters, the error only goes up by $\sqrt{\ln(K)}$

$\Rightarrow$ So we can test many different models without incurring a large penalty

- It can be extended to infinitely many models

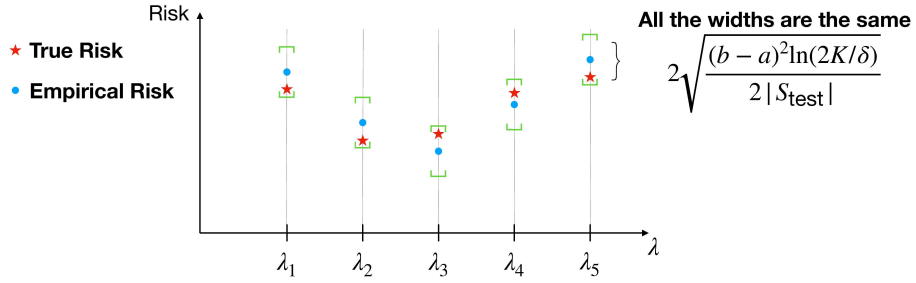
Proof: A simple union bound

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

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

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

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

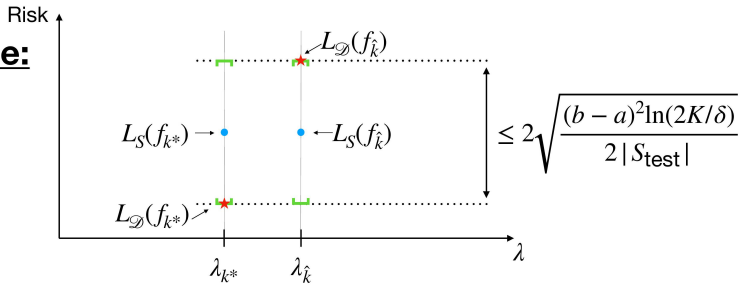
Function with

Function with

the smallest empirical risk 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 $k^* = \text{argmin}_k\, L_{\mathscr{D}}\,(f_k)$ and $\hat{k} = \text{argmin}_k\, L_{S_{\text{test}}}\,(f_k)$ then

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

Function with

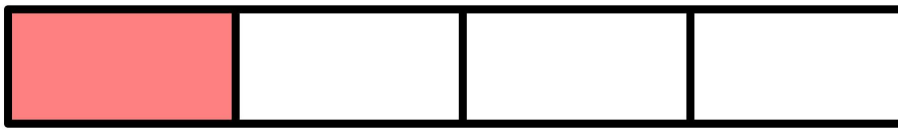
Function with

Cross-Validation

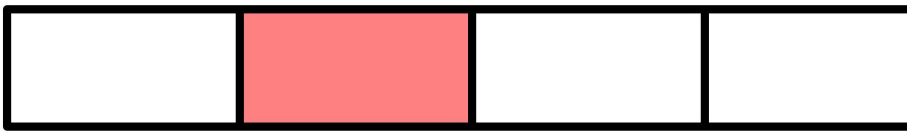
- Splitting the data once into two parts (one for training and one for testing) is not the most efficient way to use the data
- Cross-validation is a better way

K-fold Cross-Validation

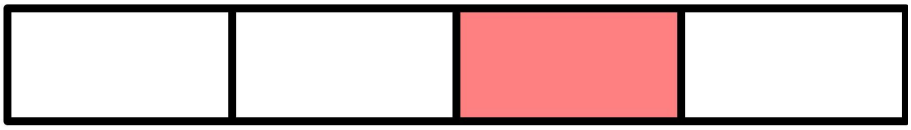
1. Randomly partition the data into K groups



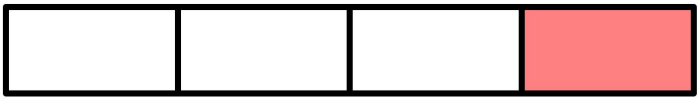
run 1



run 2 out exactly one of the K groups for testing and use the remaining $K-1$ groups for training.



run 3



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

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

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

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

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

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

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

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

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

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