LECTURE 5

GENERALIZATION

from data distributions to Bias-Variance the interpolation threshold

PRESS → OR SPACE.

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Learning outcomes

Distinguish approximating the training data from generalizing to unseen data.

Not comfortable — Very comfortable

Click to respond

Explain datasets as samples from distributions we shape, and the i.i.d. assumption.

Not comfortable — Very comfortable

Click to respond

Distinguish in- from out-of-distribution data, and covariate, concept, and label shift.

Not comfortable — Very comfortable

Click to respond

Explain optimization in the hypothesis space and the bias–variance trade-off.

Not comfortable — Very comfortable

Click to respond

Explain generalization beyond the interpolation threshold, where VC theory fails.

Not comfortable — Very comfortable

Click to respond

Describe how scaling laws make performance predictable and unlocked LLMs.

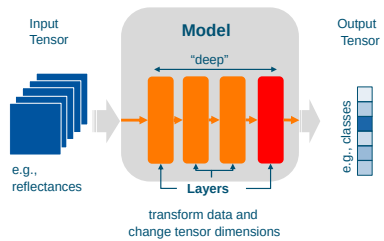
Not comfortable — Very comfortable

Click to respond

Recap Lecture 4

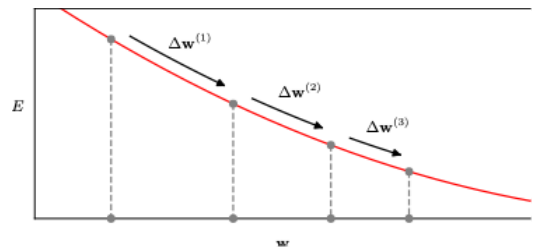
Models

Linear regression → Logistic regression → MLP



Parameter Optimization

Loss → Backpropagation → Gradient descent



Takeaway: We can now fit a model (almost) perfectly to the training data.

But how good will this model be on other data?

Approximation vs Generalization

Approximation

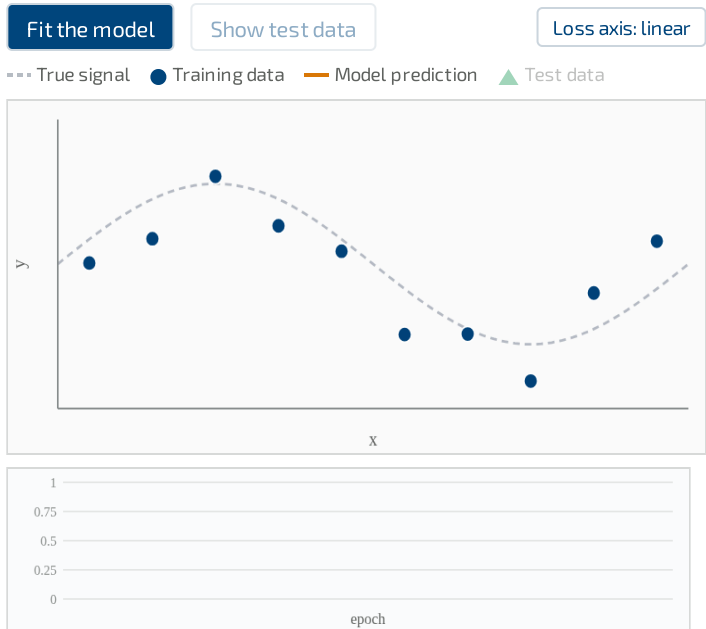
When training, we minimize the empirical risk

$$\widehat{\mathcal{R}}(\theta) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}\big(f_\theta(\mathbf{x}_i), \mathbf{y}_i\big)$$

Generalization

But in practice, we want the population (test) risk to be small

$$\mathcal{R}(\theta) = \mathbb{E}_{(\mathbf{x},\mathbf{y})\sim\mathcal{P}}\mathcal{L}\big(f_\theta(\mathbf{x}), \mathbf{y}\big)$$



A perfect training fit can still generalize poorly.

Today: Three Parts

1

Data Samples and Distributions

How does a dataset relate to the world?

Distributions and the i.i.d. assumption · train, validation, test · in- vs. out-of-distribution · distribution shifts

2

Classical Generalization Theory

When does fitting the training data generalize?

Hypothesis space · Occam's razor · bias–variance trade-off · VC dimension

3

Generalization beyond the Interpolation Threshold

Why do huge models still generalize?

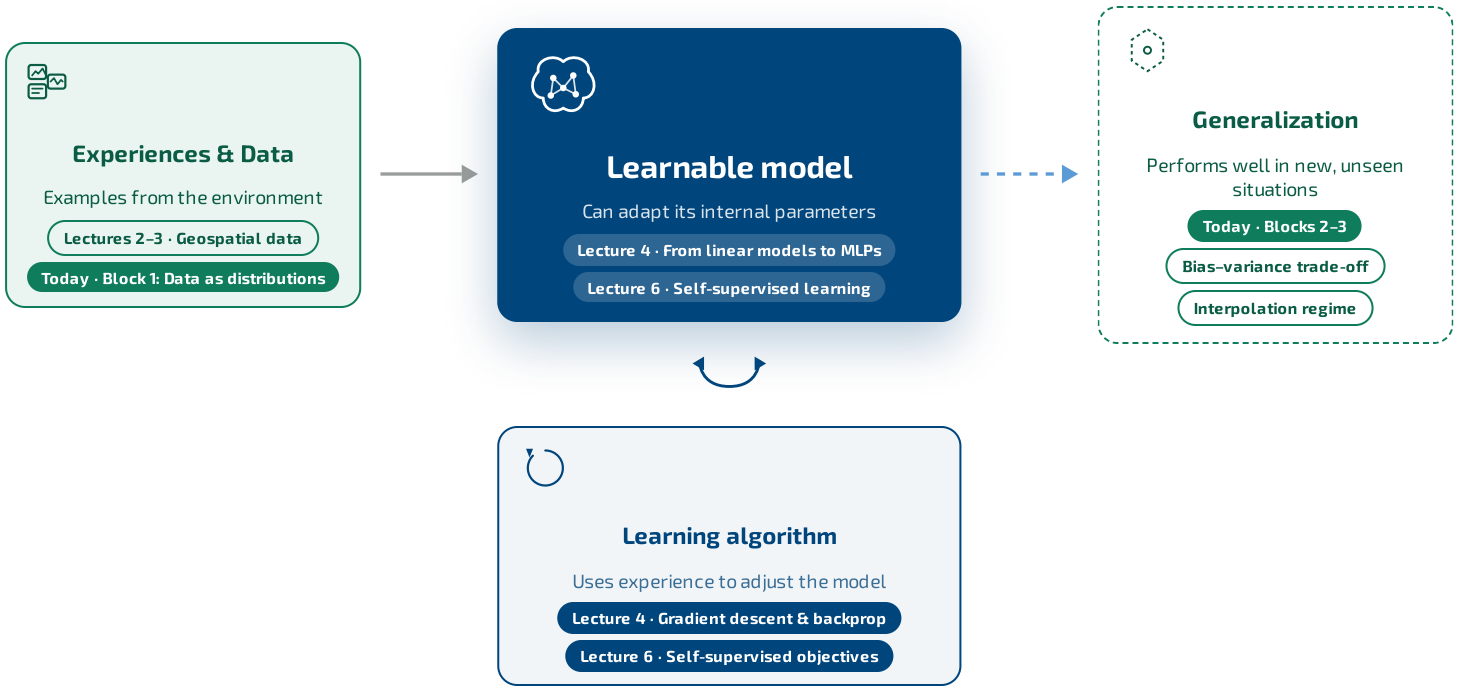
Double descent · effective capacity · inductive biases · scaling laws and the modern AI acceleration

What is wrong here?

👨‍🍳 Takeaway: The Pizza Baker Apprentice does not need to hold 📦 boxes to pick up a 🍕 pizza.



What is needed for a system to learn?



INGREDIENTS FOR LEARNING

SUCCESS CRITERION

Part 1

Data Samples and Distributions



Reality → Distribution → Dataset

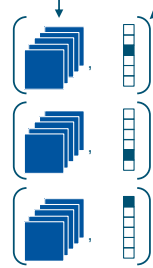
Data we use in machine learning are not the world itself, but **samples drawn** (often imperfectly) from an **underlying distribution**

reality **distribution** **dataset samples**



design → P(X, Y) → sampling → $\mathcal{D} = \{x_i, y_i\}_i^N$

e.g, S2 images e.g., Land Cover



Geospatial Specialists design:

- Which input space X (e.g., S2 satellite)
- Which label space Y (e.g., 16 Land Covers)
- Which distribution P (e.g., location and time)

Reality → Distribution: Generative Perspective

Generative Perspective
(experimental data)

$$P(X, Y) = P(Y)P(X|Y)$$

1. **first** choosing desired **labels/areas of interest** $P(Y)$ e.g., according to a (stratified) strategy
2. **then** generating (i.e., acquiring, downloading) the (image) **data** $P(X|Y)$

e.g., Experimental Flight with UAV



Reality → Distribution: Discriminative Perspective

Discriminative Perspective
(non-experimental data)

$$P(X, Y) = P(X)P(Y|X)$$

1. **first** collecting remote sensing **images** $P(X)$
2. **then** annotating the data through manual **annotation** $P(Y|X)$

e.g., download and annotate of EO data



Data as Samples from a Distribution

Data Distribution → **Data Samples**

machine learning terminology: we "s ample" data

Remote sensing terminology: we " collect " data

supervised case:

$$P(X, Y)$$

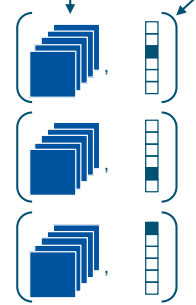
Random Variable X represents input data (e.g., S2 bands)

Random Variable Y represents output data e.g., Land Cover classes or Regression variables

$$\mathcal{D} = \{x_i, y_i\}_i^N$$

e.g, S2 images

e.g., Land Cover



Distribution → Dataset: I.I.D Assumption

Machine Learning Models assume most often that data is sampled **I** dentically and **I** ndependently **D** istributed **(I.I.D)** from the underlying distribution

development time

collected once:

$$\mathcal{D} = \{x_i, y_i\}_{i=1}^{N} \sim P(X, Y)$$

2. random sampling after data collection

then partitioned randomly:

$$\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}} \sim P(X, Y)$$

Distribution → Dataset: In-Distribution Generalization

development time

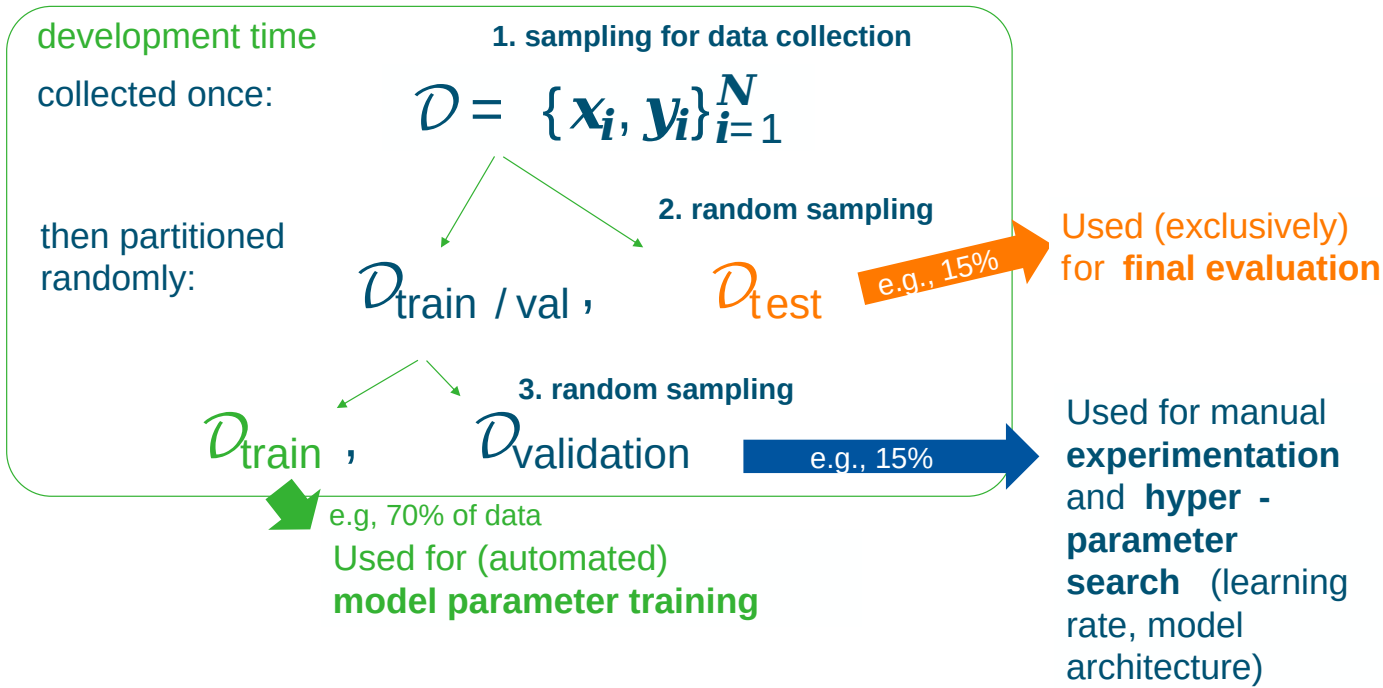
$$\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}} \sim P(X, Y)$$

Test the model's generalization **in-distribution**

trained model

Random Sampling is sufficient for model comparisons

In Practice: Training, Validation, Test Data



Distribution → Dataset: Random Sampling

Collecting (i.e., sampling) data once ensures that data is sampled **I**dentically and **I**ndependently **D**istributed **(I.I.D)** but only measures **in-distribution generalization**

development time

collected once:

$$\mathcal{D} = \{X_i, y_i\}_{i=1}^{N} \sim p(X, Y)$$

then partitioned randomly:

random sampling

$$\mathcal{D}_{\text{train}} \leftrightarrow \mathcal{D}_{\text{test}} \sim p(X, Y)$$

in-distribution generalization

Real-World Models need to generalize Out-of-Distribution

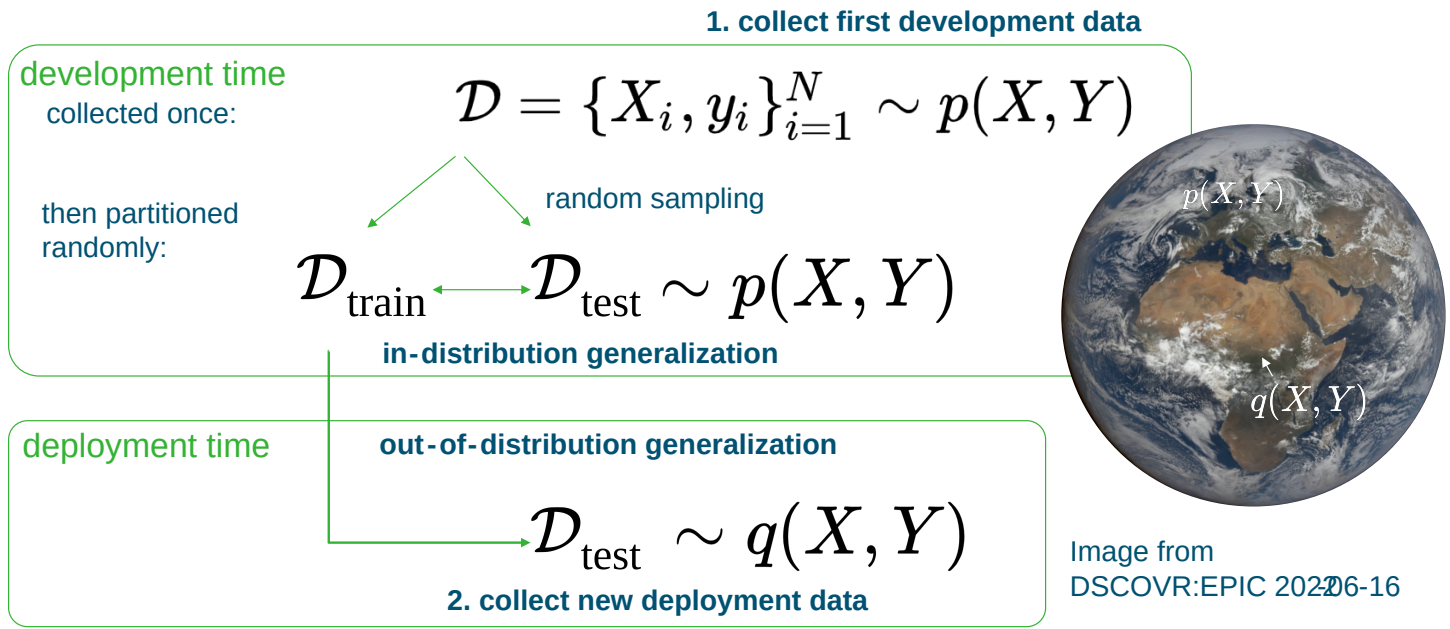


Image from DSCOVR:EPIC 2022-06-16

Types of Distribution Shifts

Covariate Distribution Shifts $P(X) \neq Q(X)$

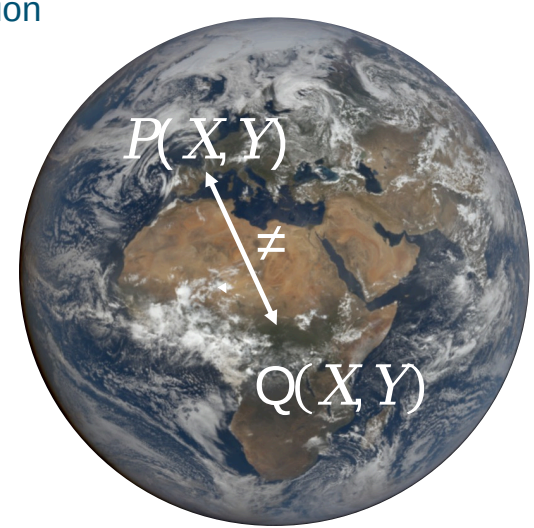
- **Different Location** : deploy model on different location
- **Different Time:** Summer/Winter
- **Different Sensors:** Sentinel - 2A vs 2B, Atmospheric correction algorithms

Concept Shifts $P(Y|X) \neq Q(Y|X)$

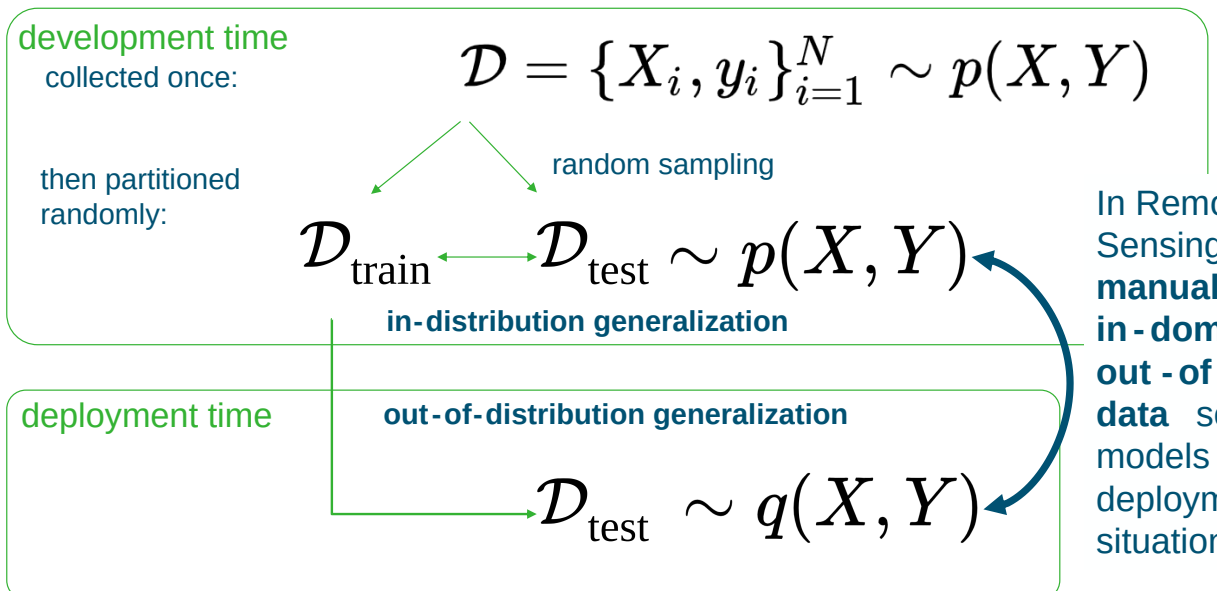
- **Different Intra - Class Variability** : Mixed Marine Debris, Different Forest Compositions
- **Different Data Annotators**

Label Shifts $P(Y) \neq Q(Y)$

- **Different Class Frequency:** One Category not present in test location.



Geospatial Models Need to Generalize Out-of-Distribution



In Remote Sensing we often **manually align in-domain and out-of-domain data** so that models work in deployment situations

Takeaway: Data

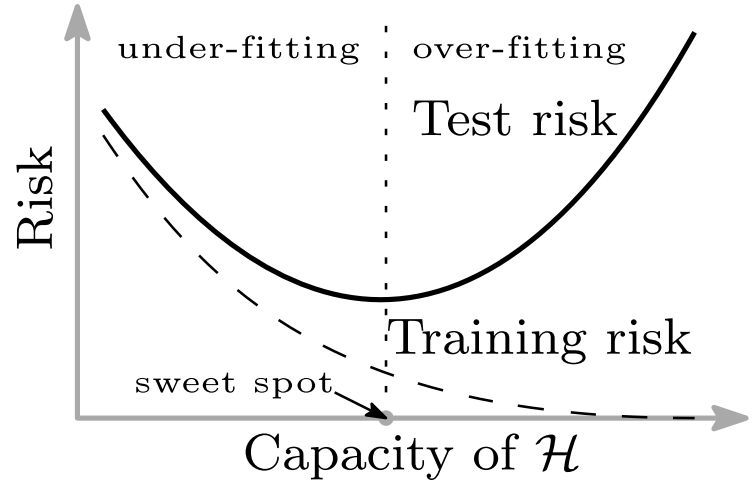
> **Data is the window through which a learner has access to our world.**

- Data are **samples from a distribution** $P(X, Y)$
- **We design the distribution** by how we sample and create data
- **Generative** (labels first) vs. **discriminative** (annotate later)
- The **i.i.d. assumption** is often violated in practice
- **Distribution shifts:** covariate, concept, and label shift



Part 2

Classical Generalization Theory



The Hypothesis Space $\mathcal{H}$

A **hypothesis** is a prediction function:

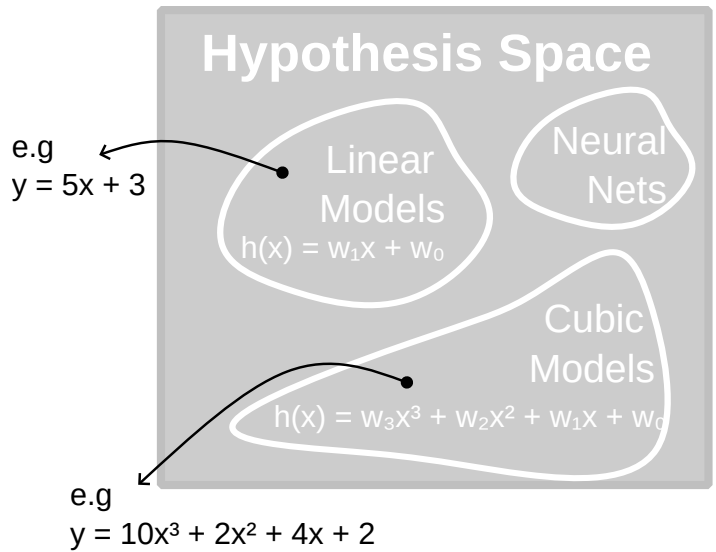
$$h : \mathcal{X} \to \mathcal{Y}$$

The **hypothesis space** is the set of functions the model can represent:

$$\mathcal{H} = \{h_\theta : \theta \in \Theta\}$$

- Θ is the **parameter space**
- $\theta \in \Theta$ is one parameter choice
- $h_\theta \in \mathcal{H}$ is the corresponding prediction function
- Training selects a hypothesis from $\mathcal{H}$

$$\boxed{\text{parameters } \theta \quad \longrightarrow \quad \text{hypothesis } h_\theta}$$



Example $\mathcal{H}_{\text{linear}}$

A **hypothesis** is a prediction function:

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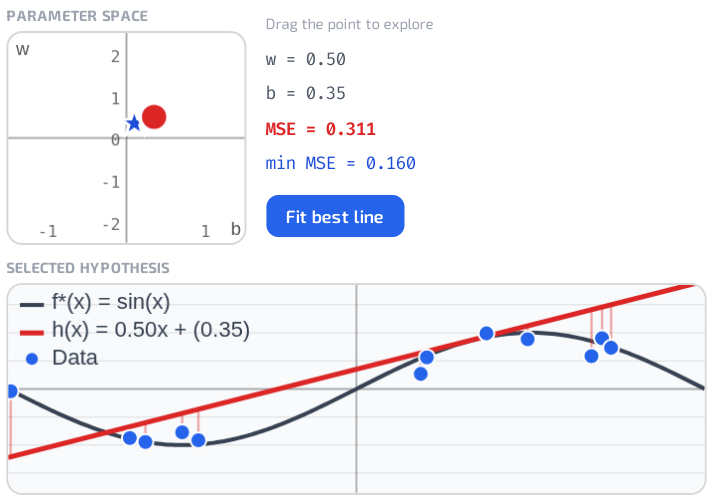
Example: $\mathcal{H}_{\text{linear}} = \{h_{w,b}(x) = wx + b : (w, b) \in \mathbb{R}^2\}$



Parameter Space and Hypothesis Space

Two parameter sets can map to the same Hypothesis

The **parameter space** contains the numerical values optimized during training:

$$\theta \in \Theta$$

The **hypothesis space** contains the prediction functions the model can represent:

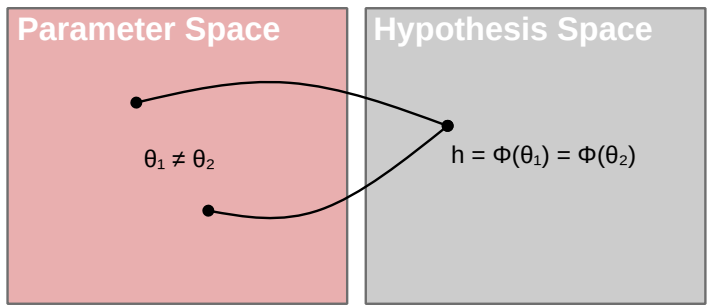
$$h_\theta \in \mathcal{H}$$

A parameterization maps parameter values to hypotheses:

$$\Phi : \Theta \to \mathcal{H}, \qquad \theta \mapsto h_\theta$$

This mapping does not have to be one-to-one:

$$\theta_1 \neq \theta_2 \qquad \text{but} \qquad \Phi(\theta_1) = \Phi(\theta_2)$$

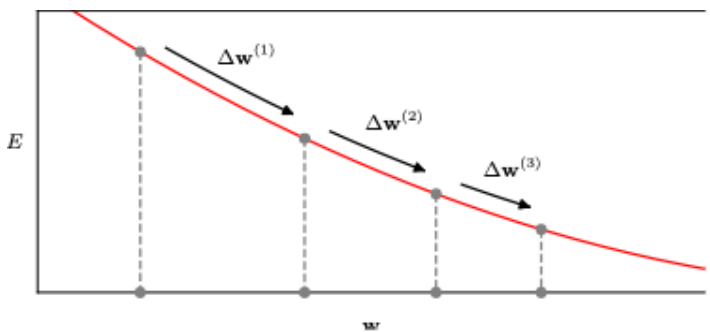


Training moves through parameter space, but predictions are determined by the corresponding hypothesis.

From Optimization to a Learned Hypothesis

Navigate parameter space

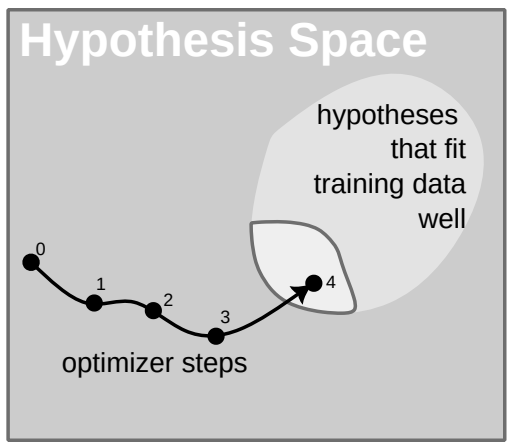
Gradient descent updates the parameters in a direction that aims to reduce the empirical risk:



Induce a path through $\mathcal{H}$

Every parameter value represents a prediction function:

$$h_{\theta^{(0)}} \to h_{\theta^{(1)}} \to \cdots \to h_{\theta^{(T)}}, \text{ so that } \hat{h}_D = h_{\theta^{(T)}} \in \mathcal{H}$$

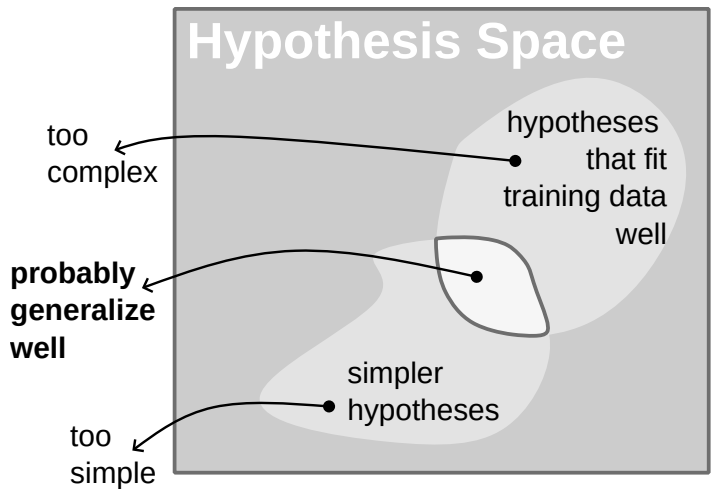


Occam's Razor Idea

Simpler functions should generalize better.

Willian of Ockham (c. 1287 – 9/10 April 1347)





Bias and Variance

$$\text{test risk} = \underbrace{\text{training risk}}_{\text{related to bias}} + \underbrace{(\text{test risk} - \text{training risk})}_{\text{related to variance}}$$

Bias

How systematically wrong is the model?

$$\text{Bias}(x) = \mathbb{E}_D[\hat{f}_D(x)] - f^*(x)$$

- Difference between the average learned model and the true function
- Often caused by a restrictive hypothesis space
- High bias leads to underfitting
- Both training and test error are typically high

Variance

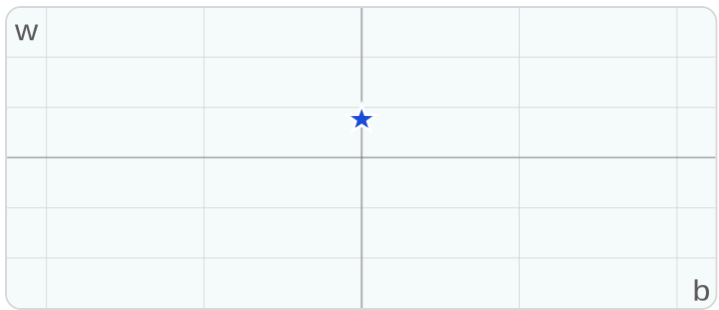
How much does the model depend on the dataset?

$$\text{Var}(x) = \mathbb{E}_D\left[\left(\hat{f}_D(x) - \mathbb{E}_D[\hat{f}_D(x)]\right)^2\right]$$

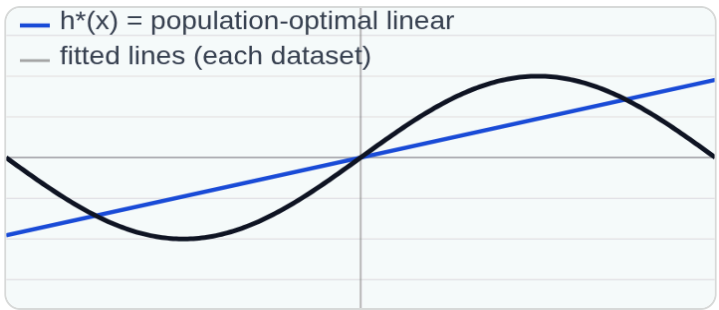
- Measures variation across different training datasets
- Often increases with model flexibility
- High variance leads to overfitting
- Test error can be much higher than training error

Example: Linear Regression

PARAMETER SPACE



X-Y PLANE SHOWING HYPOTHESES FUNCTIONS



Draw another dataset | Reset | N = 12 | M = 0

Task 1: Discuss the bias and variance of Linear Regression models.

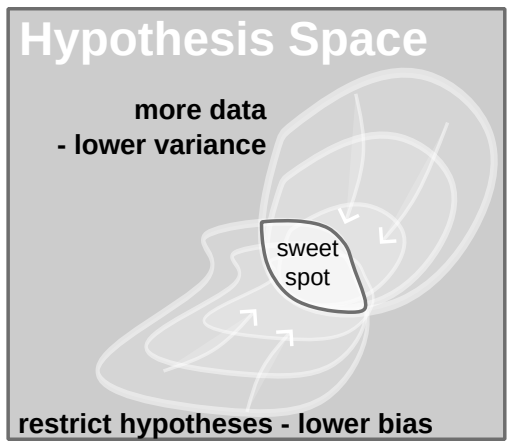
Task 2: Increase and Decrease the dataset size N, how does the variance change?

Controlling Bias and Variance

Strategy 1: Introduce Inductive Bias

Use domain knowledge to **restrict or prioritize** hypotheses:

- choose informative features;
- select an appropriate architecture;
- encode known invariances;
- regularize model complexity.



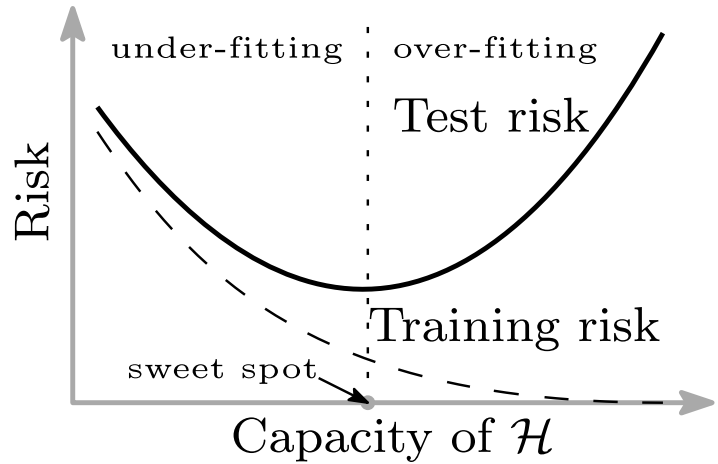
Strategy 2: Reduce Variance by more Data

Use additional information to rule out hypotheses that fit only by chance:

- collect more labelled data;
- apply valid data augmentation;
- exploit unlabelled data through pretraining.

Bias Variance Trade-Off

- **Under-fitting of simpler models** have high bias: they do not fit the training data well. Their predictions are fairly consistent across different training sets, so they have low variance.
- **Over-fitting of complex models** have lower bias: they fit the training data closely, sometimes perfectly. Their predictions depend more strongly on the training sample, so they have high variance and may perform poorly on new data.
- The classical **sweet spot** balances bias and variance to minimize test risk.

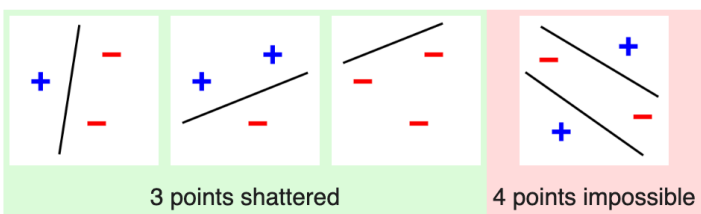


Vapnik-Chervonenkis (VC) Dimension

How to measure the Capacity of H

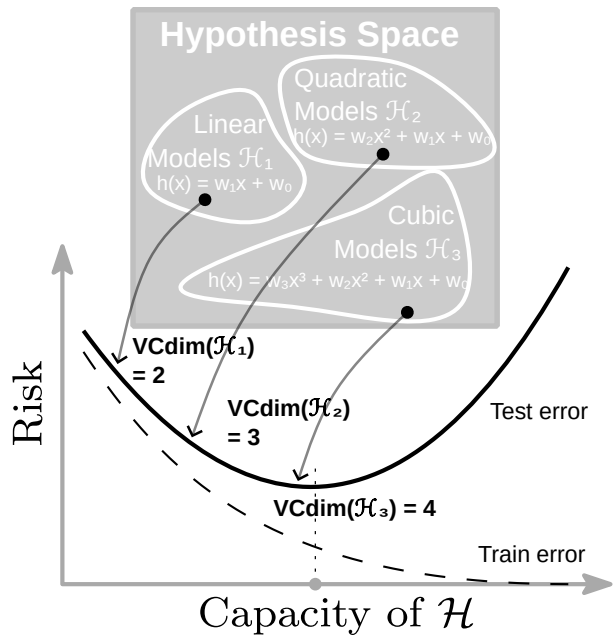
A set of n points is **shattered** by $\mathcal{H}$ if classifiers in $\mathcal{H}$ can realize all 2^n possible binary labelings. The **VC dimension** is the largest number of points that $\mathcal{H}$ can shatter:

$$\mathrm{VCdim}(\mathcal{H}) = \max\{n : \text{some } n \text{ points are shattered by } \mathcal{H}\}.$$



Linear classifier in 2D: 3 parameters (w_1, w_2, b) → VCdim = 3

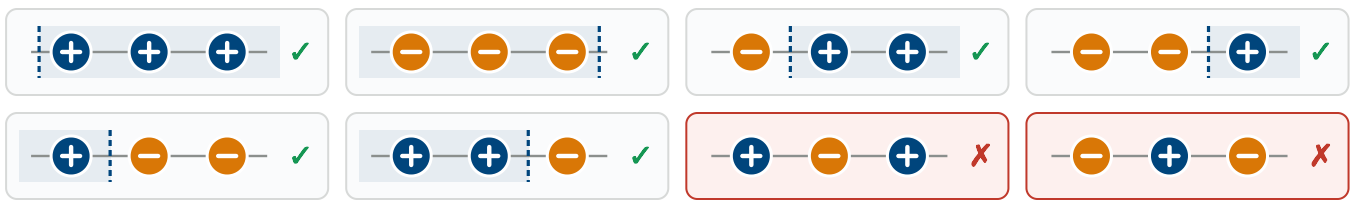
Image: Wikipedia, CC BY-SA 3.0



VC Dimension of $\mathcal{H}_1$

Linear classifier in 1D: $h(x) = \text{sign}(w_1 x + w_0)$ is a threshold with 2 parameters

3 points: only 6 of $2^3 = 8$ labelings are realizable → not shattered



dashed line = threshold · shaded = classified as +

A threshold lets the label change **only once** from left to right, so + − + is impossible: **VCdim($\mathcal{H}_1$) = 2**. For linear classifiers, VCdim = number of parameters (d + 1); in general the two can differ.

Worst-Case Generalization Gap

For a bounded loss, ignoring constants and logarithmic terms:

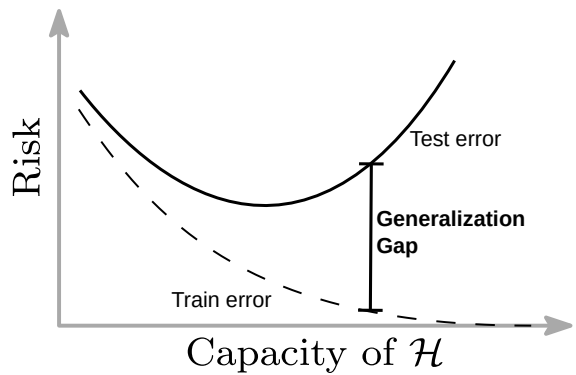
$$\left|R(h) - \widehat{R}_D(h)\right| \lesssim \sqrt{\frac{d}{n}}$$

with VC dimension d and sample size n

- A larger VC dimension gives a weaker guarantee for the same sample size.
- More training data reduces the worst-case gap approximately as $1/\sqrt{n}$.
- For a target gap ε, the required sample size scales approximately as

$$n \propto \frac{d}{\varepsilon^2}.$$

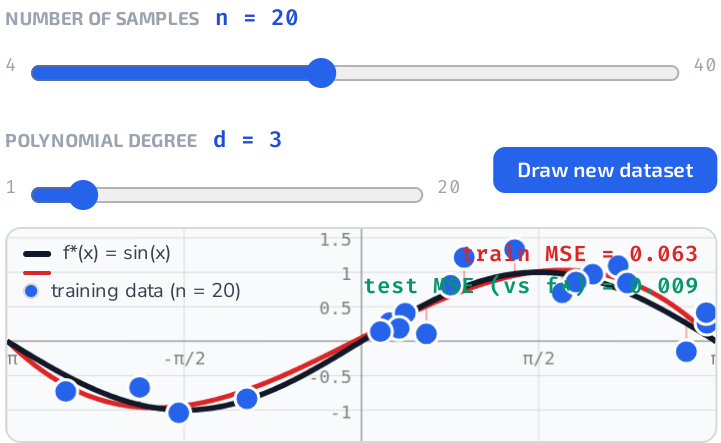
- The guarantee is useful only when $d \ll n$. When $d \approx n$, the bound becomes uninformative.

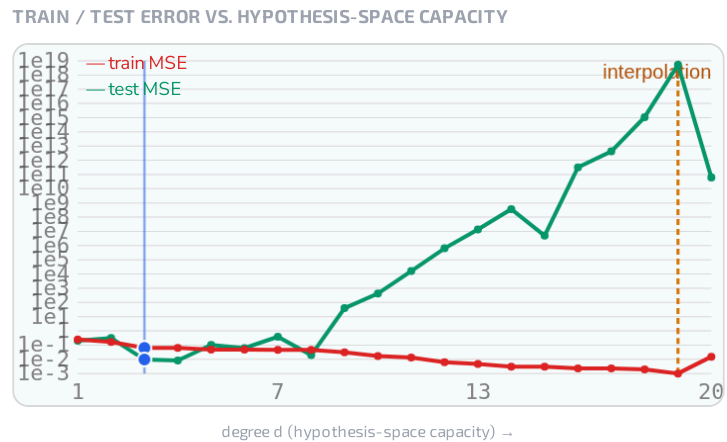


VC bounds are distribution-free and robust, but often pessimistic.

Example Polynomial Regression:

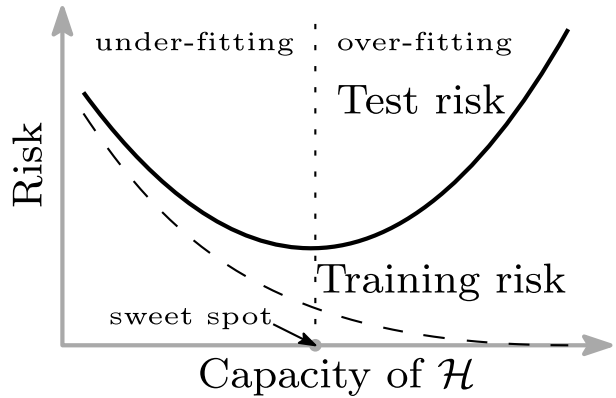
Increasing Polynomial Degree D: ↓ Bias ↑ Variance





Takeaways Classical Generalization Theory

- Training minimizes **training risk**, while the goal is low **testing risk**.
- Simpler models are more stable but may underfit because of high bias.
- More flexible models reduce bias but may overfit because of high variance.
- When overfitting, reduce model complexity, increase regularization, or use more data.
- When underfitting, increase model capacity or reduce regularization.
- Use validation data to find the model complexity that best balances bias and variance.



Part 3

Generalization beyond the Interpolation Threshold



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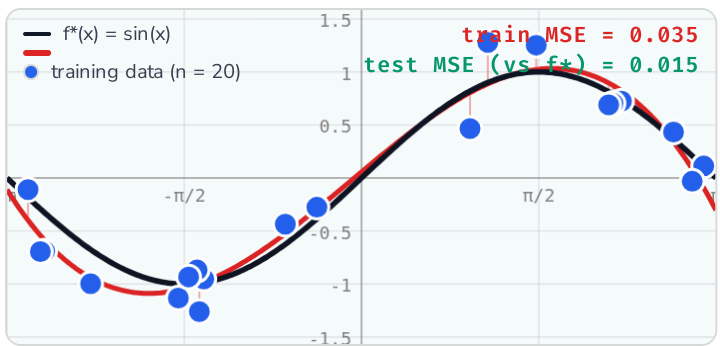
Beyond the Threshold: Double Descent in Polynomial Regression

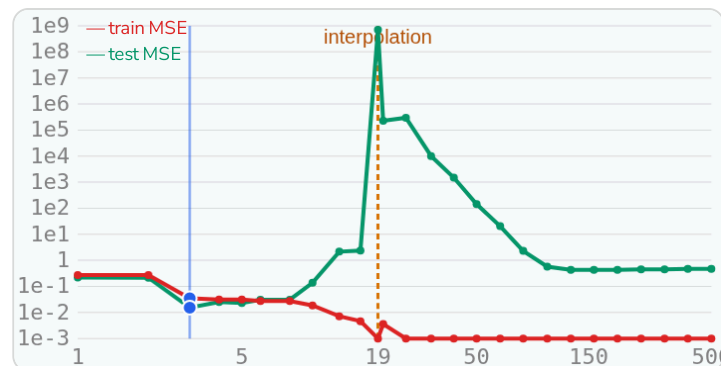
POLYNOMIAL DEGREE (LOG SCALE) **d = 3**

1 500

Draw new dataset



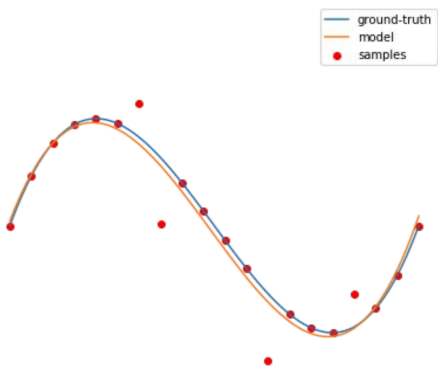
TRAIN / TEST ERROR VS. HYPOTHESIS-SPACE CAPACITY (LOG–LOG)



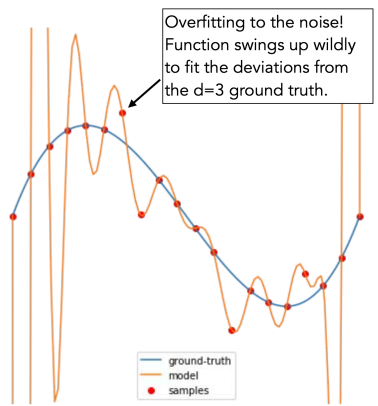
degree d (hypothesis-space capacity, log scale) →

Polynomial Regression in Interpolation Regime

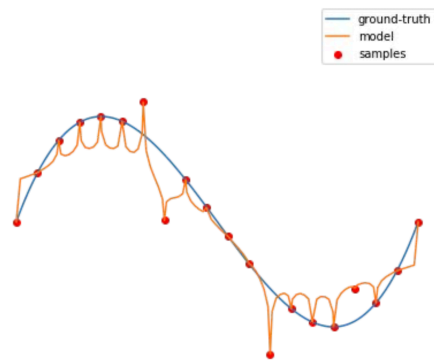
Underfitting — Degree 3



Overfitting — Degree 20



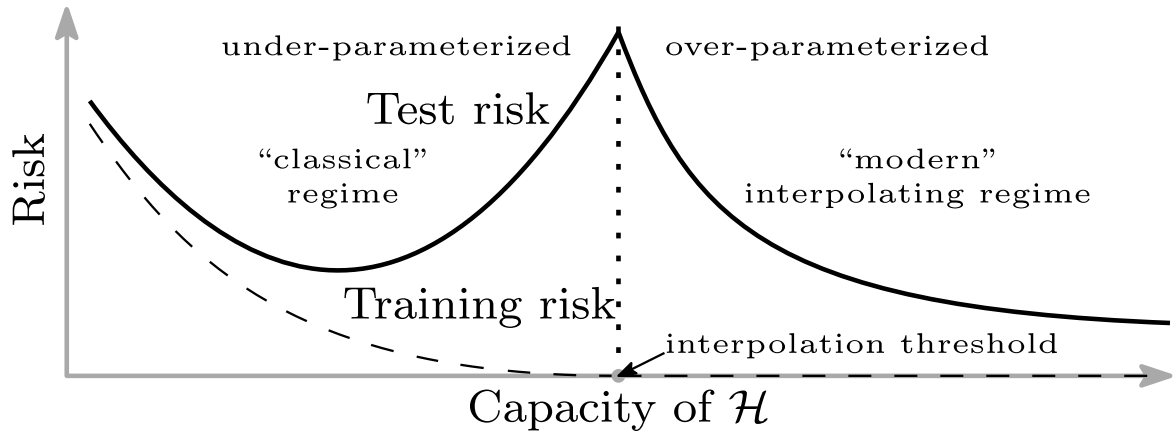
Interpolating — Degree 1000



Credit: Philip Isola, MIT 6.7960 Deep Learning (Fall 2024), Lecture 6: NN Generalization, MIT OpenCourseWare

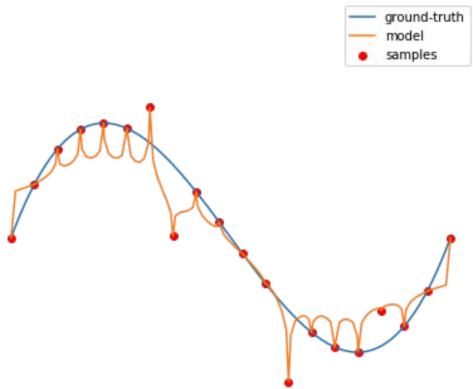
Double Descent Phenomenon

Overparamterized Models Improve Again after Overfitting



Credit: Belkin et al., 2019. Reconciling modern machine learning practice and the bias-variance trade-off

The Simple + Spiky Hypothesis



$$\text{learned model} = \underbrace{\text{“simple”}}_{\text{predictive component}} + \underbrace{\text{“spiky”}}_{\text{overfitting / memorization component}}$$

Belkin, Rakhlin & Tsybakov, 2018. Does data interpolation contradict statistical optimality?

Credit: Philip Isola, MIT 6.7960 Deep Learning (Fall 2024), Lecture 6: NN Generalization, MIT OpenCourseWare

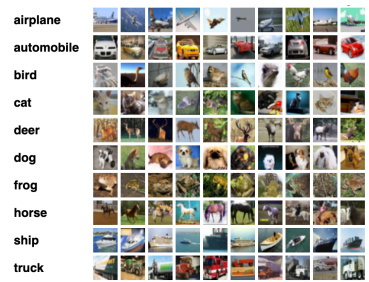
Neural Networks Interpolate and Generalize

The same hypothesis class can memorize noise and learn structure

The experiment

Inception on CIFAR-10

Training labels	Train accuracy	Test accuracy
True labels	100%	85.75%
Random labels	100%	9.78%



The VC bound becomes vacuous and does not explain Deep Networks' generalization

- **No contradiction:** The VC bound remains valid, but it is too pessimistic to distinguish the two learned solutions.

Zhang et al. (2017). *Understanding Deep Learning Requires Rethinking Generalization*. ICLR. arXiv:1611.03530

How to measure the Model Complexity now??

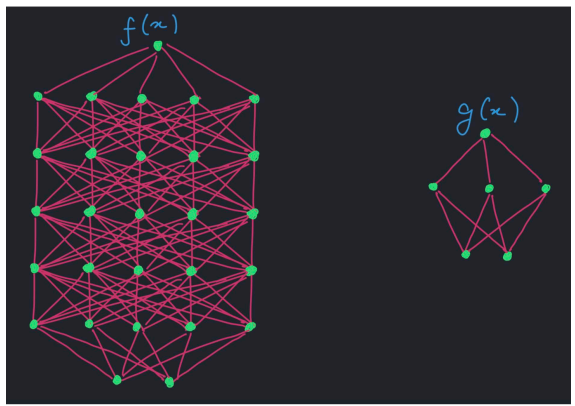
By the number of distinct functions the model can represent? (VC-dimension)

→ **No.** Not helpful — the generalization bound is too pessimistic. Following classical theory, neural networks should not generalize.

Slide from Philip Isola, MIT 6.7960 Deep Learning (Fall 2024), Lecture 6: NN Generalization, MIT OpenCourseWare

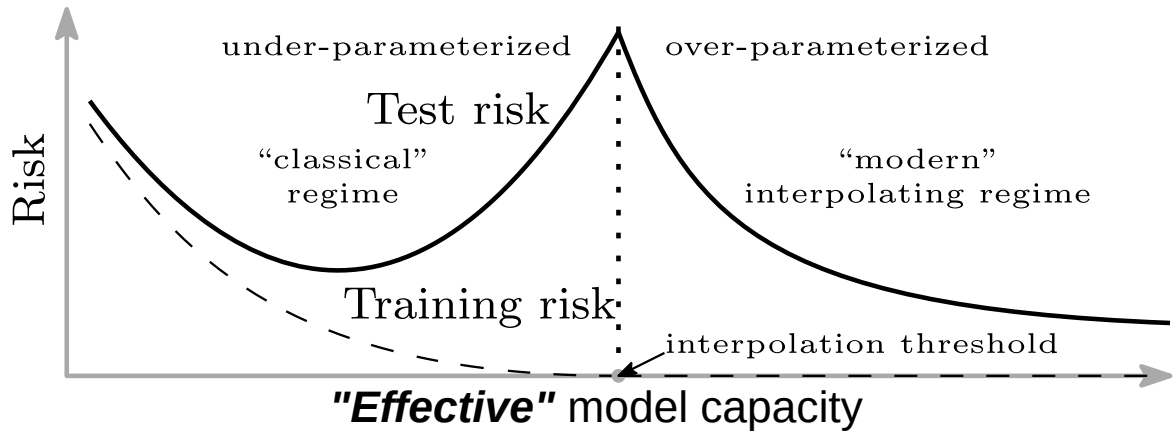
Why parameter count alone doesn't determine generalization for deep learning is still an open question.

By the number of parameters in a neural network?



Consider $h(x) = 10^{-100} f(x) + (1 - 10^{-100}) g(x)$. How many parameters does it have? Does it matter? **Not really.**

"Effective" Model Capacity



"Capacity" is intentionally abstract. Parameter count may indicate when interpolation becomes possible, but it does not determine the complexity of the learned solution or its test performance.

Recap So Far

WHAT WE OBSERVED

Deep networks generalize.
They make accurate predictions on inputs that were not part of the training data.

Deep networks also interpolate.
The same architectures can perfectly fit true labels and random labels.

Training fit alone cannot explain generalization.
Zero training error does not distinguish learning useful structure from memorizing the sample.

WHAT THIS IMPLIES

Generalization requires inductive bias.
Training must favor some interpolating solutions over many others that fit the data equally well.

Worst-case capacity is insufficient.
Parameter count and VC dimension describe the entire hypothesis space, but their bounds become vacuous for highly expressive neural networks.

The selected solution matters.
Architecture, optimization, regularization, and data properties all influence which solution training finds.

Next question: Which inductive biases make interpolating neural networks generalize?

Slide from Philip Isola, MIT 6.7960 Deep Learning (Fall 2024), Lecture 6: NN Generalization, MIT OpenCourseWare

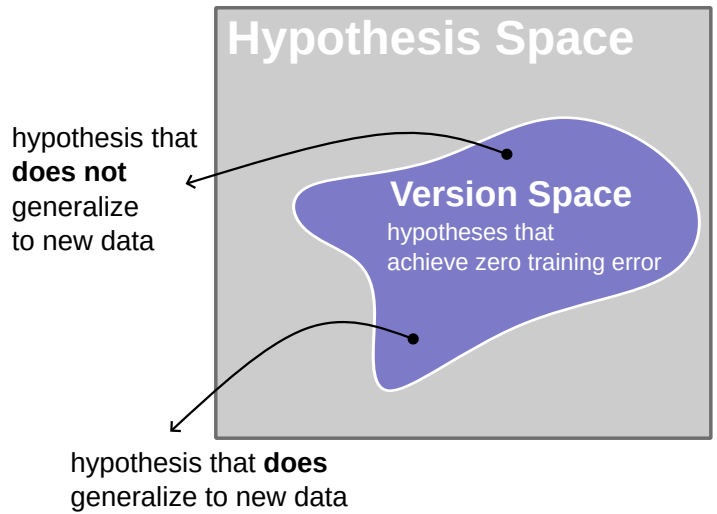
Version Space

The **version space** contains all hypotheses that fit the training data perfectly:

$$\mathcal{V}_{\mathcal{H}}(D) = \left\{ h \in \mathcal{H} : \widehat{R}_D(h) = 0 \right\}.$$

- In overparameterized models, many hypotheses belong to this set.
- Some generalize to unseen data, while others merely memorize.
- Training error cannot distinguish between them.

Deep models do generalize. Therefore, the training system must favor generalizing hypotheses within the version space.



Inductive Biases Select Interpolating Solutions

Sources of inductive bias

- **Architecture:** locality, parameter sharing, recurrence, and equivariance
- **Parameterization:** makes some functions easier to represent and reach
- **Initialization:** influences the path taken through parameter space
- **Optimization and loss:** SGD, batch size, learning rate, and loss function
- **Explicit regularization:** weight decay, dropout, and early stopping
- **Data and augmentation:** encode structure, invariances, and prior knowledge

What does “simpler” mean?

Not necessarily fewer parameters.

Depending on the setting, training may favor solutions with:

- low norm or large margin
- smoothness or invariance
- compressible representations

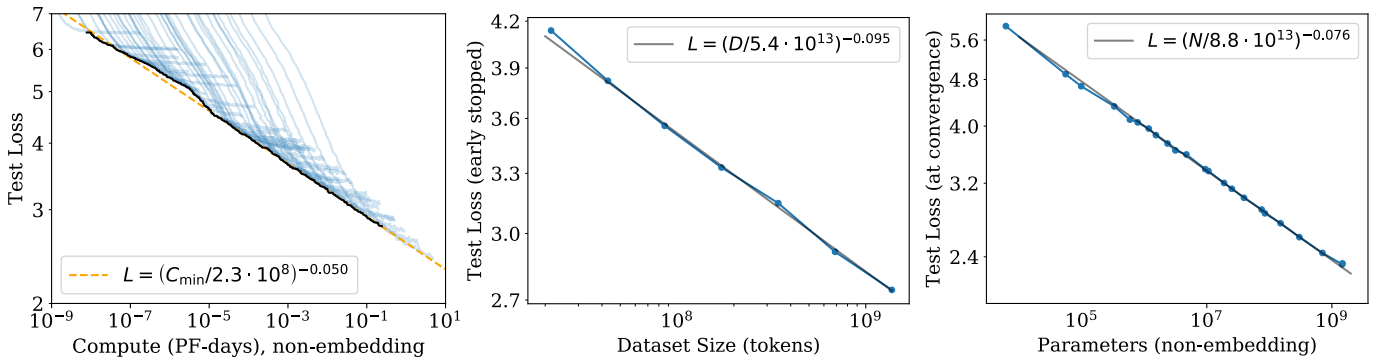
There is no single universal measure of the effective complexity of a deep network.

For concrete proposed theories, check Phillip Isola. *Lecture 6: Generalization Theory*. MIT 6.7960 Deep Learning, Fall 2024.

The Modern AI Acceleration

Scaling Laws for Transformers

Held-out loss follows power laws of compute, data, and model size



Compute

$$L(C_{\text{min}}) = \left(\frac{C_{\text{min}}}{2.3 \times 10^8}\right)^{-0.050}$$

Training data

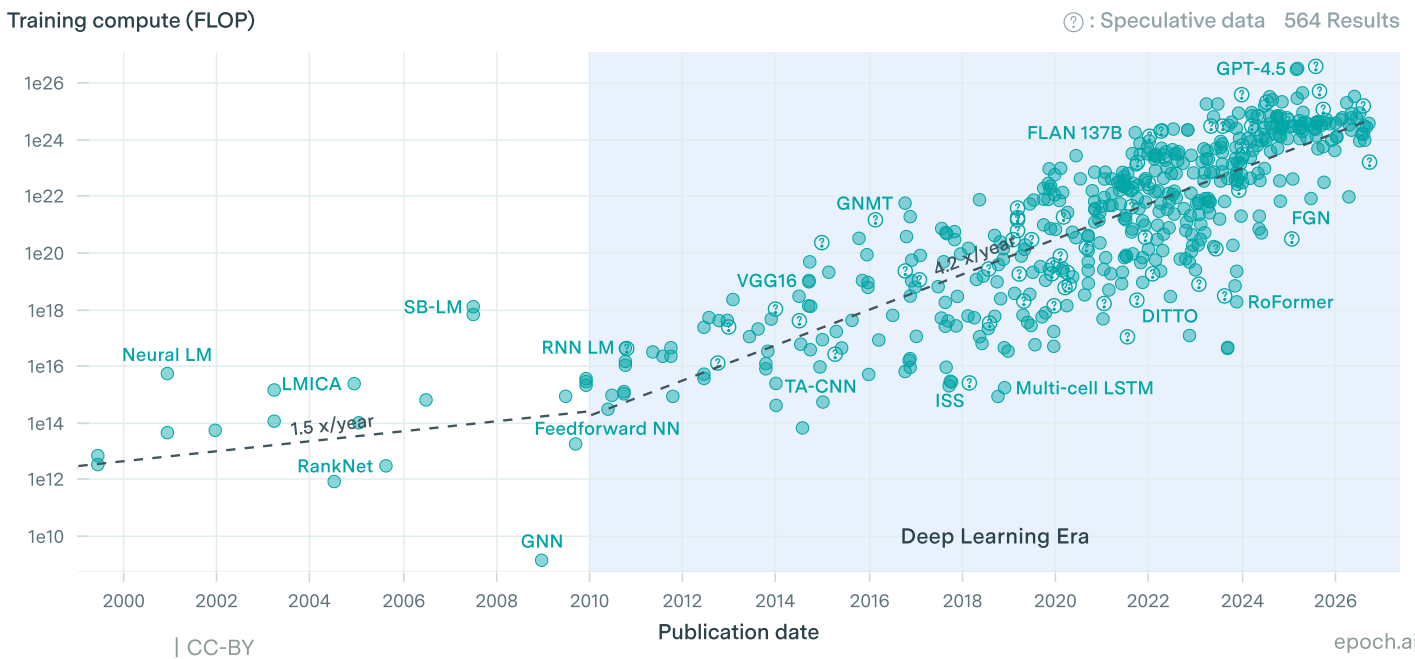
$$L(D) = \left(\frac{D}{5.4 \times 10^{13}}\right)^{-0.095}$$

Model size

$$L(N) = \left(\frac{N}{8.8 \times 10^{13}}\right)^{-0.076}$$

Kaplan et al. (2020). *Scaling Laws for Neural Language Models.*

Modern AI Acceleration



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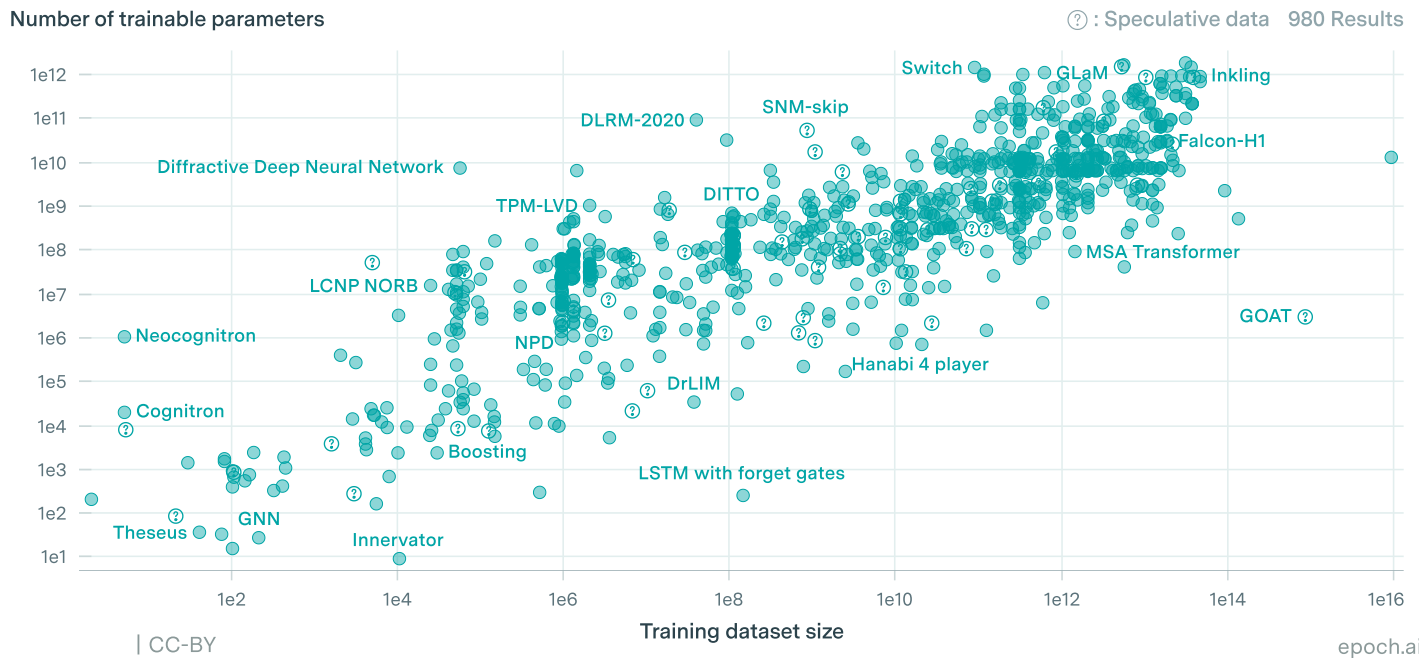
Larger Datasets and More Parameters



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Revisit the learning outcomes

Light gray fill: your group's before responses today · Click to respond again.

Distinguish approximating the training data from generalizing to unseen data.

Not comfortable — Very comfortable

Click to respond

Explain datasets as samples from distributions we shape, and the i.i.d. assumption.

Not comfortable — Very comfortable

Click to respond

Distinguish in- from out-of-distribution data, and covariate, concept, and label shift.

Not comfortable — Very comfortable

Click to respond

Explain optimization in the hypothesis space and the bias–variance trade-off.

Not comfortable — Very comfortable

Click to respond

Explain generalization beyond the interpolation threshold, where VC theory fails.

Not comfortable — Very comfortable

Click to respond

Describe how scaling laws make performance predictable and unlocked LLMs.

Not comfortable — Very comfortable

Click to respond