

Generalization Bounds

Theoretical Foundations of Deep Learning

Matteo Mazzarelli

December 17, 2024



Introduction

Motivation

- ▶ **Core Question:** How can models trained on limited data perform reliably on unseen scenarios?
- ▶ **Generalization** is a fundamental goal in machine learning: ensuring models extend their learned patterns to new, unseen data.
- ▶ A poorly generalized model risks:
 - ▶ **Overfitting:** Performing well on training data but poorly on unseen data.
 - ▶ **Underfitting:** Failing to capture the underlying patterns of the data.

The Learning Problem

- ▶ **Supervised Learning:**
 - ▶ Goal: Learn a function $f : X \rightarrow Y$ mapping inputs X to outputs Y based on labeled training data.
- ▶ **Key Question:** Can the learned function perform well on unseen data?
- ▶ **Generalization:**
 - ▶ Ability of a model to extend its learning beyond the training data.
 - ▶ **Central Problem** in machine learning: balancing *empirical performance* with *future predictions*.

Overfitting

Simulating Overfitting

- ▶ **Objective:**
 - ▶ Visualize the impact of model complexity on overfitting in a linear regression model.
- ▶ **Dataset**
 - ▶ The experiment uses the **Boston Housing dataset**, where the target variable is `medv` (median value of owner-occupied homes), and the 13 features represent housing characteristics.

► **Experimental Setup:**

► **Model Complexity:**

- Complexity is defined by the number of features included in the model.
- Additional random features are generated to simulate increasing complexity beyond the real features in the dataset.

► **Train-Test Split:**

- The dataset is split into 70% training and 30% test data.

► **Range of Complexity:**

- Models are trained with 1 to 200 features. Beyond the actual features in the dataset, random noise features are added incrementally.

- ▶ **Procedure:** For each level of complexity:
 1. A subset of features (real and random) is used to train a linear regression model.
 2. Predictions are made on both the training and test datasets.
 3. Mean Squared Errors (MSE) are calculated for both datasets.
- ▶ **Results:**
 - ▶ Training error decreases consistently as model complexity increases.
 - ▶ Test error initially decreases but then increases, demonstrating the overfitting phenomenon.
- ▶ **Visualization:**
 - ▶ A line plot shows the relationship between model complexity (number of features) and mean squared error for both the training and test datasets.

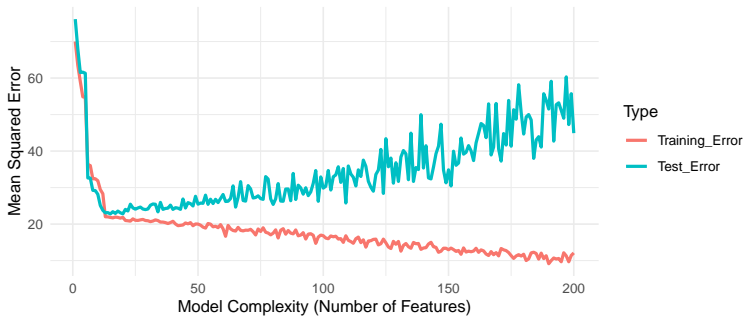


Figure 1: Overfitting Phenomenon in Linear Regression

► **Highlights:**

- The **bias-variance tradeoff**.
- The point where overfitting begins, indicated by the divergence of training and test errors.

Key Insights

- ▶ Increasing model complexity without consideration of the underlying data structure can lead to overfitting.
- ▶ Simple models that focus on the true underlying pattern often generalize better to unseen data.

Double Descent

- ▶ However, modern machine learning introduces a fascinating twist: **Double Descent**, where increasing model complexity can sometimes lead to improved generalization after an initial overfitting phase.
- ▶ Unlike traditional models where increasing complexity leads to overfitting, further increasing the complexity (e.g., using overparameterized neural networks) can eventually reduce the generalization error after an initial peak.
- ▶ This challenges the classical view of overfitting and highlights the complex relationship between model complexity and generalization in modern machine learning.

Classical Bounds

Introducing Generalization Bounds

- ▶ **What Are Generalization Bounds?**
 - ▶ Theoretical tools offering guarantees about a model's performance on unseen data.
 - ▶ Relate:
 - ▶ **Generalization Error**: How well the model performs on unseen data.
 - ▶ **Empirical Risk**: Performance observed on training data.
 - ▶ **Model Complexity**: How expressive the model is.

► **Purpose:**

- Provide insights into the trade-offs between:
 - **Model Accuracy:** How well the model captures the data patterns.
 - **Model Complexity:** The expressiveness of the model and its ability to fit intricate patterns.
 - **Training Data Size:** How much data is required to achieve reliable generalization.

Hoeffding's Inequality: A Starting Point

- ▶ **What is Hoeffding's Inequality?**
 - ▶ A fundamental result in probability theory used to bound the difference between the **empirical risk** and the **generalization error** for a fixed hypothesis.
 - ▶ Provides a way to measure how closely a model's performance on training data reflects its performance on unseen data.

Mathematical Formulation of Hoeffding's Inequality

► Hoeffding's Inequality:

$$P(|R(h) - R_{\text{emp}}(h)| > \varepsilon) \leq 2 \exp(-2m\varepsilon^2)$$

- $R(h)$: Generalization error (true performance on unseen data).
- $R_{\text{emp}}(h)$: Empirical risk (error on training data).
- ε : A small positive value (tolerance).
- m : Size of the dataset.

Key Insights

- ▶ The probability that the generalization error $R(h)$ deviates significantly from the empirical risk $R_{\text{emp}}(h)$ decreases **exponentially** with:
 - ▶ Larger dataset size m .
 - ▶ Smaller tolerance ε .

Rates of Convergence

► What Are Rates of Convergence?

- Quantify how quickly the generalization error approaches the empirical risk as the dataset size m grows.
- Provide a guideline for determining the dataset size needed to achieve a desired level of generalization.
- In Hoeffding's inequality:

$$P(|R(h) - R_{\text{emp}}(h)| > \varepsilon) \leq 2 \exp(-2m\varepsilon^2)$$

- The **exponential term** $\exp(-2m\varepsilon^2)$ shows that the convergence is faster with larger datasets.

► Key Factors:

- **Dataset Size (m)**: Larger datasets reduce the gap between $R(h)$ and $R_{\text{emp}}(h)$ more quickly.
- **Tolerance (ε)**: Smaller tolerances require larger datasets for the same level of confidence.

Interpretation of Hoeffding's Inequality

► What Does It Mean?

- As the dataset size (m) increases, the empirical risk becomes a more reliable indicator of the generalization error.
- For a fixed hypothesis, we can be confident that the performance observed on training data is close to what can be expected on unseen data.
- The **rate of convergence** shows how quickly this reliability improves as m grows.

Key Insights

- ▶ Hoeffding's inequality gives a **quantitative guarantee** about the relationship between training performance and unseen data performance.
- ▶ Understanding convergence rates helps in planning how much data is needed for robust generalization.

Limitations of Hoeffding's Inequality

- ▶ **Beyond Fixed Hypotheses:**
 - ▶ Hoeffding's inequality assumes a single, fixed hypothesis.
 - ▶ In practice, machine learning involves selecting the best hypothesis from a **large hypothesis class** \mathcal{H} , increasing the risk of overfitting.
- ▶ **Need for Complexity-Aware Bounds:**
 - ▶ Simple bounds like Hoeffding's do not consider the complexity of the hypothesis class, which influences generalization.

The Union Bound

- ▶ **What is the Union Bound?**
 - ▶ A probability tool used to extend bounds like Hoeffding's inequality to apply across an entire hypothesis space \mathcal{H} .
 - ▶ Helps estimate the probability that **at least one hypothesis** in \mathcal{H} has a large generalization gap.
- ▶ **Key Idea:**
 - ▶ Instead of considering a single fixed hypothesis, the Union Bound aggregates the probabilities of generalization gaps over all hypotheses in \mathcal{H} .

Formalization of The Union Bound

► Mathematical Expression:

$$P\left(\sup_{h \in \mathcal{H}} |R(h) - R_{\text{emp}}(h)| > \epsilon\right) \leq \sum_{h \in \mathcal{H}} P(|R(h) - R_{\text{emp}}(h)| > \epsilon)$$

- $\sup_{h \in \mathcal{H}}$: The supremum ensures we account for the worst-case scenario across all hypotheses.
- $P(|R(h) - R_{\text{emp}}(h)| > \epsilon)$: The probability of a significant generalization gap for each hypothesis.
- **How It Works:**
 - By summing up the probabilities for all hypotheses, the Union Bound provides a way to analyze the worst-case scenario over the hypothesis space.

Implications of The Union Bound

- ▶ **Impact of Hypothesis Space Size:**
 - ▶ The bound depends directly on the **size of the hypothesis space** $|\mathcal{H}|$.
 - ▶ Larger hypothesis spaces increase the sum, making the bound looser.
- ▶ **Takeaway:**
 - ▶ The Union Bound highlights a trade-off:
 - ▶ **Small hypothesis space:** Tighter bounds, but limited model capacity.
 - ▶ **Large hypothesis space:** Higher capacity, but risk of overfitting and looser bounds.

Transition to Advanced Bounds

- ▶ **Connection to Practical Learning:**
 - ▶ In practice, hypothesis spaces are often infinite or too large to enumerate explicitly. This motivates the need for alternative ways to measure hypothesis complexity.
- ▶ **From Simple to Sophisticated:**
 - ▶ The Union Bound provides a conceptual basis for understanding how hypothesis space size affects generalization.
 - ▶ Next, we delve into **complexity measures** that allow us to extend generalization bounds to more practical, infinite hypothesis spaces.

Advanced Bounds

Motivation for Advanced Bounds

- ▶ **Advanced bounds** address a variety of the limitations we have outlined by incorporating:
 - ▶ **VC Dimension:** A measure of the capacity or expressiveness of a hypothesis class. Higher VC dimensions indicate more complex models, which may require more data to generalize well.
 - ▶ **Rademacher Complexity:** A data-dependent measure of how well a hypothesis class can fit random noise in the training data. It captures both the hypothesis class and the specifics of the data distribution.

► Extending Convergence Rates:

- Advanced bounds refine the rates of convergence by linking the generalization error to:
 - The size of the dataset m .
 - The complexity of the hypothesis class (e.g., **VC dimension** or **Rademacher complexity**).
- For example, the generalization error is often bounded as:

$$R(h) - R_{\text{emp}}(h) \leq \mathcal{O} \left(\sqrt{\frac{\text{Complexity}(\mathcal{H})}{m}} \right)$$

- Larger datasets m reduce error, but higher complexity increases the required data for a desired level of generalization.

► Practical Implications:

- These bounds provide actionable insights for balancing model complexity and dataset size.

Vapnik-Chervonenkis (VC) Theory

► Growth Function

- The **Growth Function** is a measure of the expressiveness of a hypothesis space \mathcal{H} .
- **Definition:**
 - The growth function, $\Pi_{\mathcal{H}}(m)$, is the maximum number of distinct ways a hypothesis space can label m data points.
- **Key Idea:**
 - A more expressive hypothesis space can label datasets in a greater number of ways, indicating higher complexity.
- **Growth Behavior:**
 - For small m , $\Pi_{\mathcal{H}}(m) = 2^m$.
 - For larger m , the growth may be limited by the structure of \mathcal{H} .

▶ VC Dimension

▶ The **VC Dimension** is a scalar value that quantifies the capacity of a hypothesis space \mathcal{H} .

▶ Definition:

▶ The VC dimension d_{VC} is the size of the largest dataset that can be **shattered** by \mathcal{H} .

▶ Shattering:

▶ A dataset is shattered if every possible labeling of the dataset can be perfectly captured by hypotheses in \mathcal{H} .

▶ Examples:

▶ A linear classifier in 2D space has a VC dimension of 3 (it can shatter any 3 points, but not all configurations of 4 points).

VC Generalization Bound

► What is the VC Generalization Bound?

- A theoretical result that connects the **generalization error** with the **empirical risk**, the **VC dimension**, and the size of the dataset.
- **Mathematical Formulation:**

$$R(h) \leq R_{\text{emp}}(h) + \sqrt{\frac{8d_{\text{VC}} \left(\ln \left(\frac{2m}{d_{\text{VC}}} \right) + 1 \right) + 8 \ln \left(\frac{4}{\delta} \right)}{m}}$$

- $R(h)$: Generalization error.
- $R_{\text{emp}}(h)$: Empirical risk.
- d_{VC} : VC dimension.
- m : Dataset size.
- δ : Confidence level ($1 - \delta$ is the probability that the bound holds).

Key Insights

- ▶ As d_{VC} increases (more complex hypothesis space):
 - ▶ The bound becomes looser, reflecting a higher risk of overfitting.
- ▶ As m increases (larger dataset size):
 - ▶ The bound tightens, improving generalization guarantees.

Summing Up VC Theory

- ▶ **Expressiveness vs. Generalization:**
 - ▶ The VC dimension captures the **expressiveness** of a hypothesis space:
 - ▶ Higher d_{VC} : More complex, more expressive.
 - ▶ A balance is required to avoid overfitting (high complexity) or underfitting (low complexity).
- ▶ **Implications for Learning:**
 - ▶ The VC dimension helps understand:
 - ▶ Why simpler models often generalize better.
 - ▶ Why increasing data size improves generalization, especially for complex models.
- ▶ **Foundation for Algorithm Design:**
 - ▶ VC theory guides the development of learning algorithms by quantifying the trade-offs between hypothesis complexity, data size, and generalization performance.

Distribution-Based Bounds

- ▶ **From General Bounds to Data-Driven Insights:**
 - ▶ Generalization bounds like Hoeffding's inequality and VC bounds rely on worst-case scenarios.
- ▶ **Distribution-Based Bounds:**
 - ▶ Leverage specific properties of the data distribution to achieve **tighter bounds**.
 - ▶ Exploit **data structure** to understand how well a model generalizes in practice.

Example: Support Vector Machines (SVMs)

- ▶ **SVMs and Margin-Based Bounds:**
 - ▶ Support Vector Machines (SVMs) introduce the concept of a **margin**, the distance between the decision boundary and the nearest data points.
 - ▶ **Intuition:**
 - ▶ A larger margin indicates better separation between classes, leading to better generalization.
 - ▶ **Margin-Based Generalization Bounds:**
 - ▶ Generalization error decreases as the margin increases, even for infinite hypothesis spaces.

Alternative Capacity Measures

- ▶ **Why Explore Alternative Measures?**
 - ▶ VC dimension assumes worst-case datasets, often leading to overly conservative bounds.
 - ▶ Alternative measures provide more nuanced insights into hypothesis space complexity, especially for modern machine learning models like neural networks.

► **Examples of Alternative Measures**

1. **Covering Numbers:** The minimum number of small “balls” needed to cover the hypothesis space under a certain metric. Smaller covering numbers indicate a simpler hypothesis space, leading to tighter generalization bounds.
2. **Rademacher Complexity:** Measures the ability of a hypothesis class to fit random noise. A lower Rademacher complexity indicates that the hypothesis space is less prone to overfitting.

► **Next Steps:**

- We want to explore how these theoretical tools are applied to modern machine learning methods.

Key Insights

- ▶ These measures allow for tighter, data-adaptive generalization bounds, particularly useful for complex or large-scale models.
- ▶ There's no one-size-fits-all measure. The choice of capacity measure depends on:
 - ▶ The hypothesis space.
 - ▶ The structure of the data.
 - ▶ The learning algorithm.

Conclusion

References

1. Bousquet, O., Boucheron, S., & Lugosi, G. (2003). Introduction to statistical learning theory. *Advanced Lectures on Machine Learning*.
2. Samir, M. (2016). *A gentle introduction to statistical learning theory*. <https://mostafa-samir.github.io/ml-theory-pt2/>.
3. Vapnik, V. N. (1995). *The nature of statistical learning theory*. Springer.
4. Mohri, M., Rostamizadeh, A., & Talwalkar, A. (2012). *Foundations of machine learning*. MIT Press.