6 – Generalization bounds

Mathematics of Data Science

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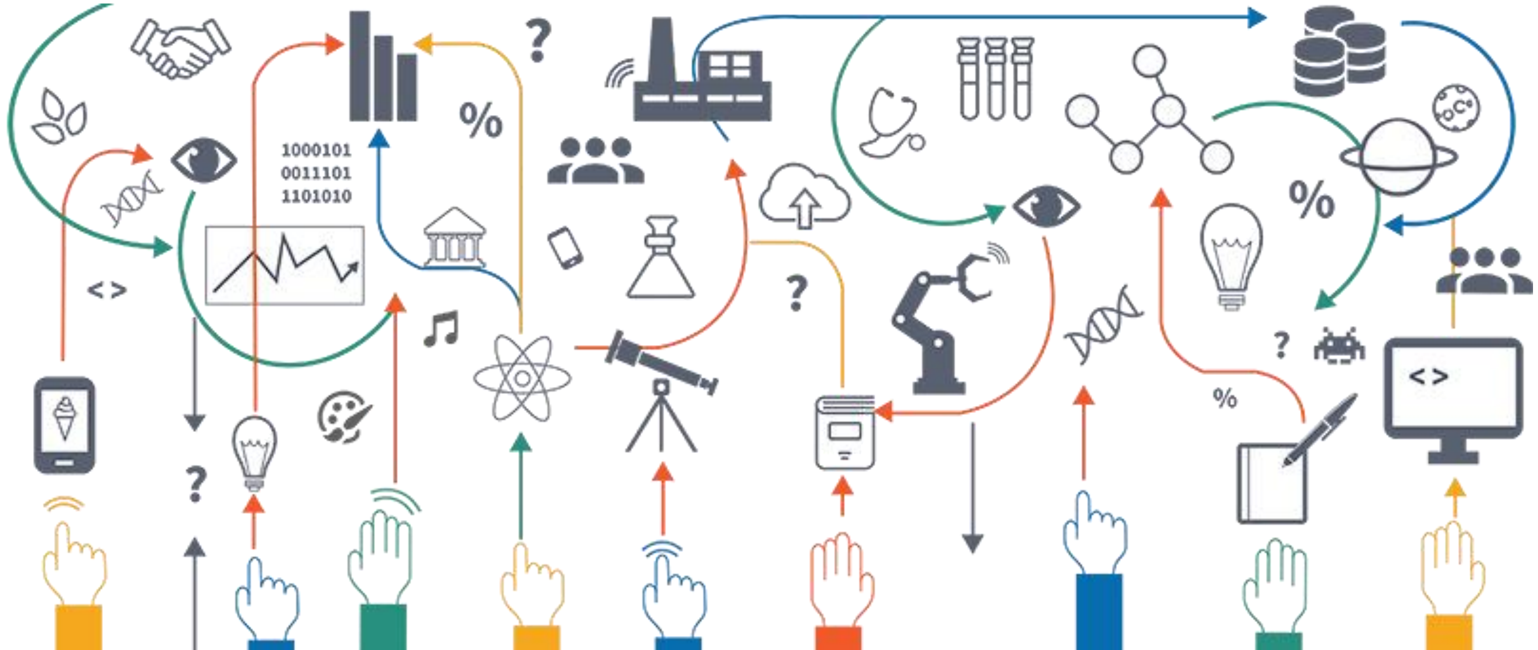


University of Vienna, WiSe 2025

Master’s programme in Data Science

Motivation

In the lecture block on *Function Approximation and Supervised Learning*, we identified the following inequality for the risk:

$$R(\hat{h}) \leq \sup_{h\in\mathcal{H}} \left| R(h) - \hat{R}(h) \right| + \inf_{g\in\mathcal{H}} \hat{R}(g)$$

The second term is the **interpolation error**. In the *Deep Neural Networks* block, we introduced the concept of **affine pieces** to bound it!

But how can we bound the first term: **the generalization error**?

Content

- Reminder: Hoeffding’s inequality
- PAC learning
- Covering numbers
- Overfitting in the under-and overparametrized regime
- Appendix: VC dimension

Return of the Hoeffding's inequality

In the lecture block *Foundations of Probability Theory*, we discussed Hoeffding's inequality:

Hoeffding's inequality: Assume independent random variables $x_1, x_2, \ldots, x_m$ from the same distribution and finite support $x \in [a, b]$. Then:

$$P\left(\left| \frac{1}{m} \sum_i x_i \ - \mathrm{E}(x_1) \right| \geq \epsilon \right) \leq 2\, e^{-\frac{2m\epsilon^2}{(b-a)^2}} \quad \forall \epsilon > 0$$

Observation:
The risk $R(h)$ is an **expectation value**,
and the empirical risk the corresponding **arithmetic mean**!
If we restrict the loss function to be between, e.g., [0,1], then the risk is an expectation value of a random variable with **finite support**!

→ **Hoeffding's inequality applies! :)**

Learning bound: finite hypothesis set

Equipped with this knowledge, lets assume we have a finite hypothesis set $\mathcal{H}$. We start with the probability that the supremum is larger than some certain error $\epsilon > 0$:

$$p\left(\sup_{h\in\mathcal{H}}\left|R(h)-\hat{R}(h)\right| \geq \epsilon\right) \leq \sum_{h\in\mathcal{H}} p\left(\left|R(h)-\hat{R}(h)\right| \geq \epsilon\right) \leq \sum_{h\in\mathcal{H}} 2\,e^{-2m\epsilon^2} \leq |\mathcal{H}|2e^{-2m\epsilon^2} = \delta$$

Union bound:
$p(\text{largest one} \geq \epsilon) \leq p(\text{at least one} \geq \epsilon)$

Hoeffding

# training samples

With this, we get:

Let $\mathcal{H}$ be a finite hypothesis set. Then for every $\delta > 0$, the following inequality holds with probability at least $1-\delta$ for all $h \in \mathcal{H}$:

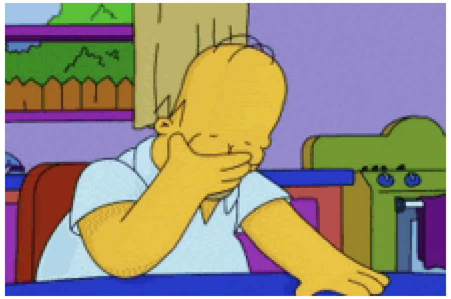
$$\left|R(h)-\hat{R}(h)\right| \leq \sqrt{\frac{\ln(|\mathcal{H}|)+\ln\left(\frac{2}{\delta}\right)}{2m}} = \epsilon$$

PAC Learning

Learning algorithms that have such a learning bound are also known as **PAC learnable**:

Probably Approximately Correct

$1 - \delta$ ϵ



We can squeeze out some more by solving ϵ for the number of training samples m:

Let $\mathcal{H}$ be a finite hypothesis set. Then for every $\delta > 0$ and $\epsilon > 0$, we have for all $h \in \mathcal{H}$

$$p\left(\left|R(h) - \hat{R}(h)\right| \leq \epsilon\right) \geq 1 - \delta$$

if we have at least $m \geq \frac{\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right)}{2\epsilon}$ training samples.

Problem: what happens in the limit of infinite hypotheses?

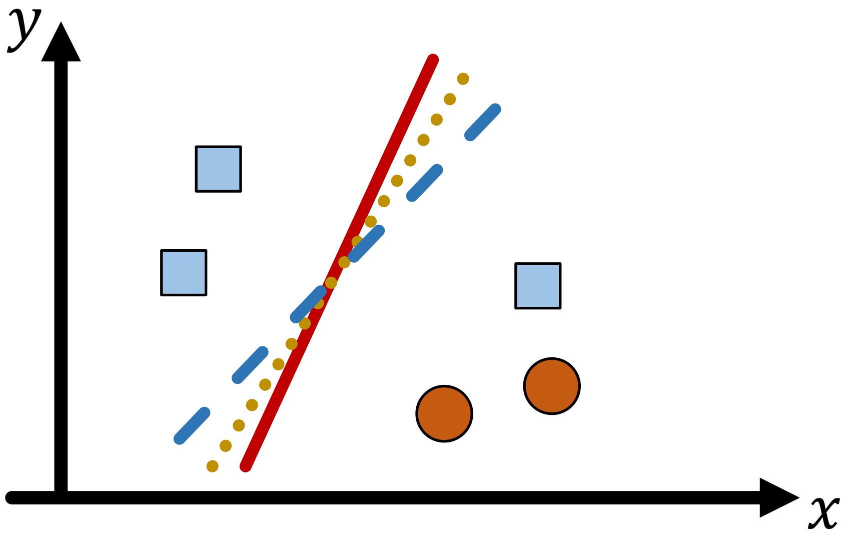
$$\sup_{h\in\mathcal{H}}\left|R(h)-\hat{R}(h)\right| \le \sqrt{\frac{\ln(|\mathcal{H}|)+\ln\left(\frac{2}{\delta}\right)}{2m}}$$

The bound goes to infinity!

But why? Obviously linear regression, neural networks, etc. all generalize to some degree!

Reason: we assumed independence of the hypotheses! But what if two hypotheses have very similar outputs for all possible inputs? We shouldn't count them separately!

Illustration: classification



All lines shown here produce similar outputs!

Thus, instead of counting them individually, we should count them as **"one class" of "equivalent" functions**!

Covering number

Let's formalize this!

Assume we have our hypothesis set $\mathcal{H}$. We will now decompose the set into "equivalence" classes. Per class $C_k \subset \mathcal{H}$, we have one representative function $h_k \in \mathcal{H}$ such that for all $h \in C_k, |h - h_k|_\infty < \kappa$ for $\kappa > 0$.

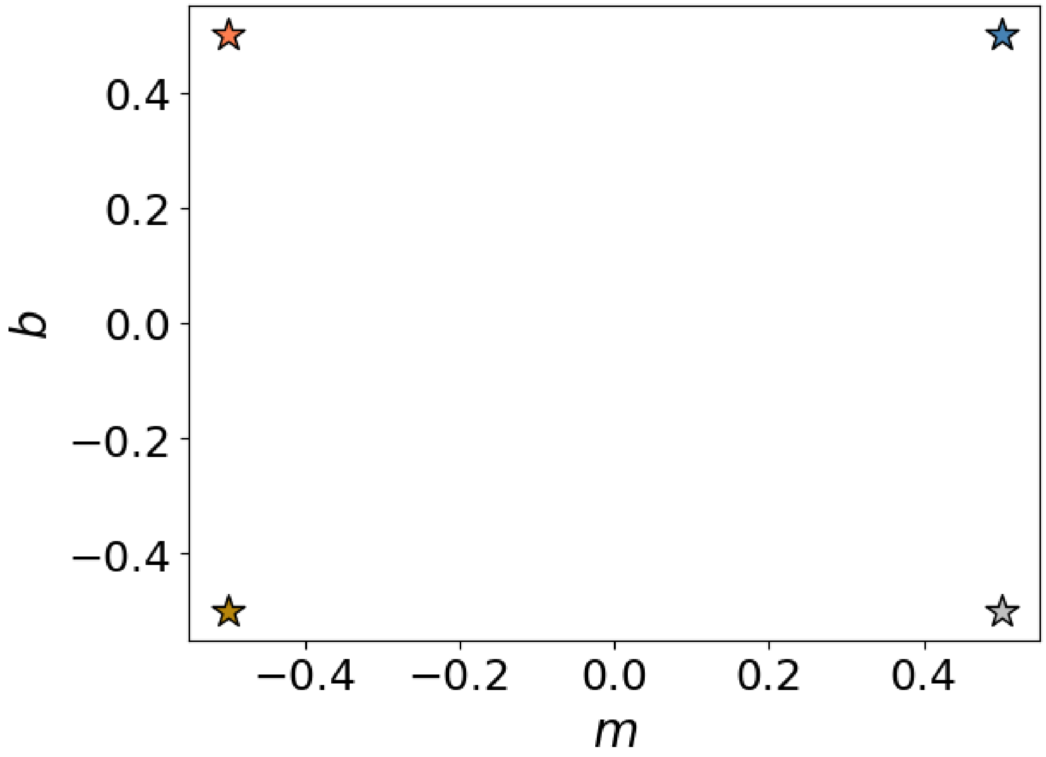
The covering number $d_C(\kappa)$ is the minimum number of classes k required to **fully cover** $\mathcal{H}$, i.e., such that "$\bigcup_{i=1}^{k} C_k = \mathcal{H}$" up to error κ.

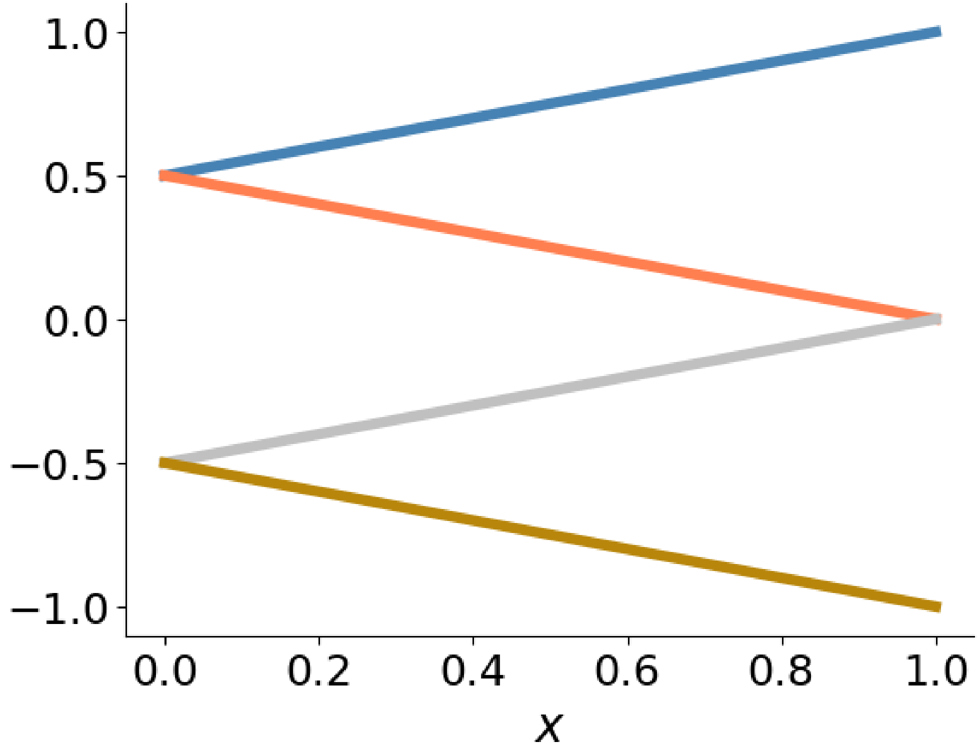
Example

Linear regression: $f_{m,b}(x) = mx + b$ with $m \in [-0.5, 0.5], b \in [-0.5, 0.5], x \in [0,1]$.

Assume $\kappa = 0.5$. Then the following four functions cover all realizations of f:

$$f_{0.5,0.5}, f_{-0.5,0.5}, f_{0.5,-0.5}, f_{-0.5,-0.5}$$





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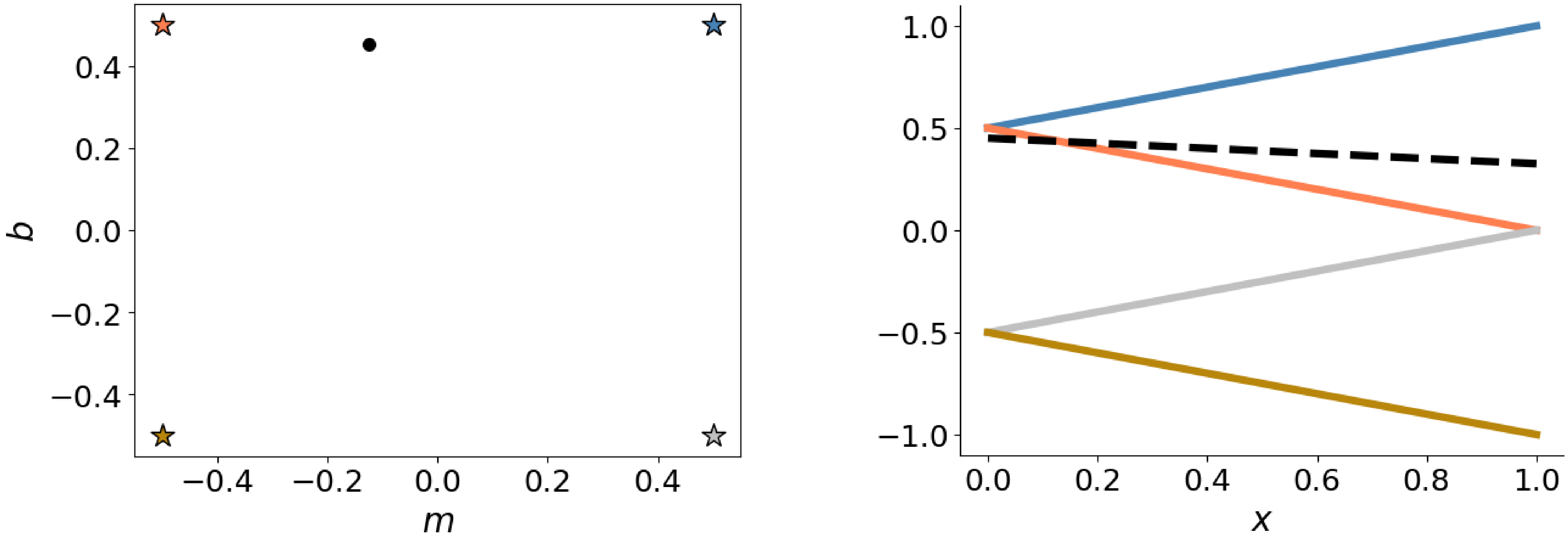

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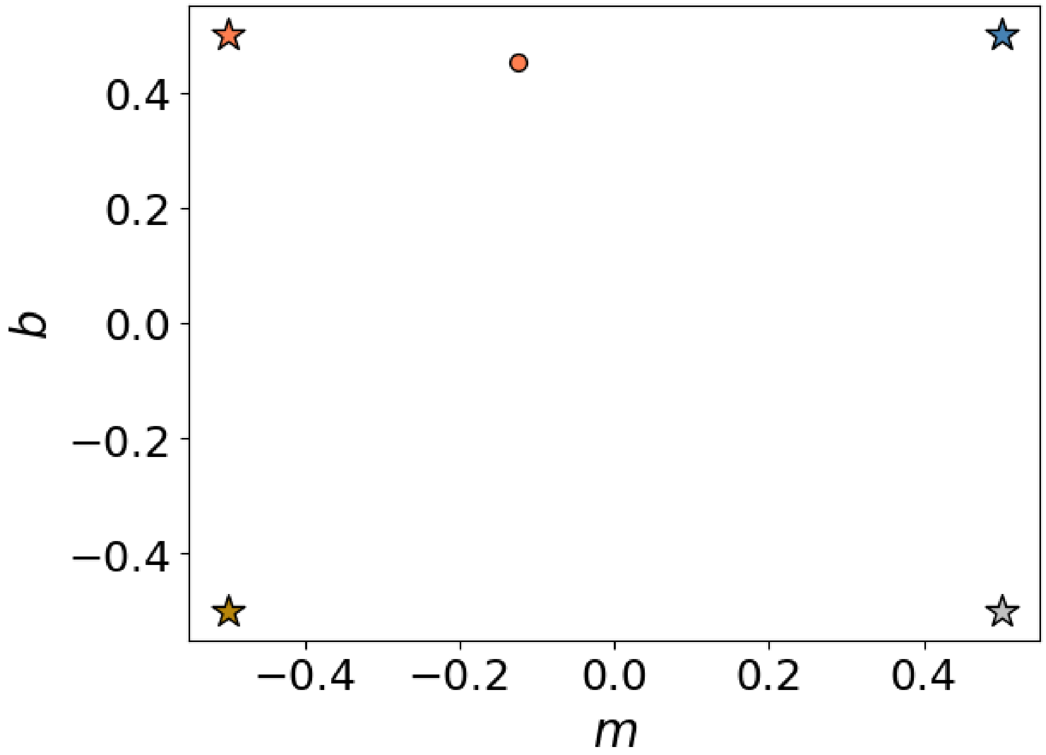

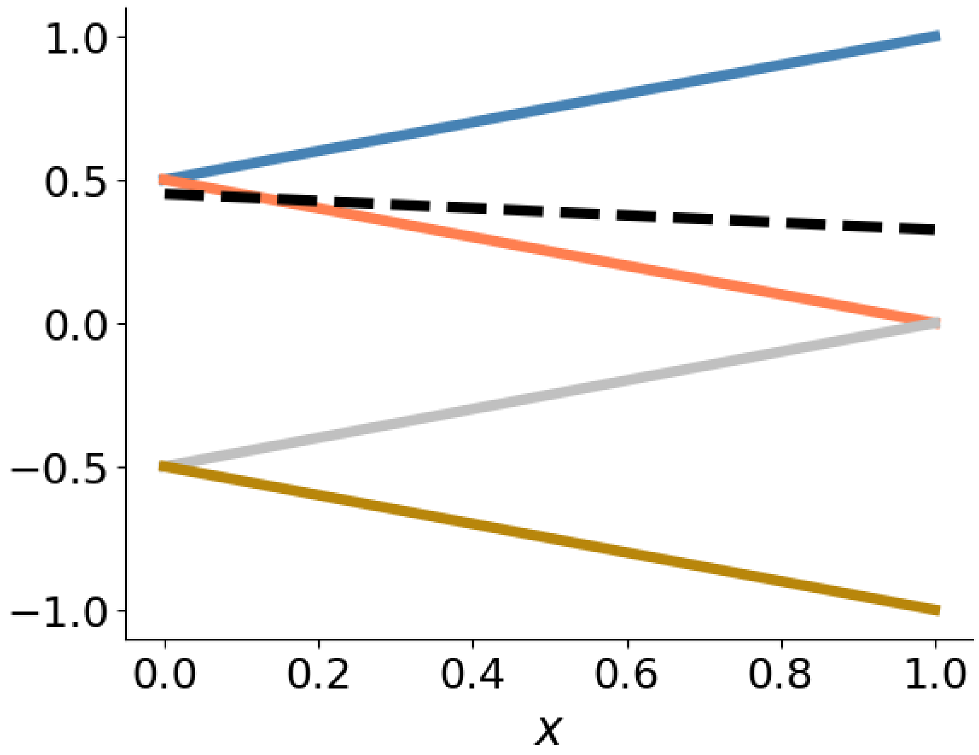

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Assume $\kappa = 0.5$. Then the following four functions cover all realizations of f:

assign random functions to one of the four classes such that the distance is smaller than κ

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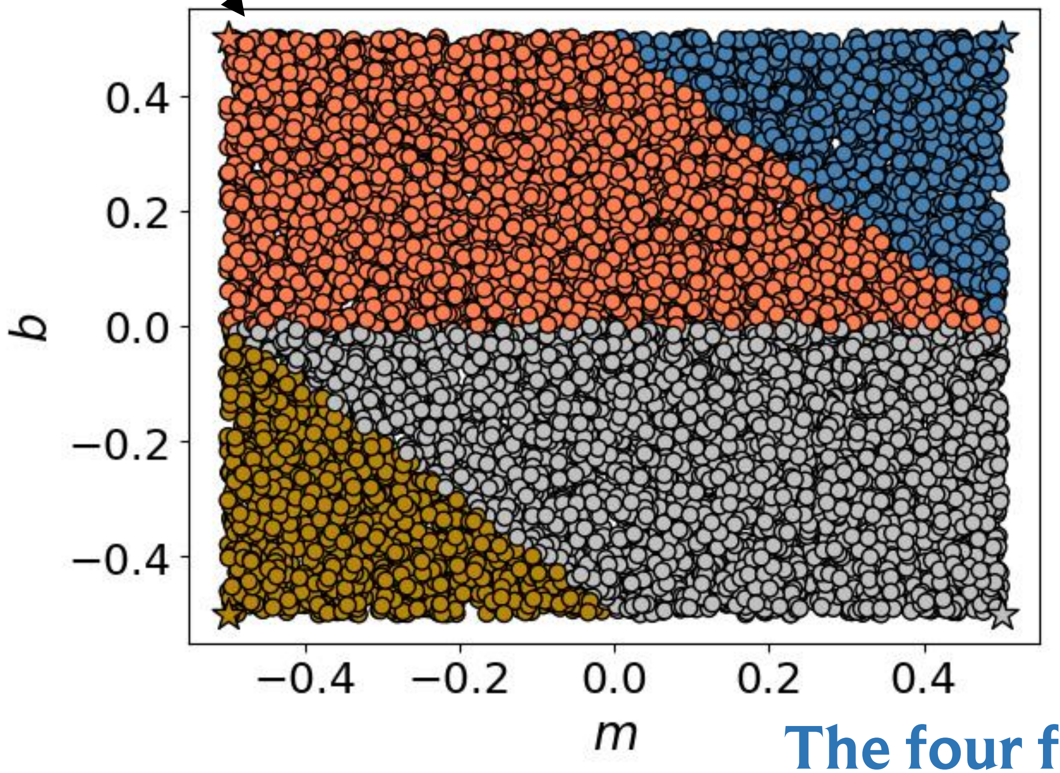
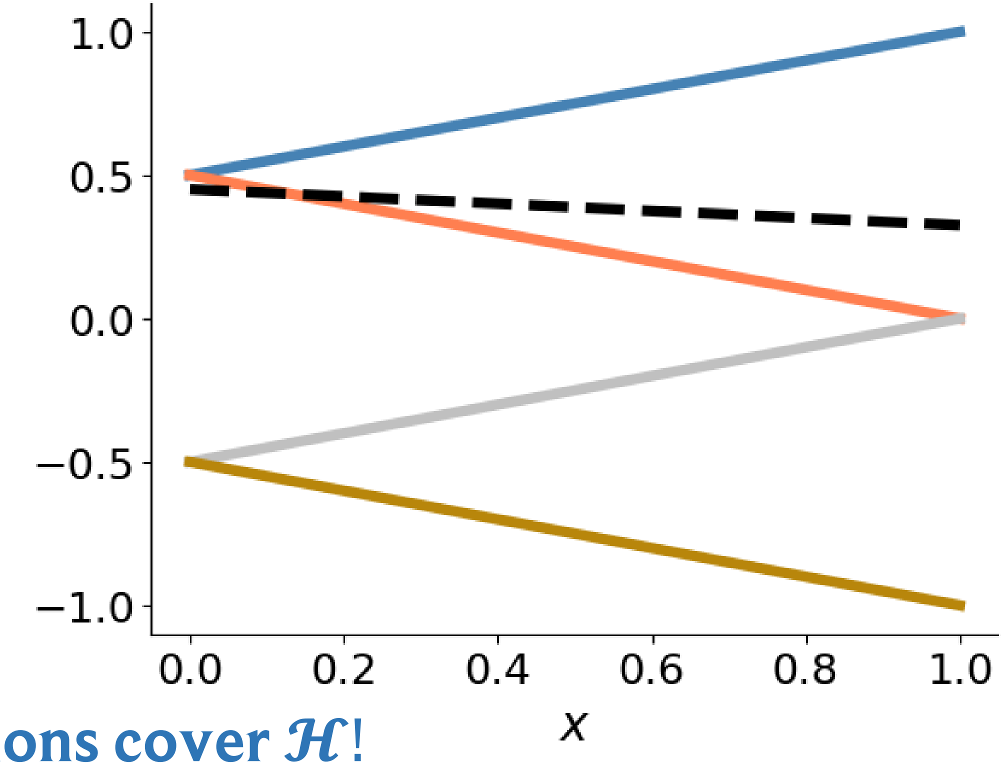




The four functions cover $\mathcal{H}$!

Learning bound: covering numbers

Previously, we had:

Let $\mathcal{H}$ be a finite hypothesis set. Then for every $\delta > 0$, the following inequality holds with probability at least $1 - \delta$ for all $h \in \mathcal{H}$:

$$\left|R(h) - \hat{R}(h)\right| \leq \sqrt{\frac{\ln(|\mathcal{H}|) + \ln(2/\delta)}{2m}}$$

Using covering numbers, we get *(using a rather similar derivation)*:

Let $\mathcal{H}$ be a hypothesis set with covering number $\mathcal{G}$. Then for every $\delta > 0$, and for C_L-Lipschitz loss function with output range $[-C, C]$, we have with probability at least $1 - \delta$ for all $h \in \mathcal{H}$ and m training data samples:

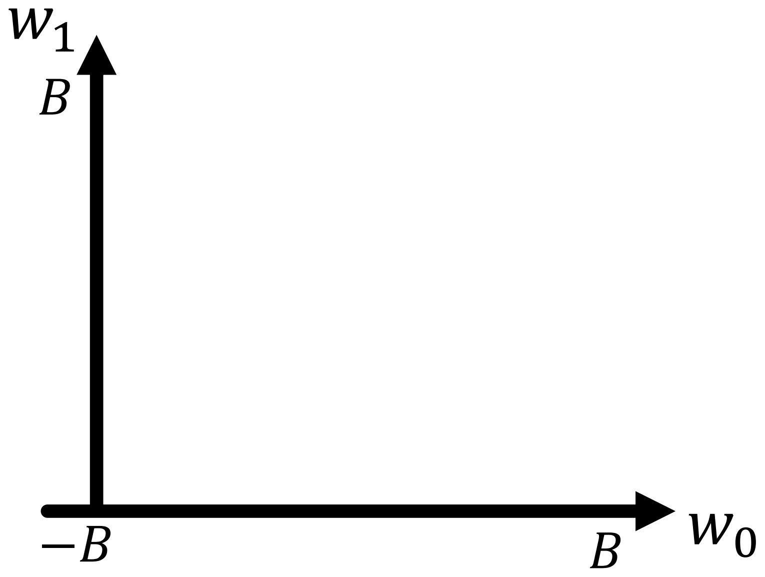
$$\left|R(h) - \hat{R}(h)\right| \leq 4C \cdot C_L \cdot \sqrt{\frac{\ln \mathcal{G} + \ln(2/\delta)}{m}} + \frac{2C_L}{m^{\alpha}}$$

size of the "balls" κ we use for covering $\mathcal{H}$

Covering numbers from Lipschitz constants

If our neural network is ***C*-Lipschitz in the parameters** *(which it is for most activation functions used in practice),* then there is a clever way of **bounding the covering number**!

Taking the reverse route: cover the parameter space!
→ Find w_i such that for all $w \in [-B, B]^n$, there is at least one α_i with $|w - \alpha_i|_\infty \leq \frac{\kappa}{C}$.



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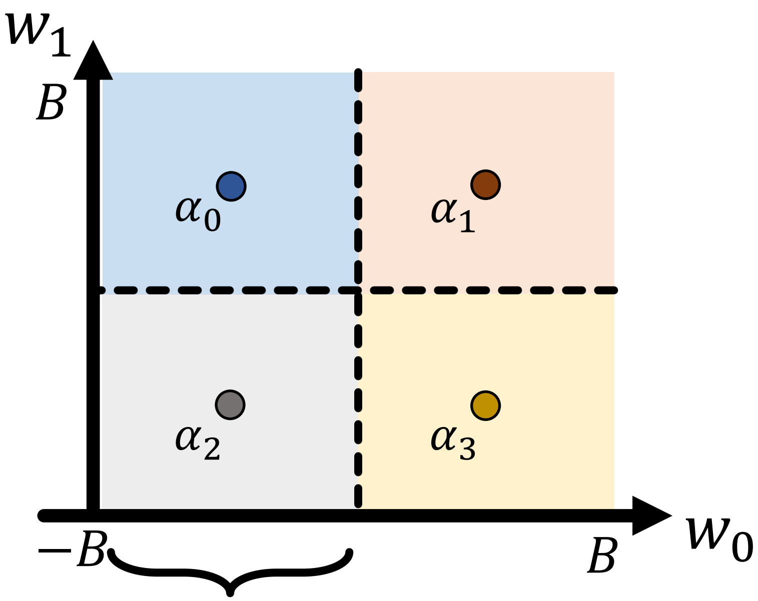

Size: κ/C

Thus: $\mathcal{G} \leq (B \cdot C/\kappa)^n$ = # of boxes here

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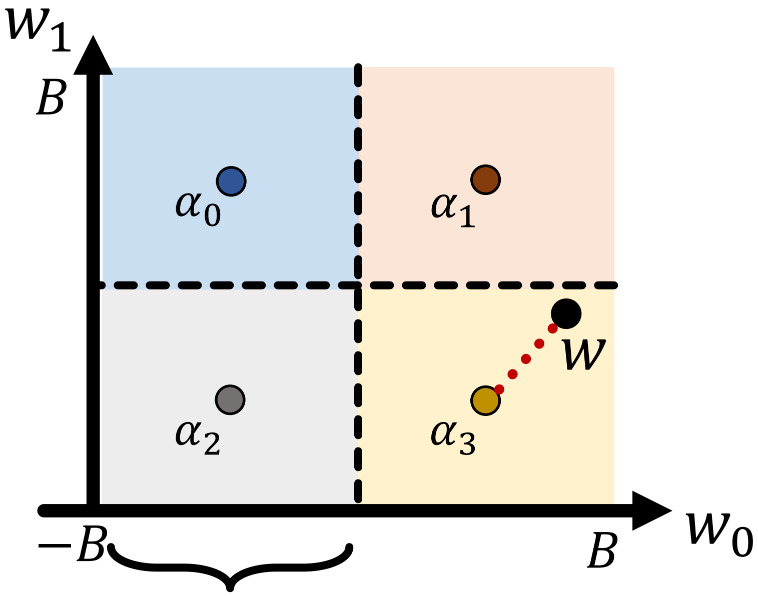
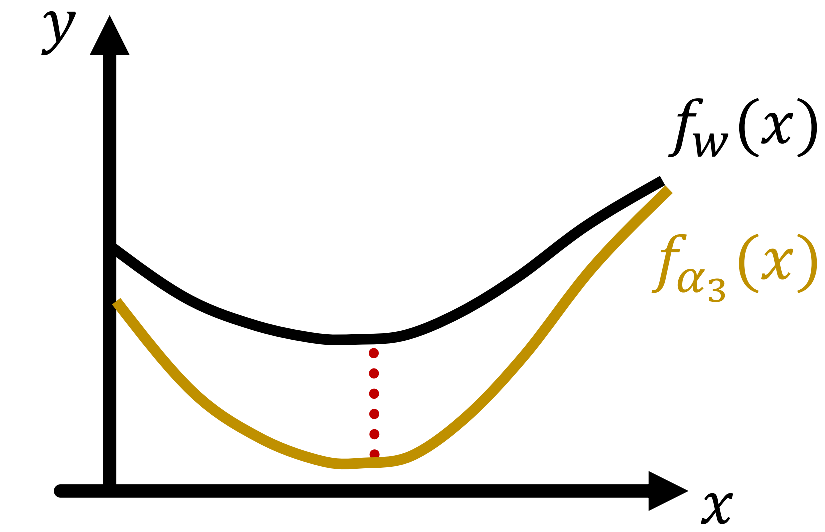


Size: κ/C

Thus: $\mathcal{G} \leq (B \cdot C/\kappa)^n = \#$ of boxes here

Look at any w!



Via Lipschitz property, we have
$\left|f_w(x) - f_{\alpha_i}(x)\right|_\infty \leq C|w - \alpha_i|_\infty = \kappa$,
→ **We also covered $\mathcal{H}$**!

Finale: Lipschitz constant of ReLU neural networks

A ReLU neural network with n parameters, max. width d, L layers, an activation function with Lipschitz constant C_ϕ, and parameters constrained to $[-B, B]$, has Lipschitz constant:

1. If $B \geq 1$: $C = n \cdot \left(2\, C_\phi B\, d\right)^L$
2. If B > 0: $C = C_\phi^L \cdot (B\, d)^{L+1}$

From which we get the covering numbers, e.g.,:

1. If $B \geq 1$: $\mathcal{G} \leq (n/\kappa)^n \cdot \left(2\, C_\phi B\, d\right)^{n \cdot L}$
2. If B > 0: $\mathcal{G} \leq \left(C_\phi^L/\kappa\right)^n \cdot (B\, d)^{nL+n}$

These can be simply inserted into our generalization bounds!

Outro: data science in the overparametrized regime

Classical piece of wisdom: the more parameters your model has, the more expressive it is. However, with many more parameters than training data, it will start overfitting!

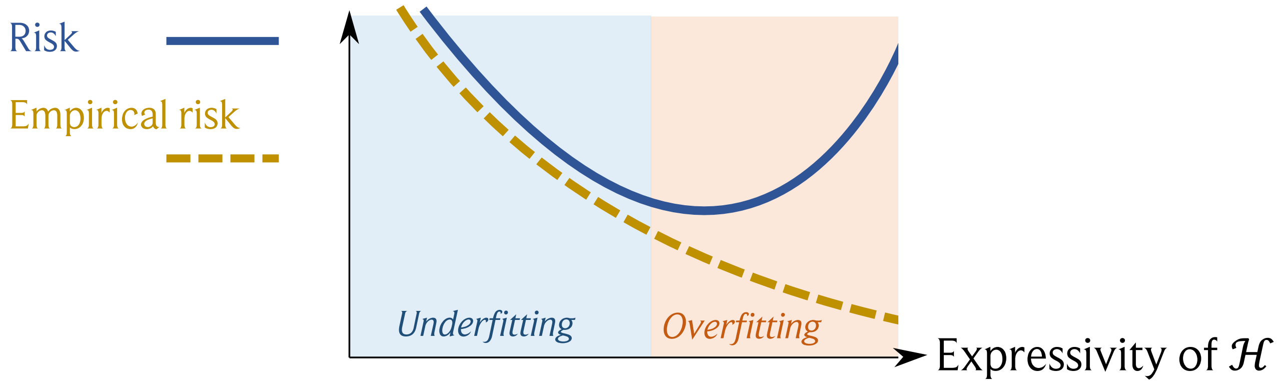


Image adapted from: Philipp Petersen, Jakob Zech. Mathematical theory of deep learning (2025)

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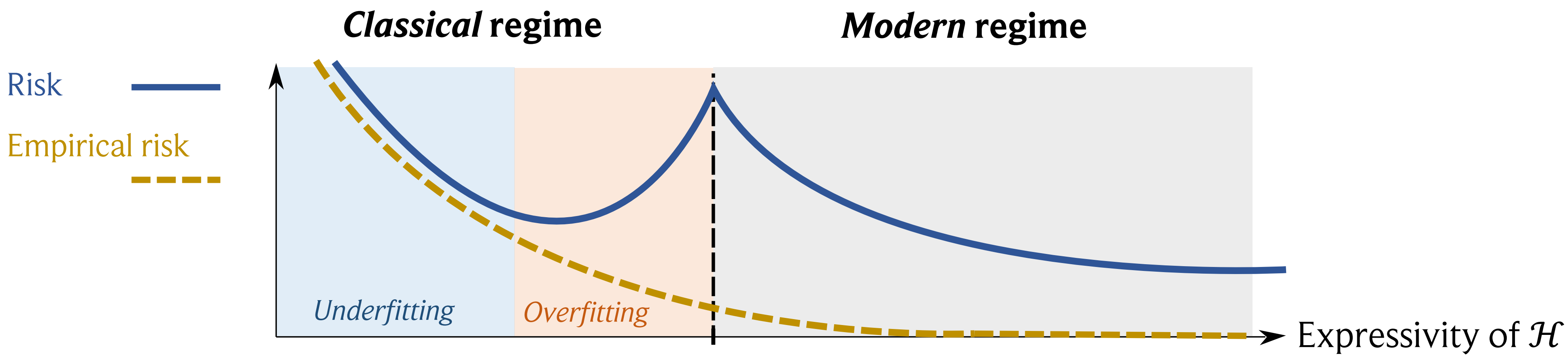


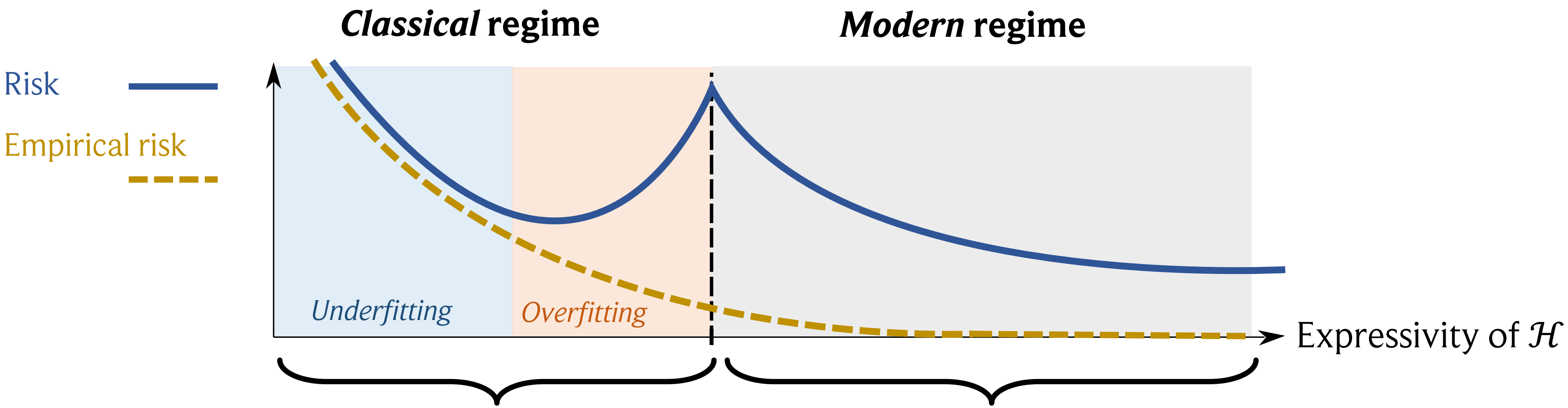
However, in practice we observe that highly overparametrized models can generalize well! A famous phenomena is the above curve, called **"double descent"** .

Note that this phenomenon is **not exclusive to neural networks**:
one can recreate it for linear models, polynomials, regression with basis functions, etc.!

There are several explanations for this behaviour … we will briefly touch on one of them.

Image adapted from: Philipp Petersen, Jakob Zech. Mathematical theory of deep learning (2025)

One explanation: the power of many, small parameters



Only few parameters, which potentially have to be large to fit the data. We have:

$$\mathcal{G} \leq (n/\kappa)^n \cdot \left(2\, C_\phi B\, d\right)^{n \cdot L}$$

Generalization bound depends on # parameters!

Many parameters, so they can be quite small*

(large values are obtained by summing up many inputs!)

Thus, we can choose $B \leq \left(d\, C_\phi\right)^{-1}$, leading to $C \approx 1$.
The hypothesis set of C-Lipschitz functions (here: $C = 1$) has a covering number** that only depends on the # input features d_0:

$$\log \mathcal{G} \leq \alpha \kappa^{-d_0} \qquad \text{with constant } \alpha > 0$$

Generalization bound is constant w.r.t. # parameters!
We see a decrease since the empirical risk still improves.

* *Note that most types of regularization ensure small weights (L1, L2, etc.)! We also often initialize neural networks with weight scales that depend on the width!*
** *Both bounds shown here are valid for both regimes. We get the "double" curve by choosing the bound that is smaller!*

Image adapted from: Philipp Petersen, Jakob Zech. Mathematical theory of deep learning (2025)