# Neural Network Training

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# Review

- Last lecture:
  - Objective function: what to learn
  - Gradient descent: how to learn
  - Training a neural network: optimization
  - Gradient descent for different activation functions

- Assignments (Canvas):
  - Problem set 1 grades out
  - Lab assignment 1 due Monday

- Questions?

# Today’s Topics

- Universal approximation theorem vs No Free Lunch theorem
- Selecting model capacity: avoid overfitting and underfitting
- Selecting model hyperparameters
- Learning efficiently: optimization methods
- Programming tutorial

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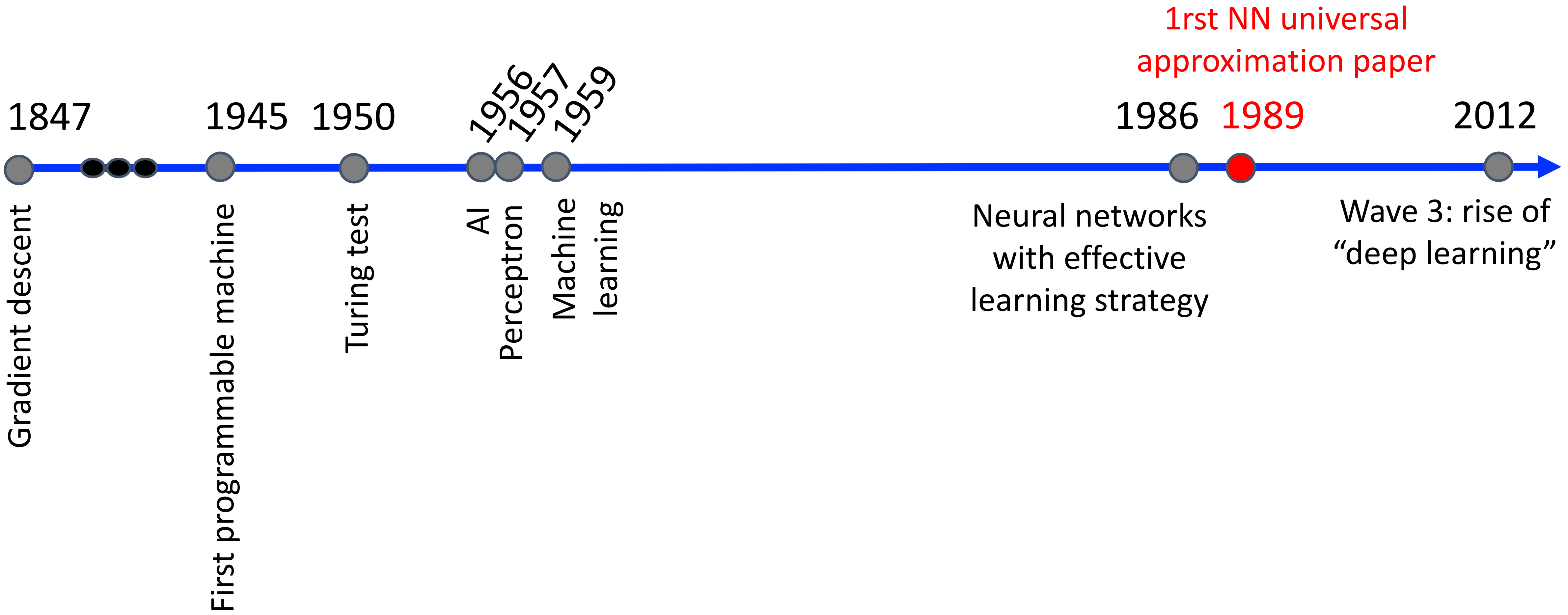
# Historical Context: Universal Approximator

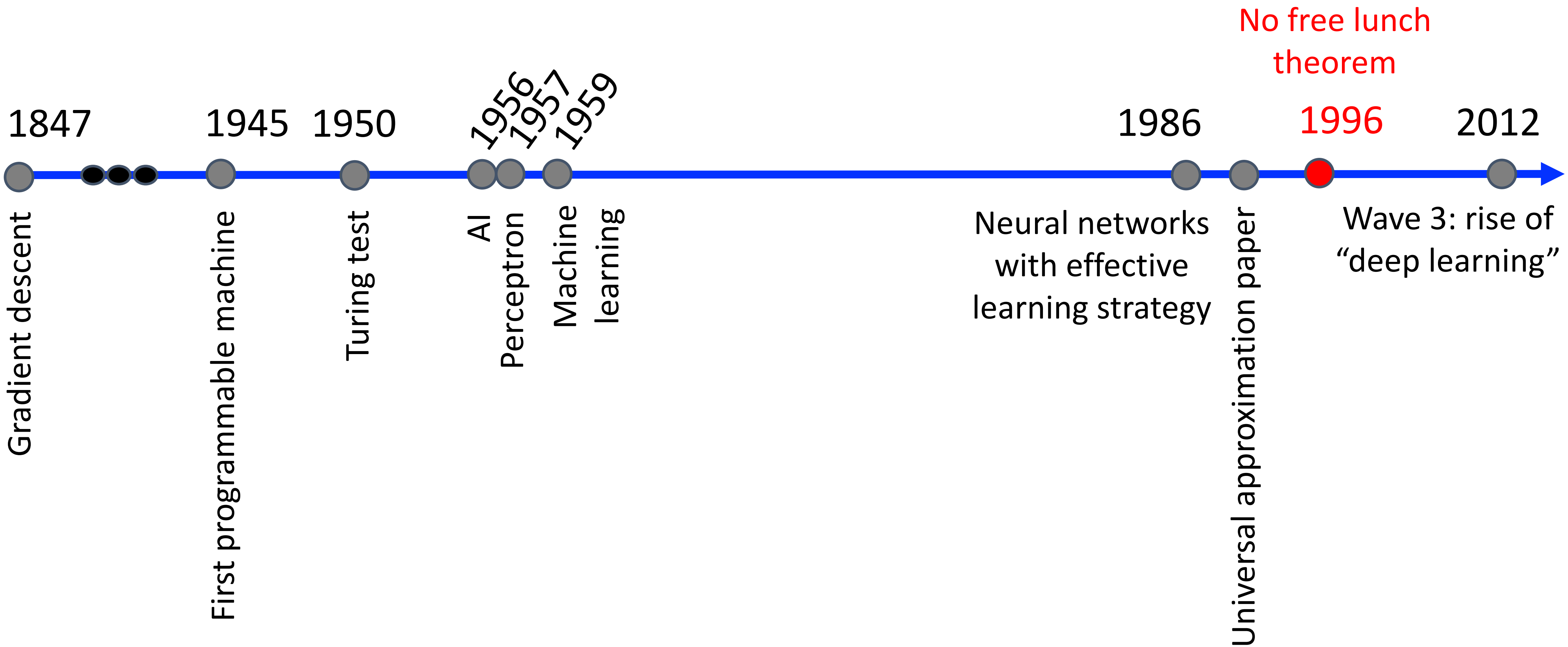



Hornik, Stinchcombe and White. Multilayer feedforward networks are universal approximators. Neural Networks, 1989

"The universal approximation theorem means that regardless of what function we are trying to learn, we know that a large MLP [multilayer perceptron] will be able to *represent* this function."

- Ch. 6.4.1 of Goodfellow book on Deep Learning

# Historical Context: Challenge




Hornik, Stinchcombe and White. Multilayer feedforward networks are universal approximators. Neural Networks, 1989 “**no free lunch theorem**… no machine learning algorithm is universally any better than any other.”

- Ch. 5.2.1 of Goodfellow book on Deep Learning

# Deep Learning Challenge

Since neural networks can in theory represent ANY function, how do we learn models that can perform well for the data generated in real world problems…

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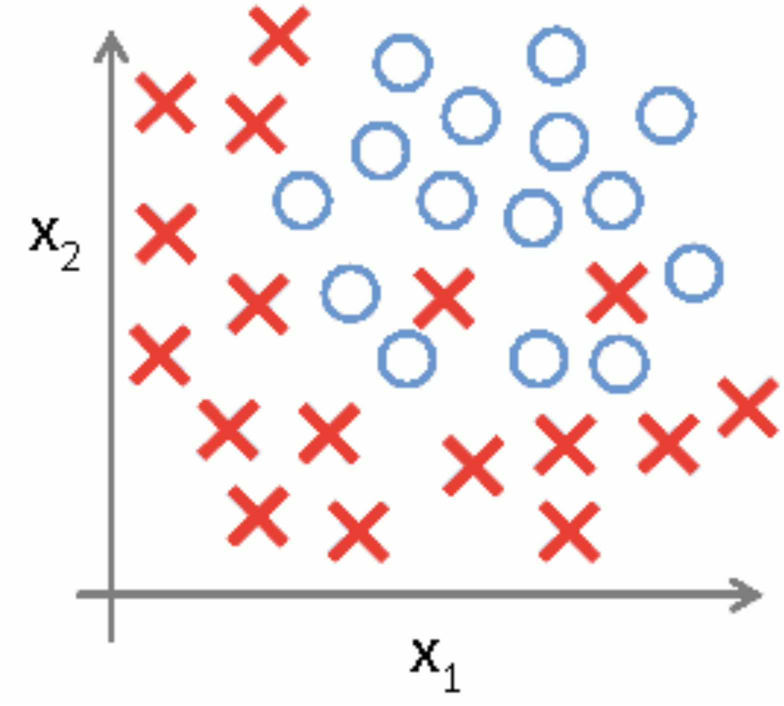
# Recall: Class Exercise from Lecture 1

- Model-based classification approach: separate x from o




Class volunteer:
1) Draw a straight line (linear equation)
2) Draw a parabola (quadratic equation)
3) Draw any curve

Models with increasing representational capacity

Figure source: https://medium.com/greyatom/what-is-underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6803a989c76

# Model Capacity

Which model would you choose to separate x from o?

(a) (b) (c)

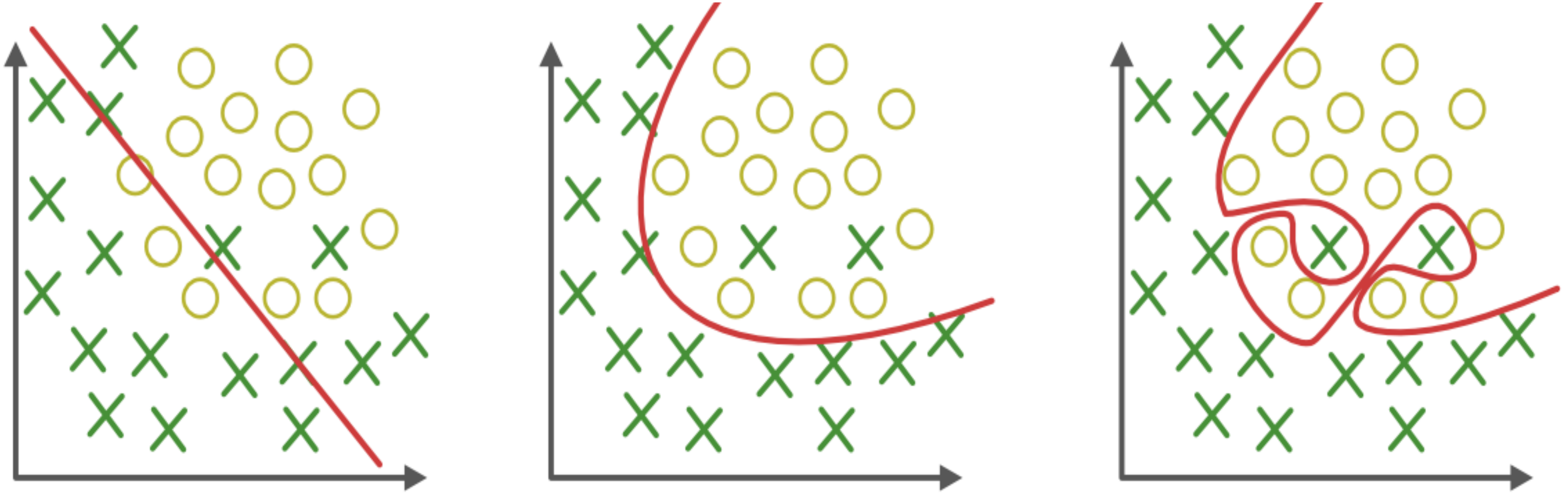


Figure source: https://towardsdatascience.com/underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6fe4a8a49dbf

# Model Capacity

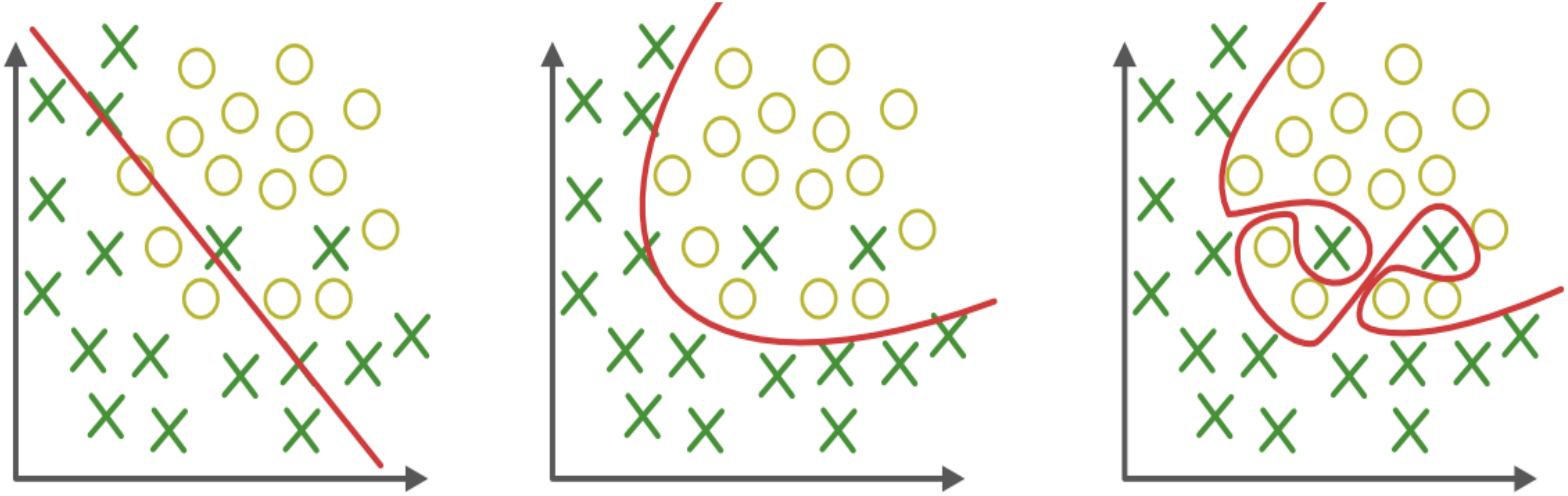
Underfits: too simple to explain the data

Overfits: too complex to generalize to a test set

(a)

(b)

(c)



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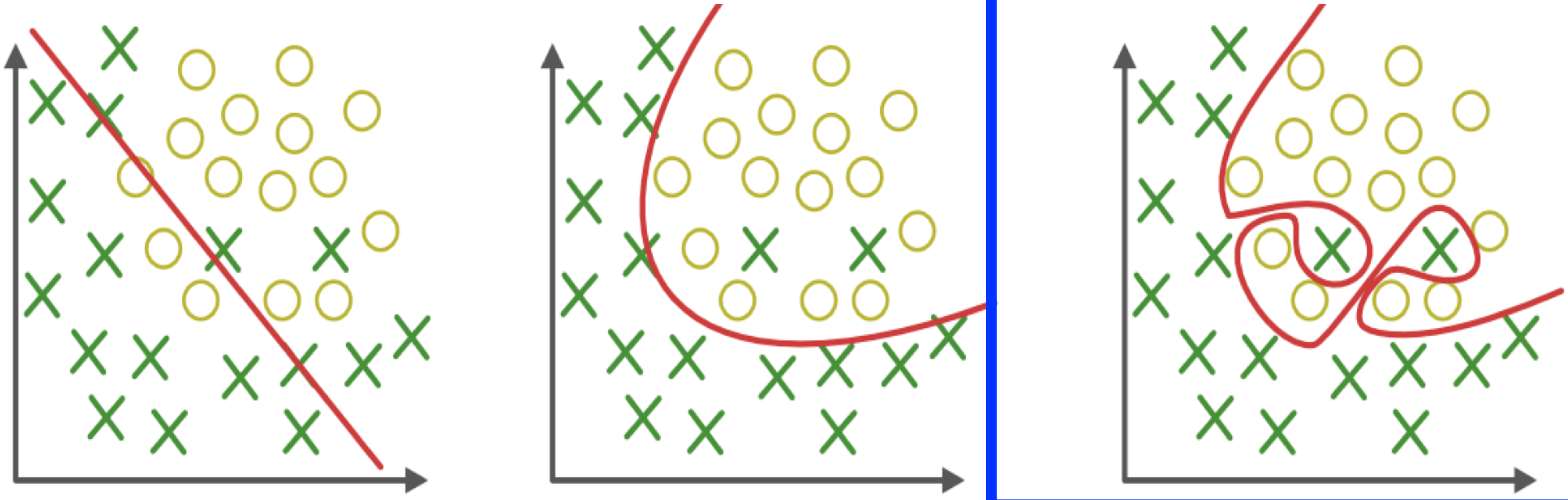
# Model Capacity

Key challenge for neural networks since they have many parameters

Underfits: too simple to explain the data

Overfits: too complex to generalize to a test set

(a) (b) (c)



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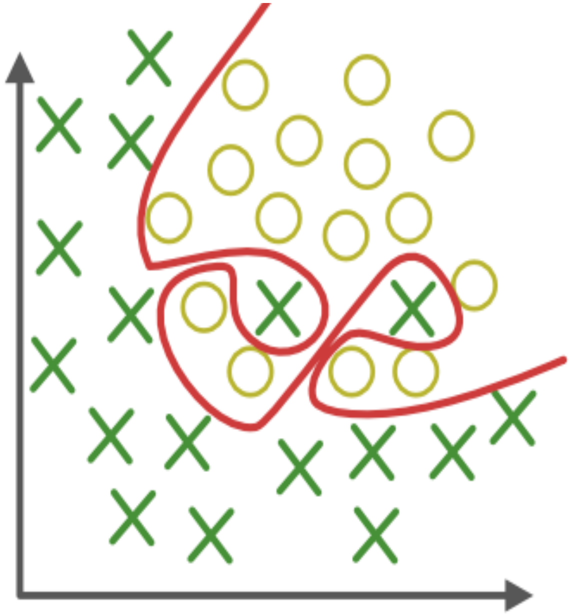
# Model Capacity: Overfitting Problem

- Problem: models can learn to model **noise** and so generalize poorly to novel examples!
- What would cause noise in a dataset?
  - e.g., incorrect data entry/labeling, hardware measurement error
- Caution: some outliers are not noise and so are data points we want models to learn



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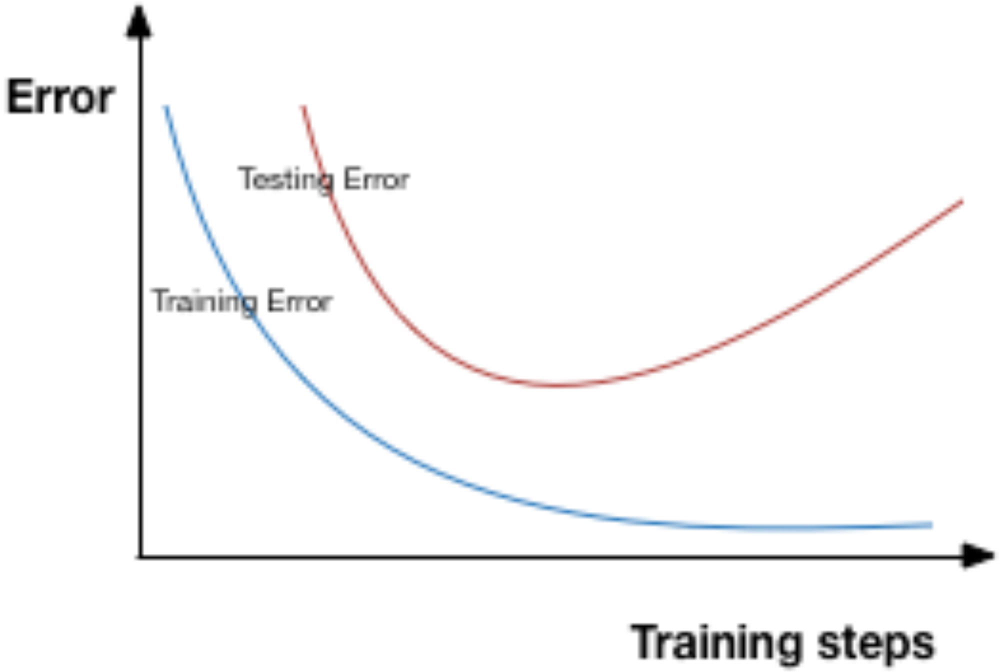
# Model Capacity: Overfitting Remedy

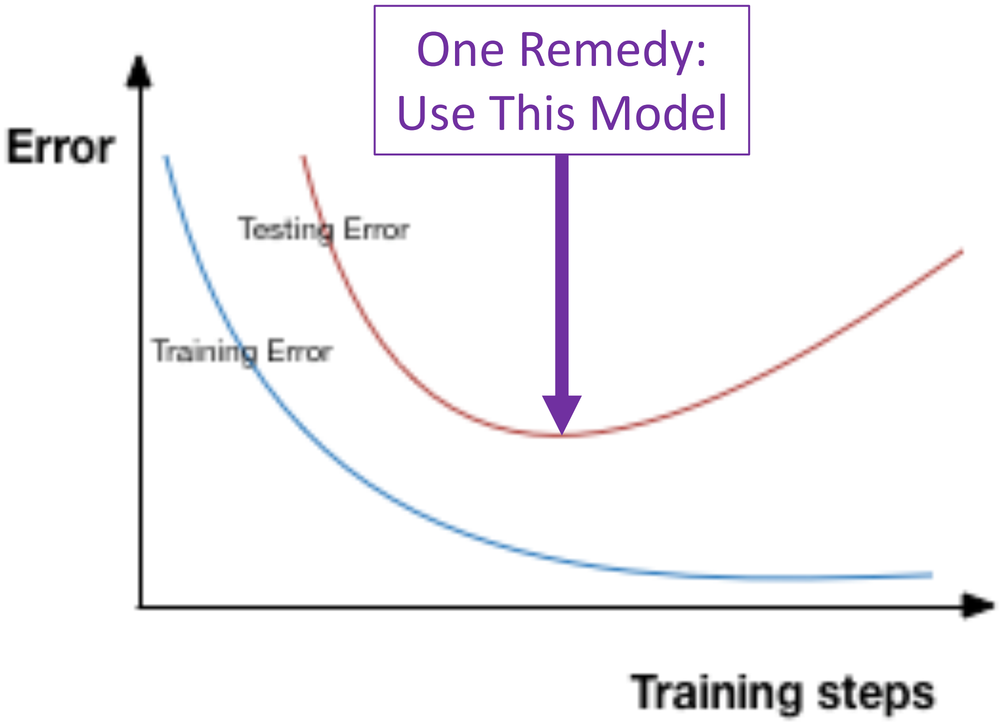



- To detect overfitting, analyze **learning curves** for models tested on training data and test data
  - What happens to training data error as number of training steps increases?
    - Error shrinks
  - What happens to test data error as number of training steps increases?
    - Error shrinks and then grows
  - Why does training error ***shrink*** and test error ***grow***?
    - Modeling ***noise*** in the training data (i.e., "overfitting") reduces training error at the expense of losing knowledge that generalizes to unobserved test data

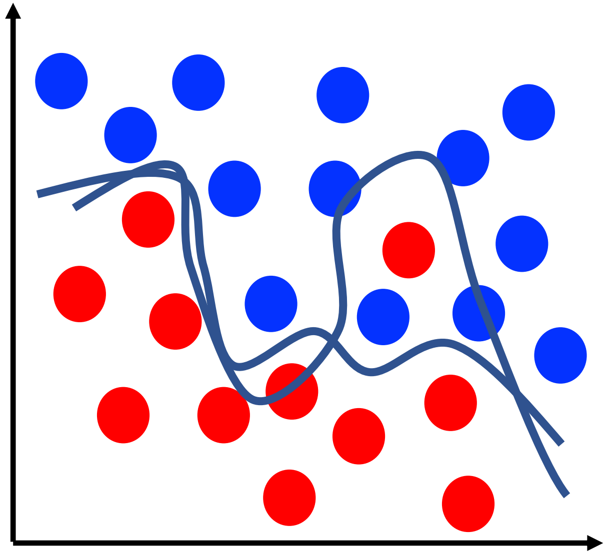
Image Source: https://chatbotslife.com/regularization-in-deep-learning-f649a45d6e0

# Model Capacity: How to Avoid Overfitting?

Early stopping




Add training data



Many more techniques to be discussed in this course…

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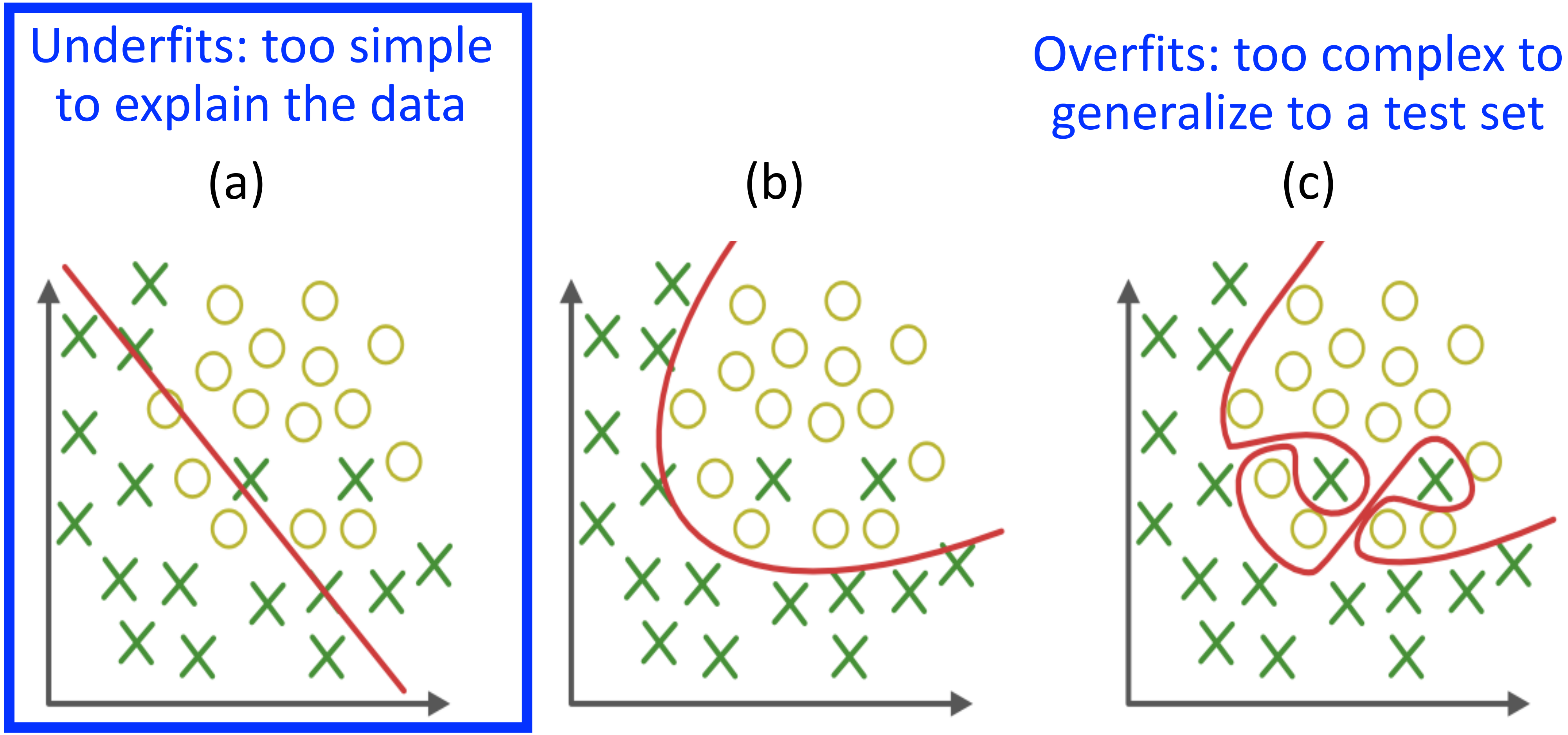
# Model Capacity

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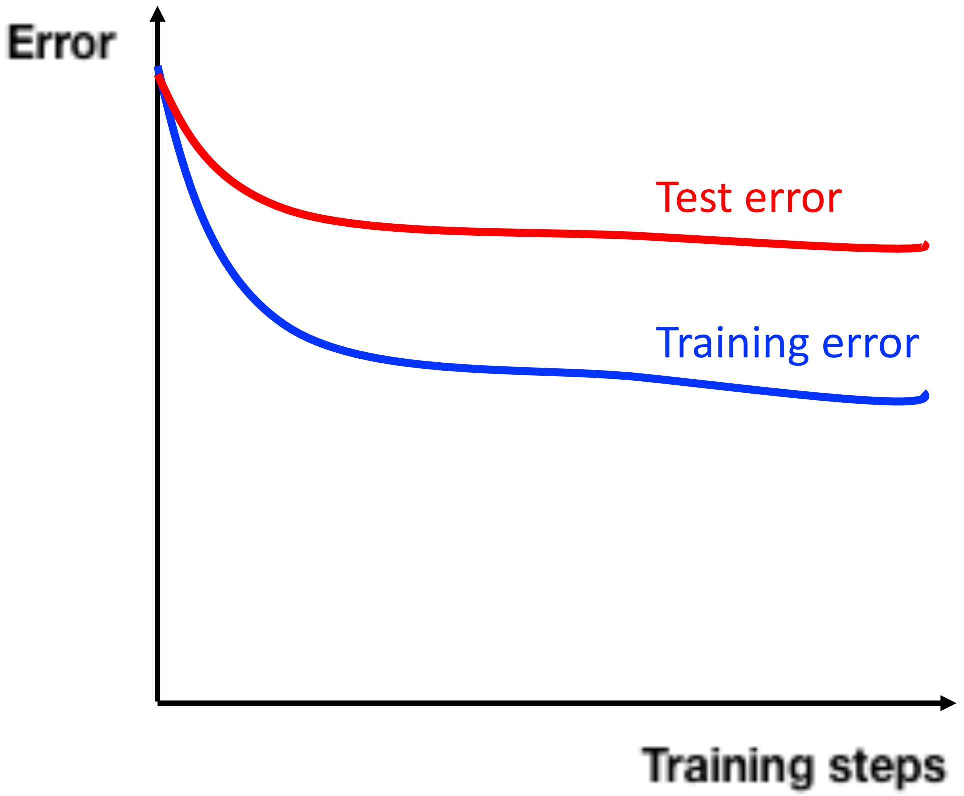
# Model Capacity: Underfitting



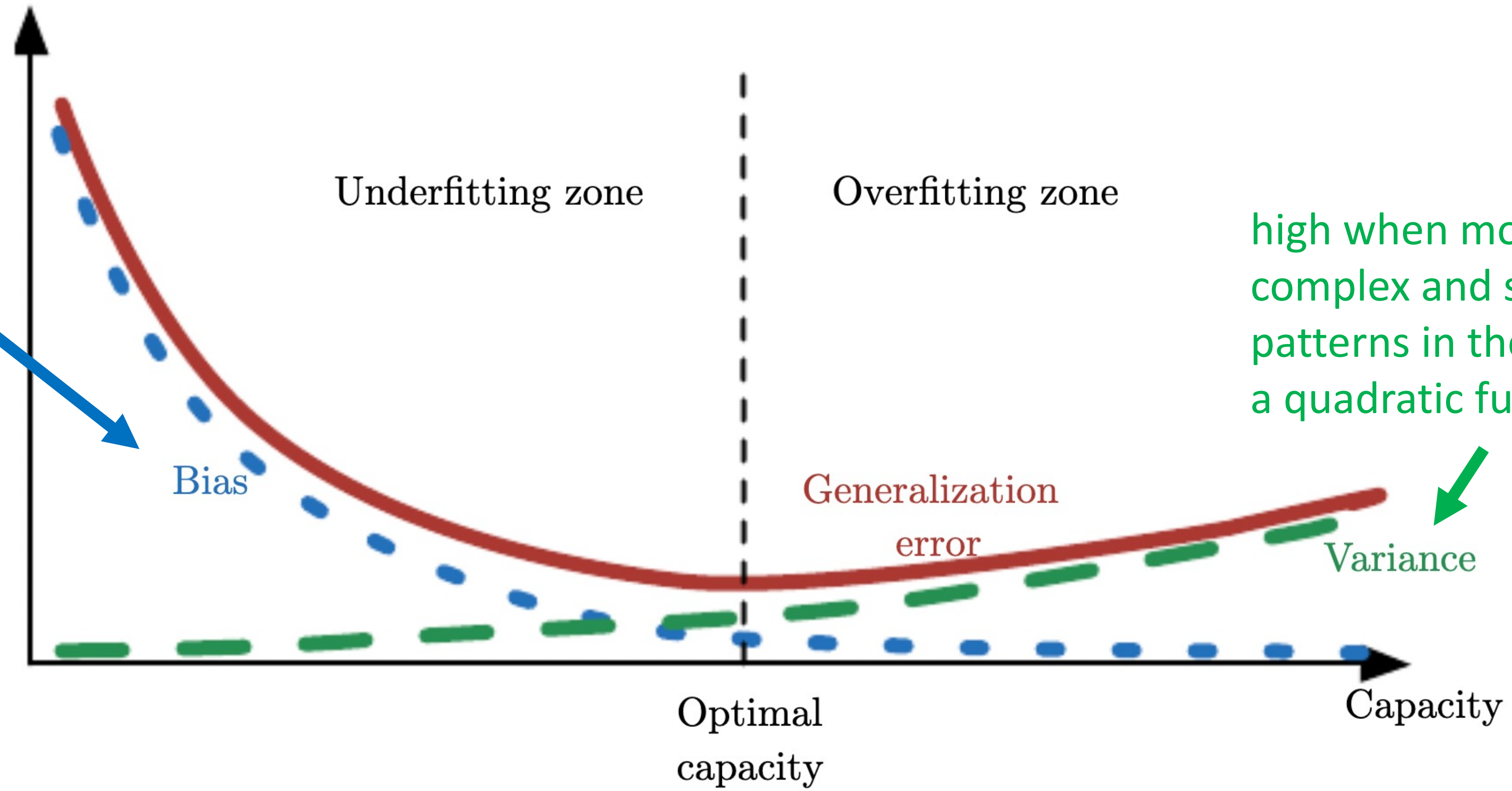

- To detect underfitting, analyze **learning curves** for models tested on training data
  - What happens to training data error as number of training steps increases?
    - Error remains high

# Model Capacity: How to Avoid Underfitting?

Increase representational complexity, for example add the number of layers and/or units in a neural network

# Model Capacity: Overfitting vs Underfitting

(not related to the "bias" parameter in neural networks): high when model is overly-simple and so assumes simpler patterns in the data (e.g., linear function)

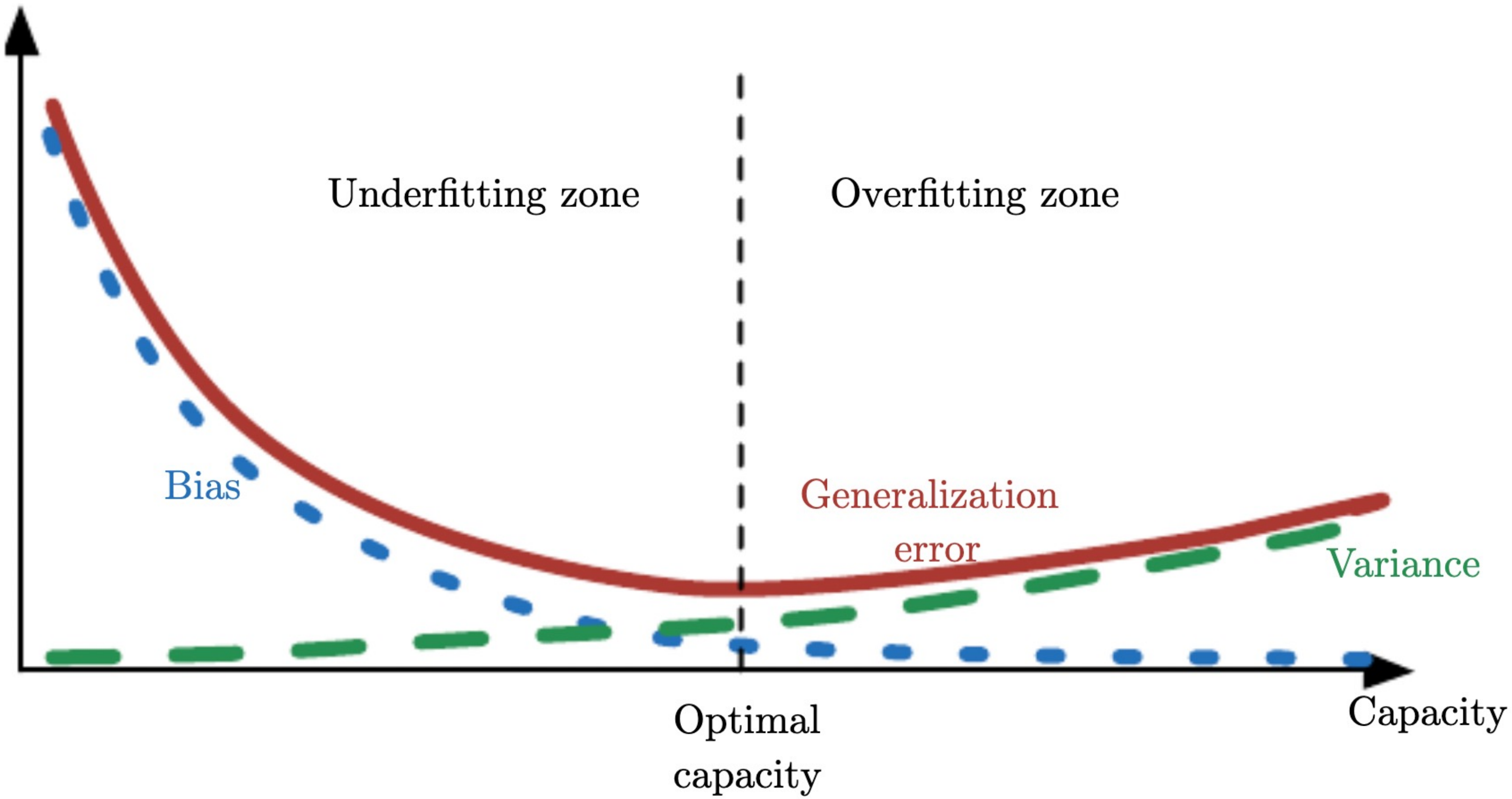



high when model is overly-complex and so misses simpler patterns in the data (e.g., does a quadratic function suffice?)

Often discussed with respect to a **bias-variance** trade-off

Source: Ian Goodfellow, Yoshua Bengio, and Aaron Courville; Deep Learning, 2016

# Model Capacity: Overfitting vs Underfitting




Overfitting linked to …

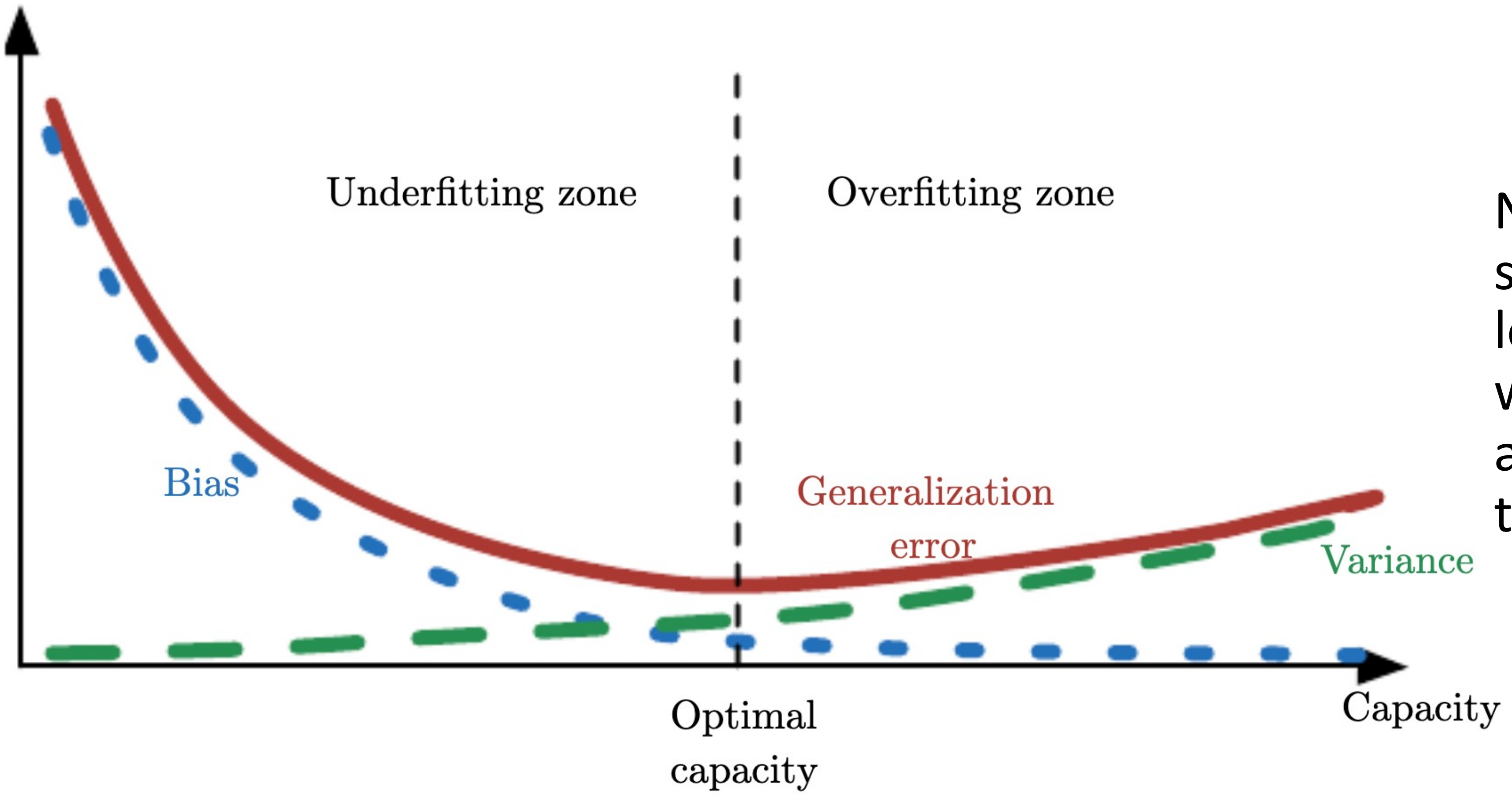
- High or low bias?
- High or low variance?

Underfitting linked to …

- High or low bias?
- High or low variance?

Source: Ian Goodfellow, Yoshua Bengio, and Aaron Courville; Deep Learning, 2016

# Model Capacity: Overfitting vs Underfitting




Neural networks can simultaneously arrive at low bias and low variance, with large neural networks and large amounts of training data

Source: Ian Goodfellow, Yoshua Bengio, and Aaron Courville; Deep Learning, 2016

# Summary: Model Capacity

- Goal: learn model with capacity that is neither too small nor too large so it generalizes well when predicting on previously unseen test data

- Challenges: choosing…
  - **Architecture** (i.e., number of layers, number of units per layer)
  - **Training algorithm** (e.g., training duration too brief/long)
  - **Training dataset** (e.g., insufficient training data)

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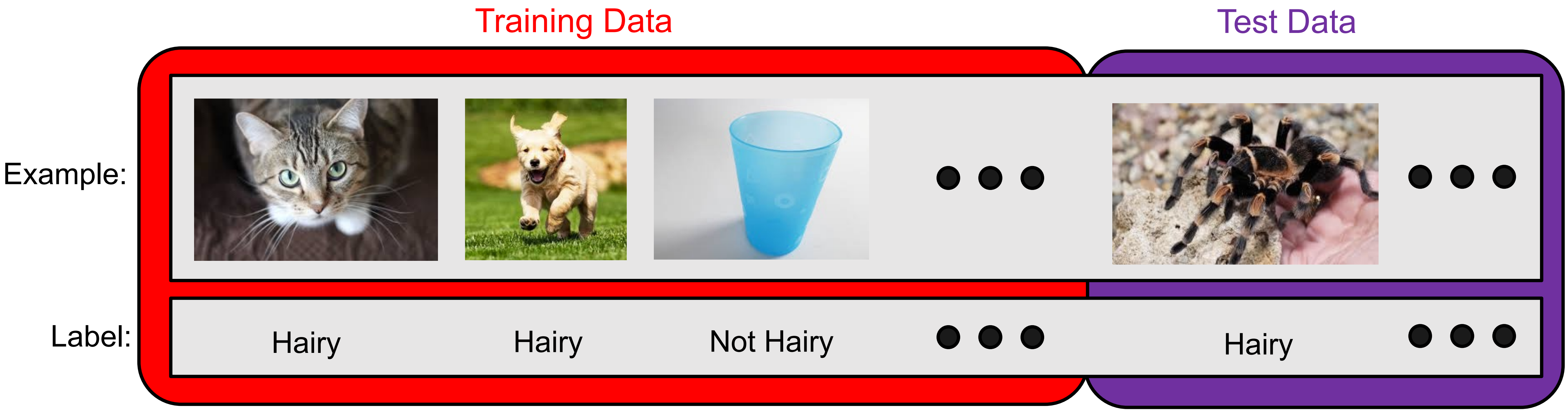
# Model Design Decisions

**Model hyperparameters (selected); e.g.,**
- Number of layers
- Number of units in each layer
- Activation function
- Batch size
- Learning rate
- …

**Model parameters (learned)**
- Weights
- Biases

Key Challenge: how to design a model without repeatedly observing the test data (which leads to overfitting)?

# Recall: Our Goal is to Design Models that **Generalize** Well to New, Previously Unseen Examples (Test Data)

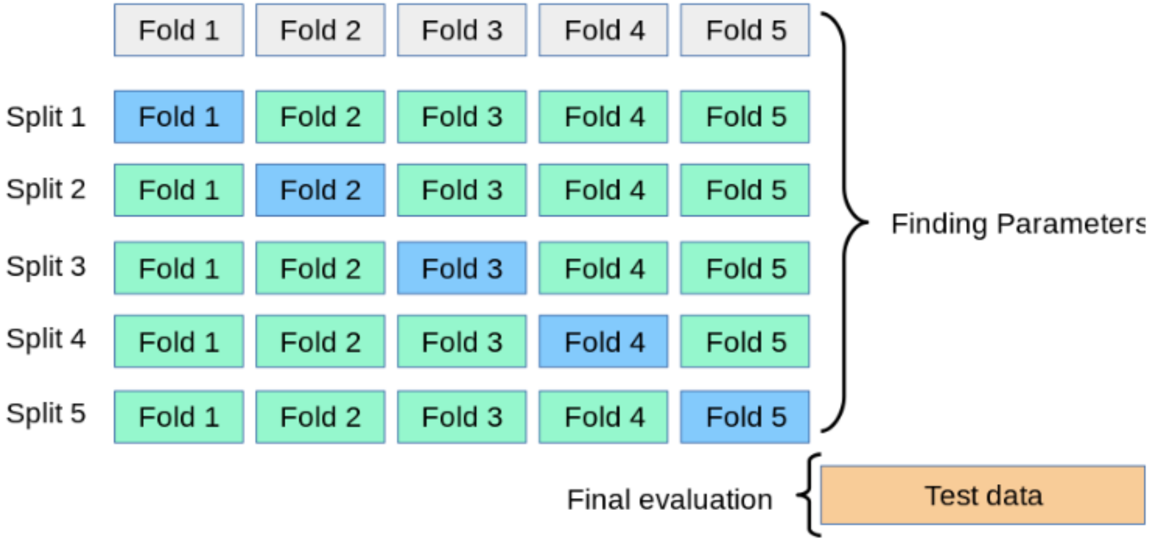



Key Challenge: how to design a model without repeatedly observing the test data (which leads to overfitting)?

# Hyperparameter Tuning: Split Training Set So It Can Be Used to Test Different Hyperparameters

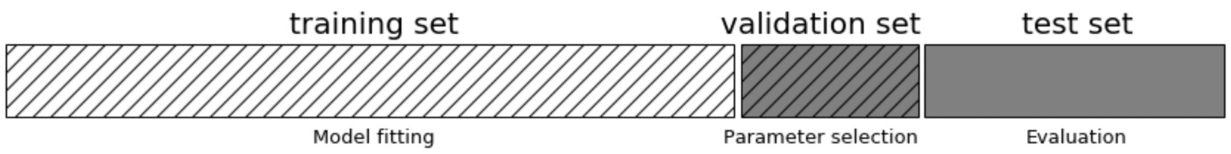
For statistically strong results:

## Small training dataset: cross validation




https://kevinzakka.github.io/2016/07/13/k-nearest-neighbor/

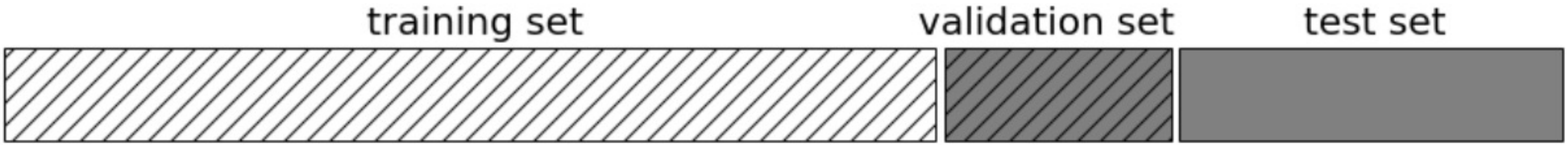
## Else: train/validation split




https://github.com/amueller/introduction_to_ml_with_python/blob/master/05-model-evaluation-and-improvement.ipynb

# Train/Validation/Test Split

- Split dataset into 3 sets: “train”, “validation”, and “test” splits
  - e.g., 60%/20%/20% train/val/test split




- **Hyperparameter selection**: test variants on validation set to identify best set of hyperparameters
- **Final model**: train a new model on data in the training AND validation splits using the best hyperparameters from hyperparameter selection

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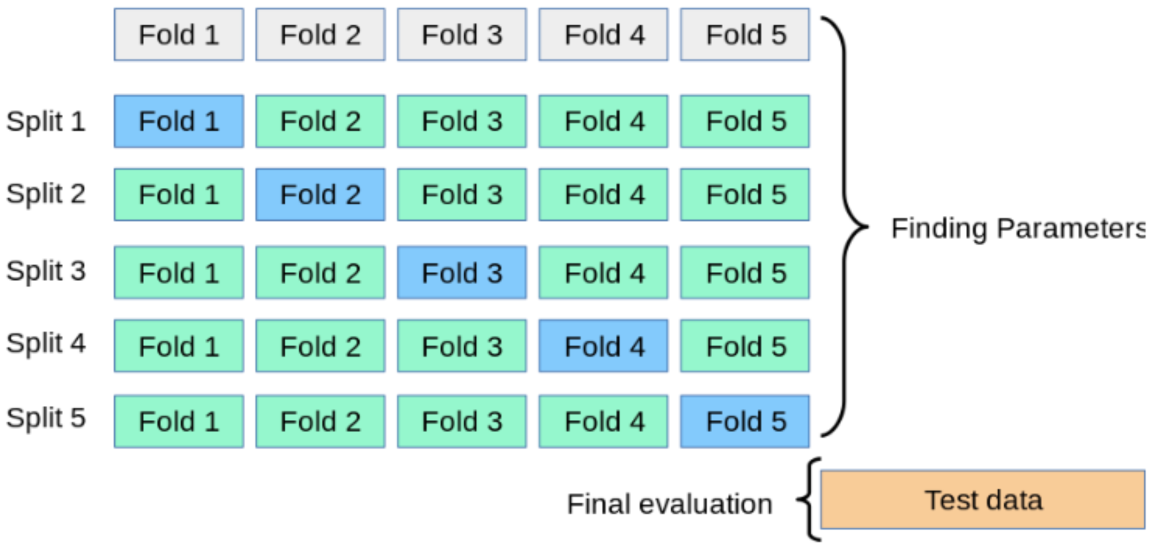


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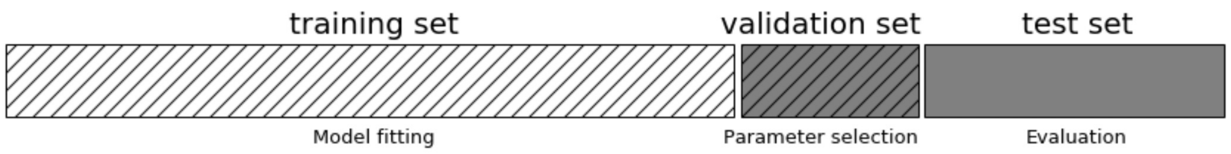


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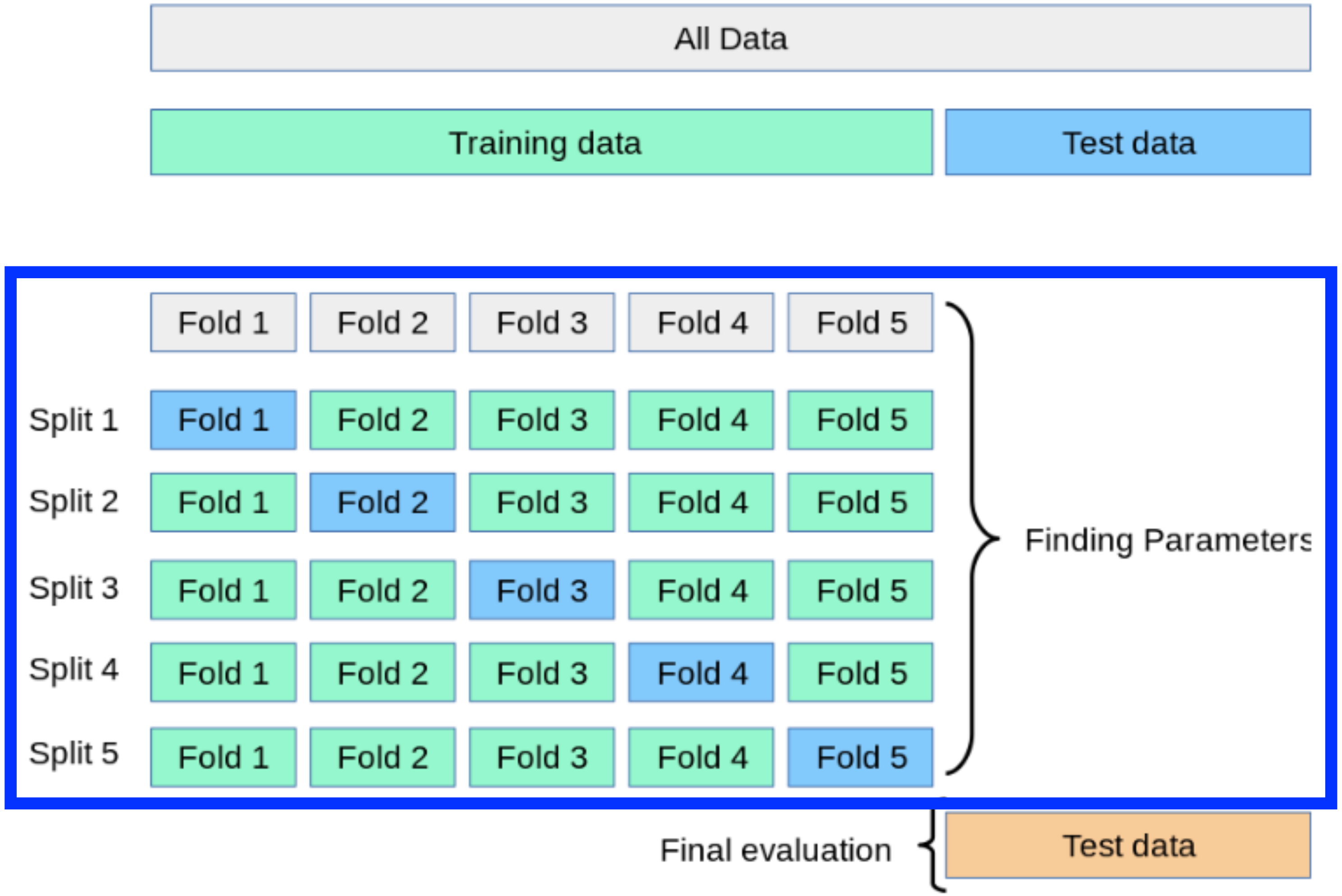
# Cross-Validation: Limit Influence of Dataset Split

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# Cross-Validation: Limit Influence of Dataset Split

**e.g., 3-fold cross-validation on training data**

Input:    ● ● ●  ● ● ●

Label: Hairy | Hairy | Not Hairy | ● ● ● | Not Hairy | ● ● ●

$\underbrace{\qquad\qquad}_{1/3}$ $\underbrace{\qquad\qquad}_{1/3}$ $\underbrace{\qquad\qquad}_{1/3}$

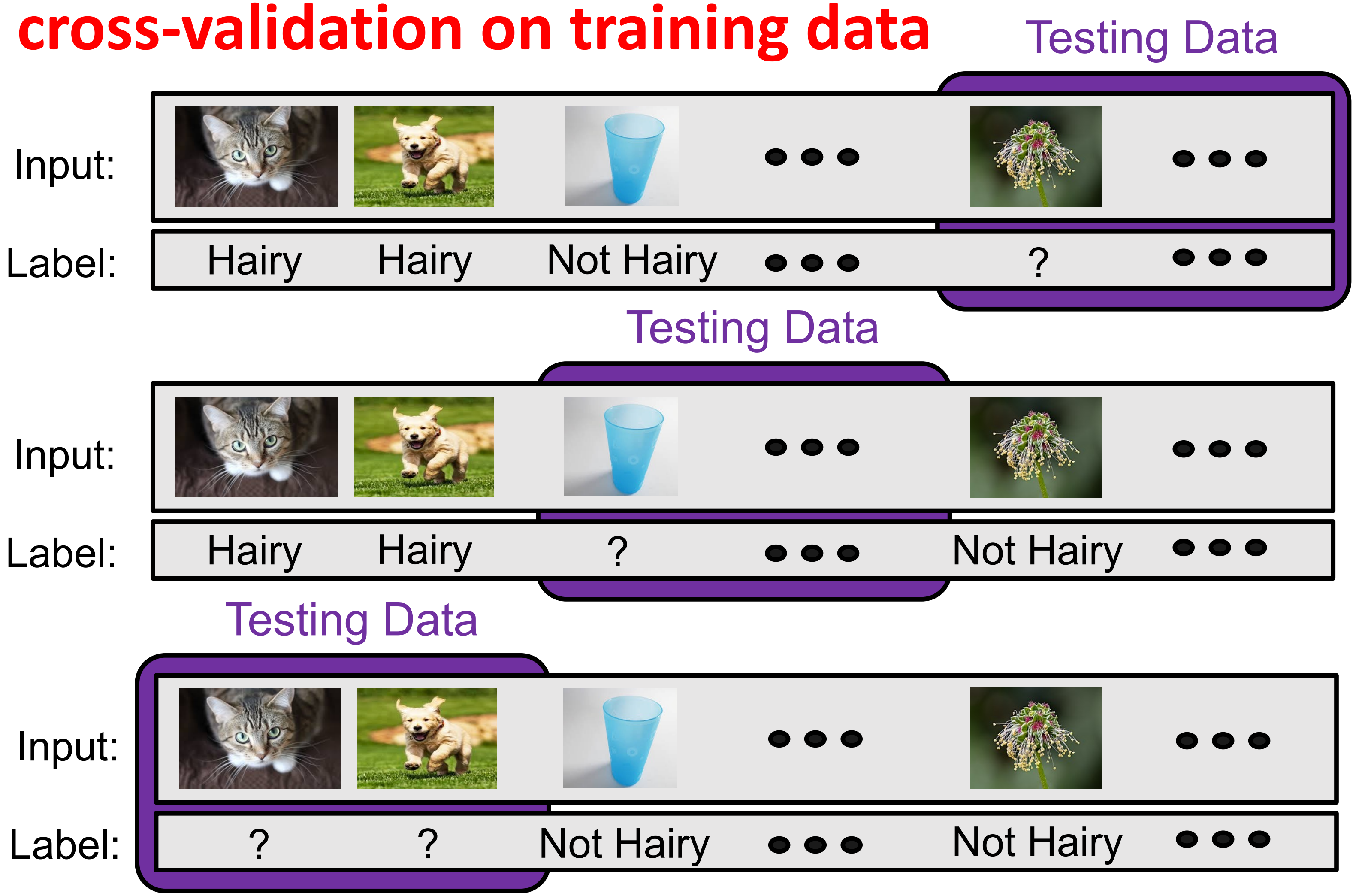
# Cross-Validation: Limit Influence of Dataset Split

**e.g., 3-fold cross-validation on training data**

**Fold 1:**
- train on k-1 partitions
- test on k partitions

**Fold 2:**
- train on k-1 partitions
- test on k partitions

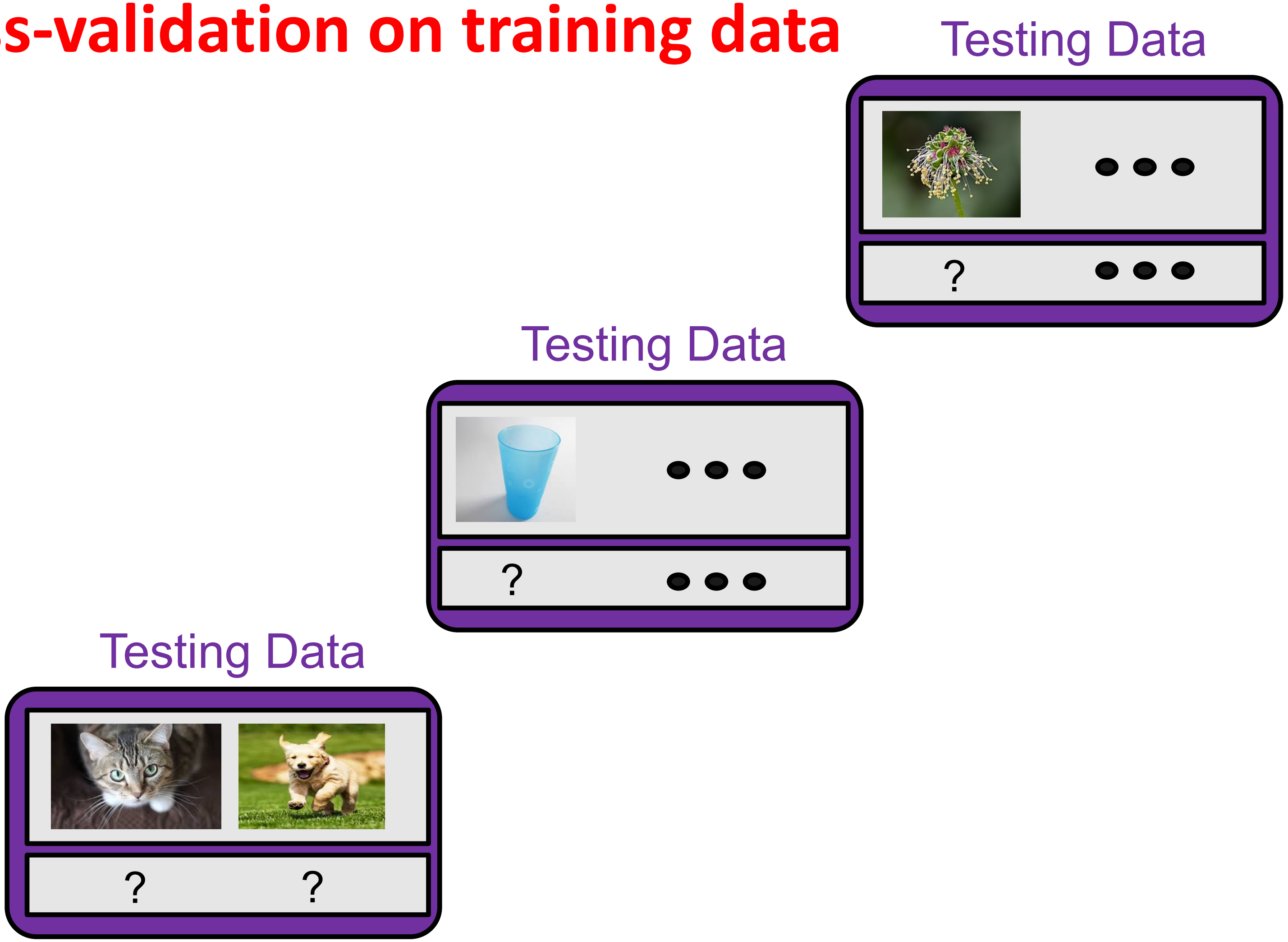
**Fold 3:**
- train on k-1 partitions
- test on k partitions



# Cross-Validation: Limit Influence of Dataset Split

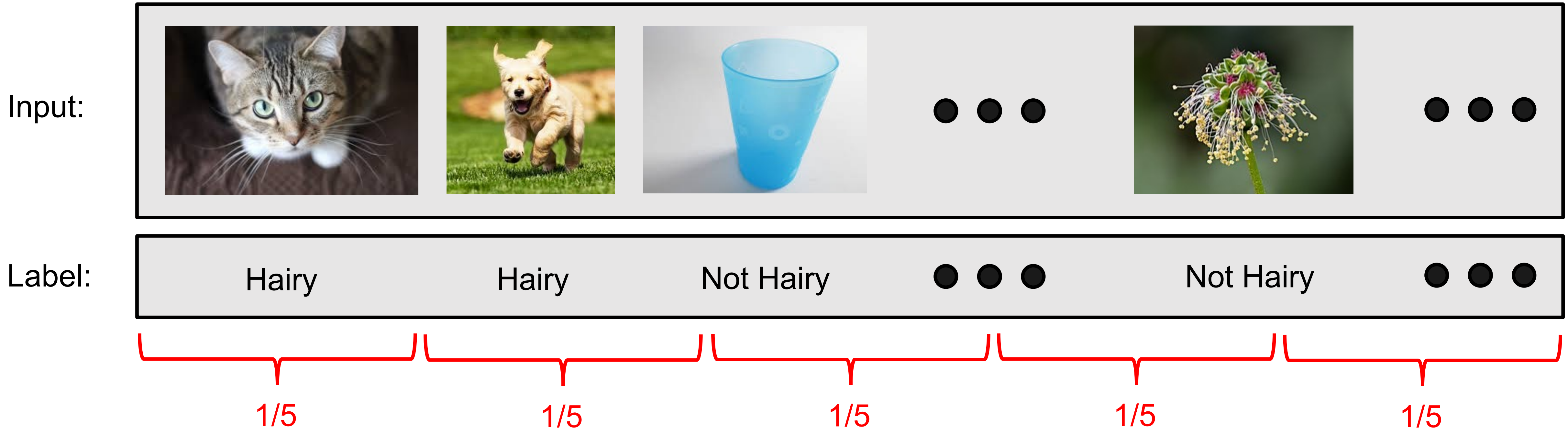
**e.g., 3-fold cross-validation on training data**

**Model performance:** performance across all folds of "test" data



# Cross-Validation: Limit Influence of Dataset Split

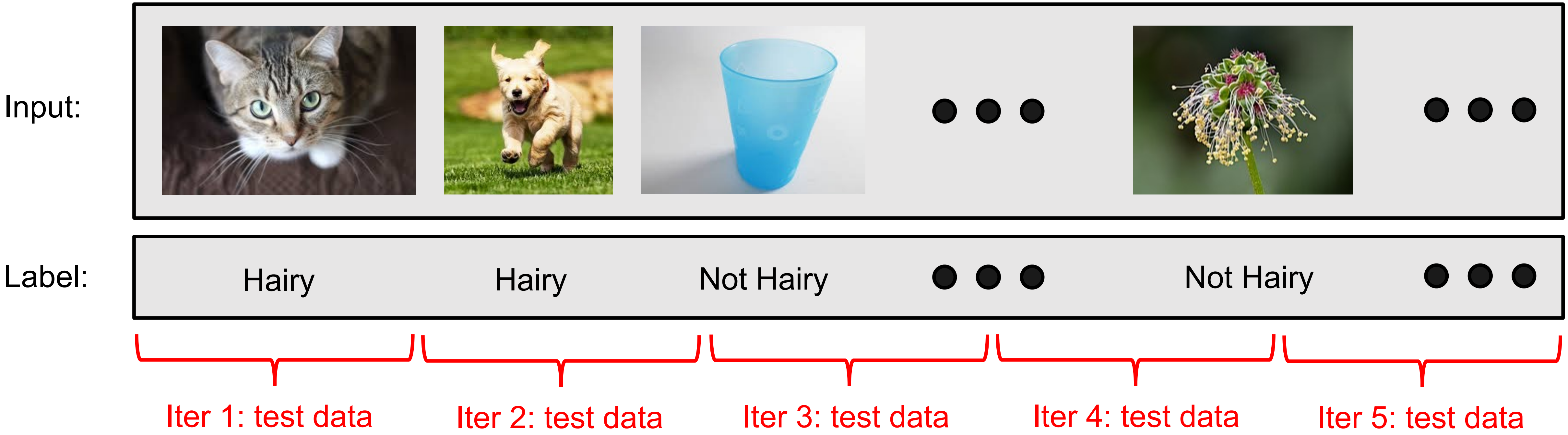
**e.g., 5-fold cross-validation on training data**




**How many partitions of the data to create?**

# Cross-Validation: Limit Influence of Dataset Split

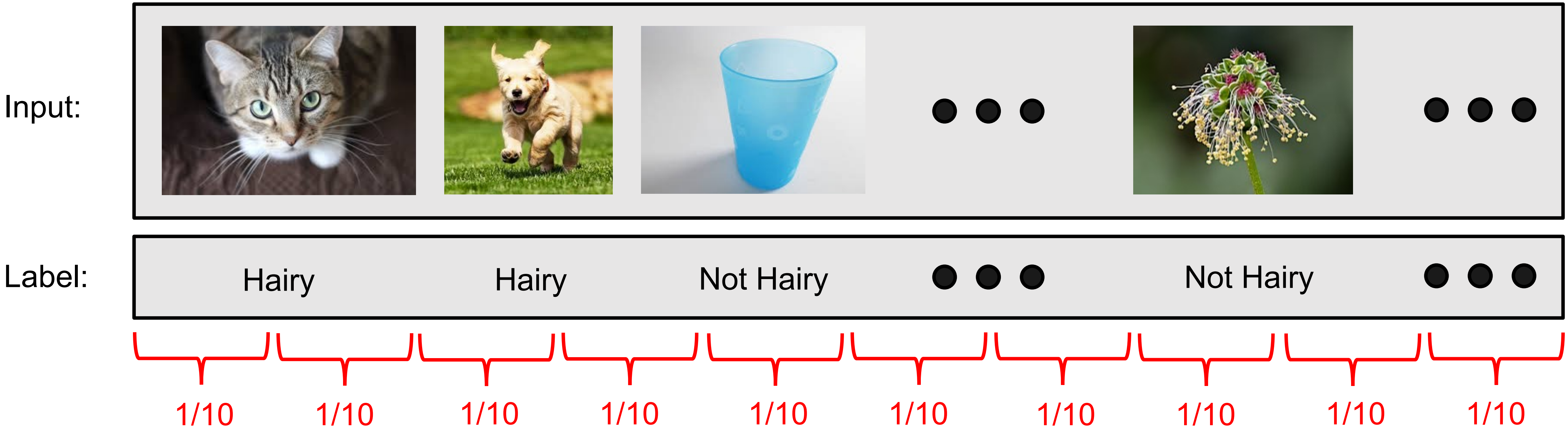
**e.g., 5-fold cross-validation on training data**




**How many iterations of train & test to run?**

# Cross-Validation: Limit Influence of Dataset Split

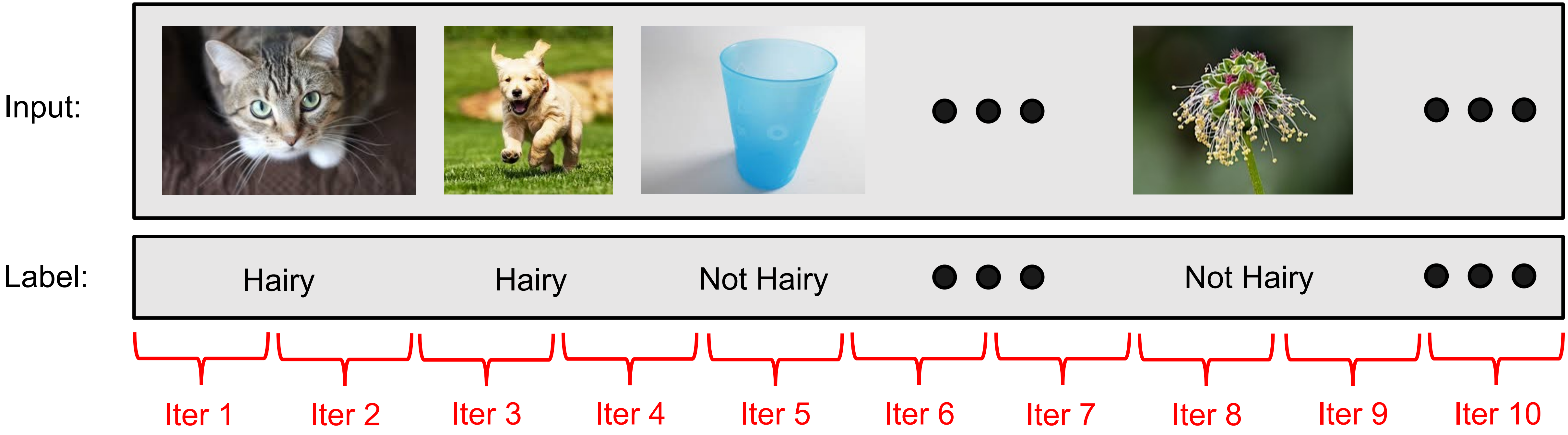
**e.g., 10-fold cross-validation on training data**




**How many partitions of the data to create?**

# Cross-Validation: Limit Influence of Dataset Split

**e.g., 10-fold cross-validation on training data**




**How many iterations of train & test to run?**

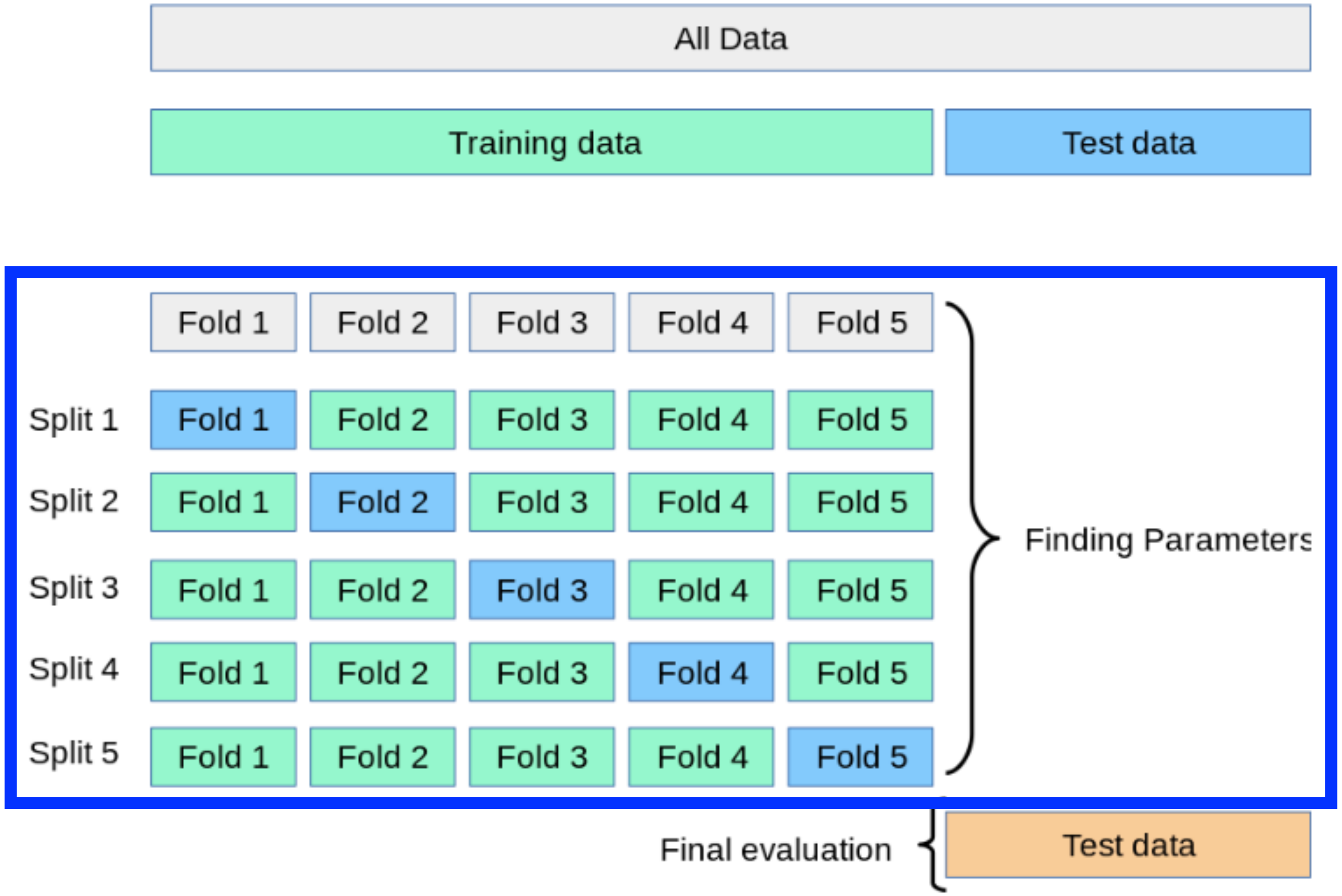
# Cross-Validation: Limit Influence of Dataset Split

**e.g., k-fold cross-validation on training data**


**What are the (dis)advantages of using larger values for "k"?**

# Cross-Validation: Limit Influence of Dataset Split

Select the hyperparameters that lead to the best results overall across all the folds

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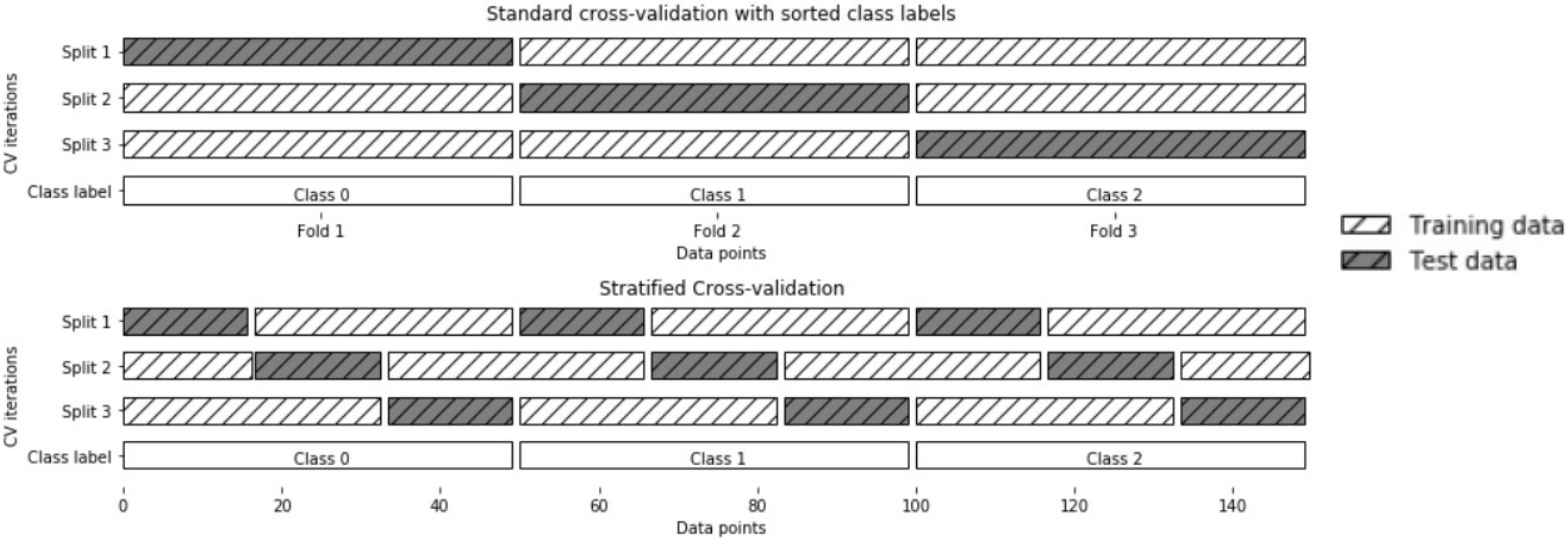
# Stratified Dataset Splits

- For imbalanced datasets, preserve frequencies of each category in each split; e.g.,

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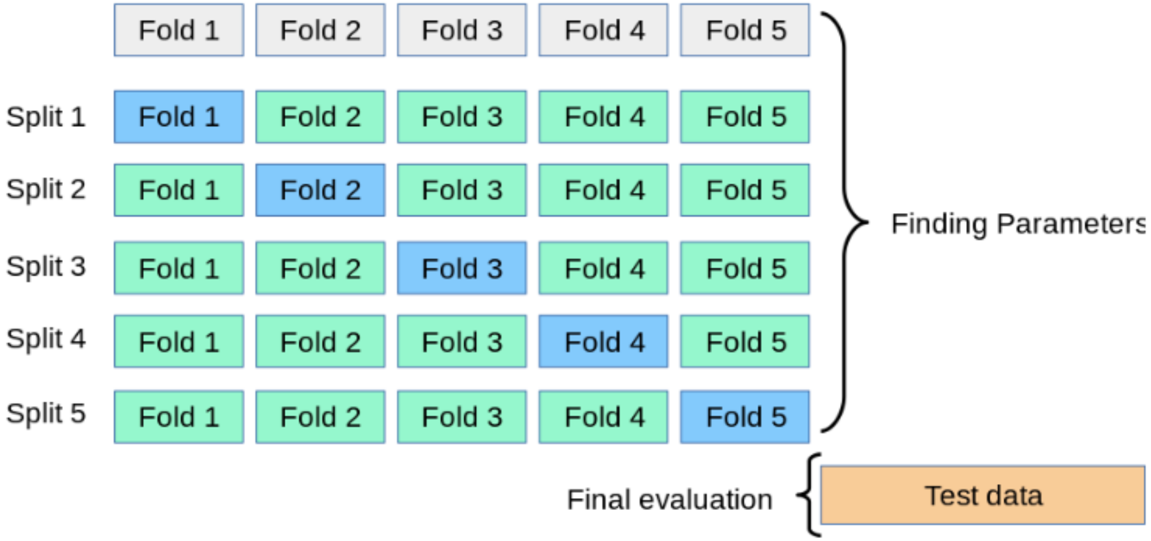
# Summary: Hyperparameter Tuning Approaches

For statistically strong results:

Small training dataset: cross validation

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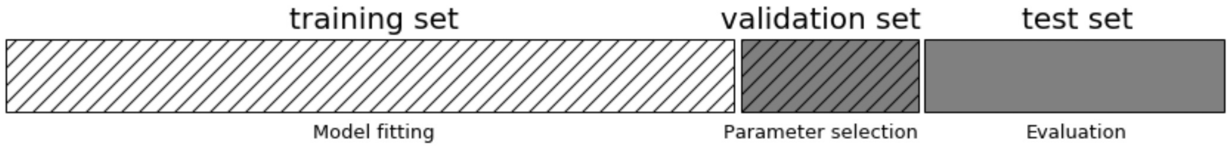


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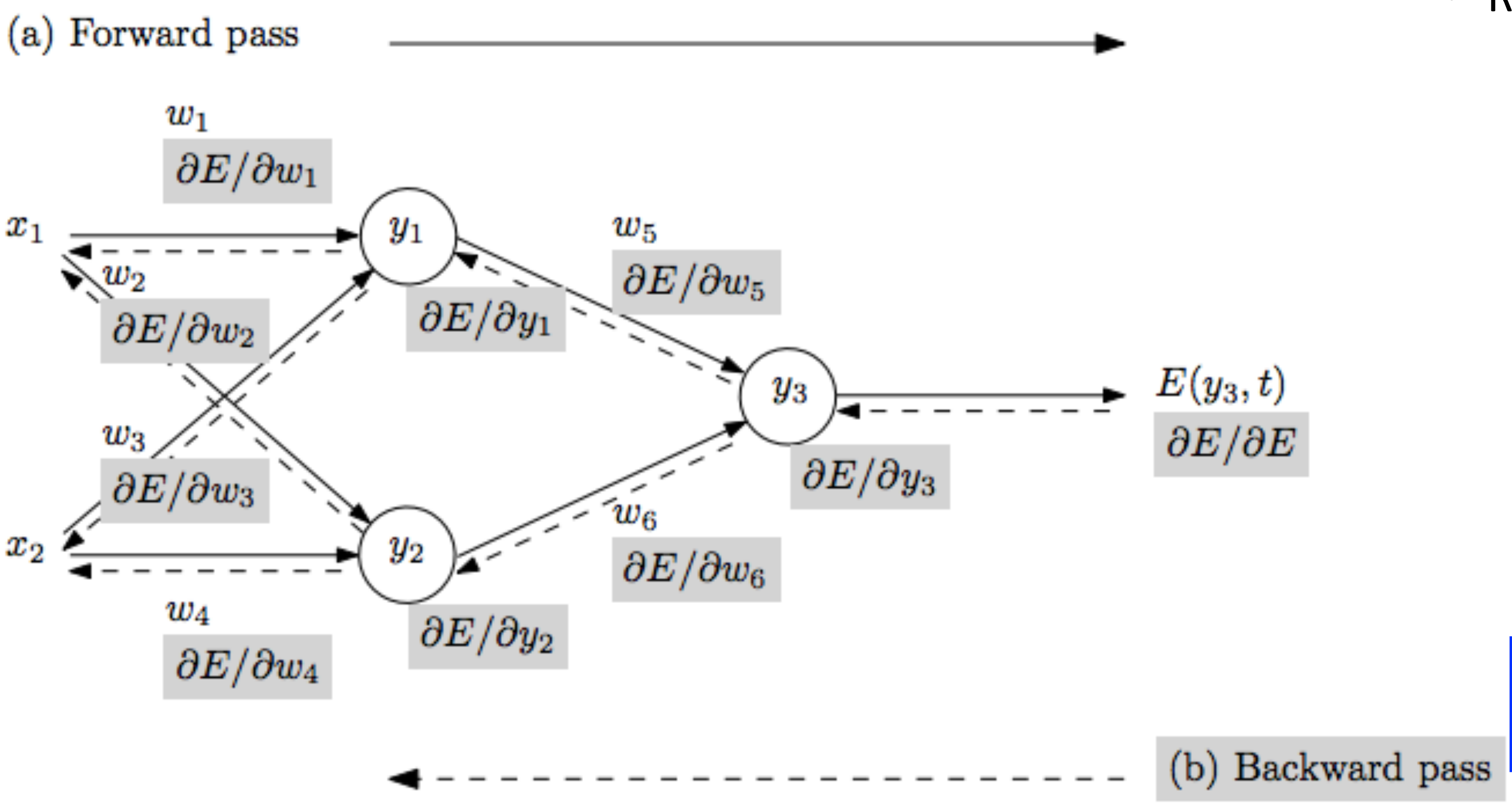
# Challenge: Train Faster!!!

Algorithm training can take hours, days, weeks, months, or more with big data and so many parameters…

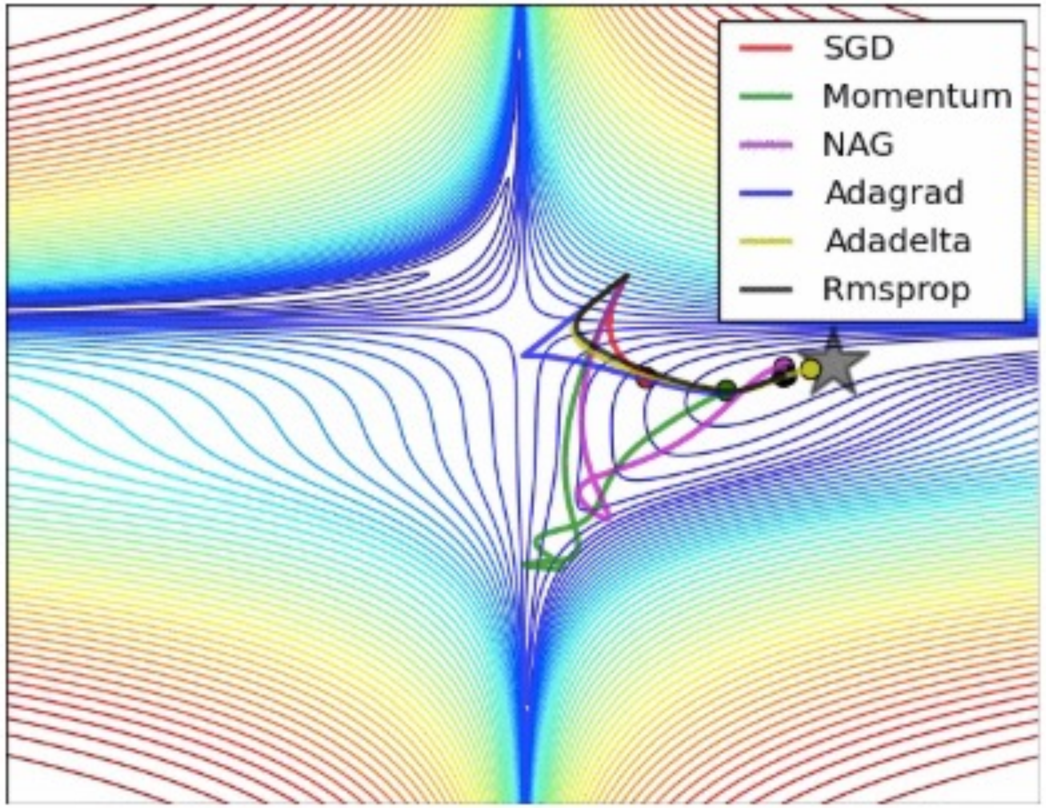
# Recall: How Neural Networks Learn

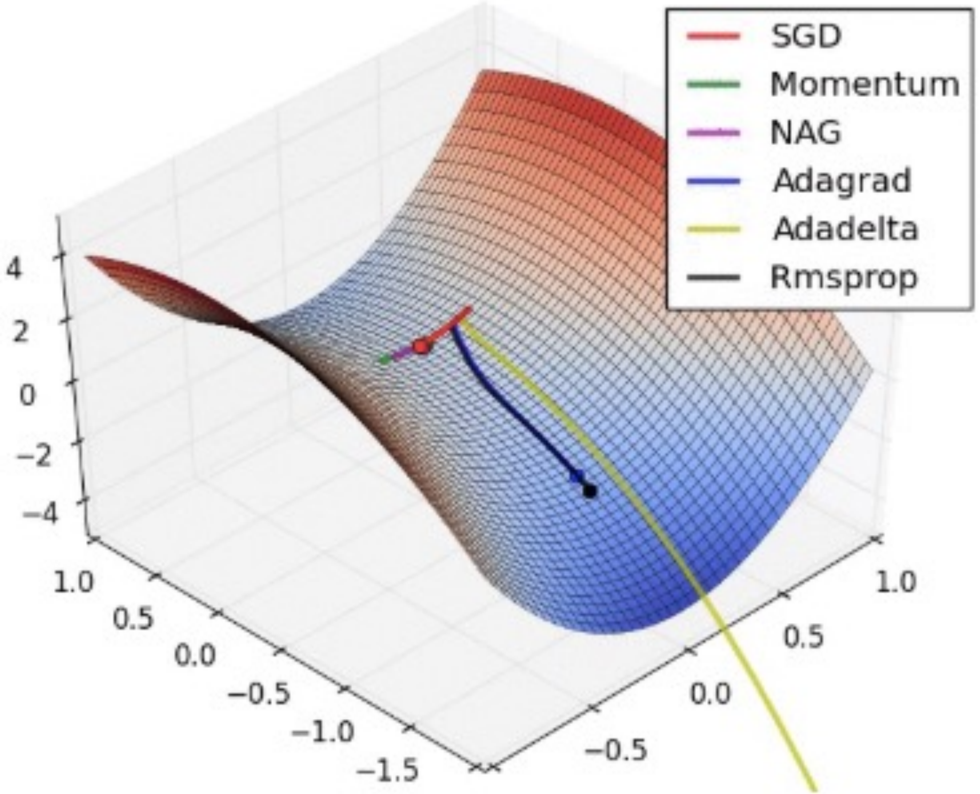



- Repeat until stopping criterion met:
  1. **Forward pass**: propagate training data through model to make prediction
  2. Quantify the dissatisfaction with a model's results on the training data
  3. **Backward pass**: using predicted output, calculate gradients backward to assign blame to each model parameter
  4. Update each parameter using calculated gradients

Figure from: Atilim Gunes Baydin, Barak A. Pearlmutter, Alexey Andreyevich Radul, Jeffrey Mark Siskind; Automatic Differentiation in Machine Learning: a Survey; 2018

# Train Faster: How to Update Using Gradient?



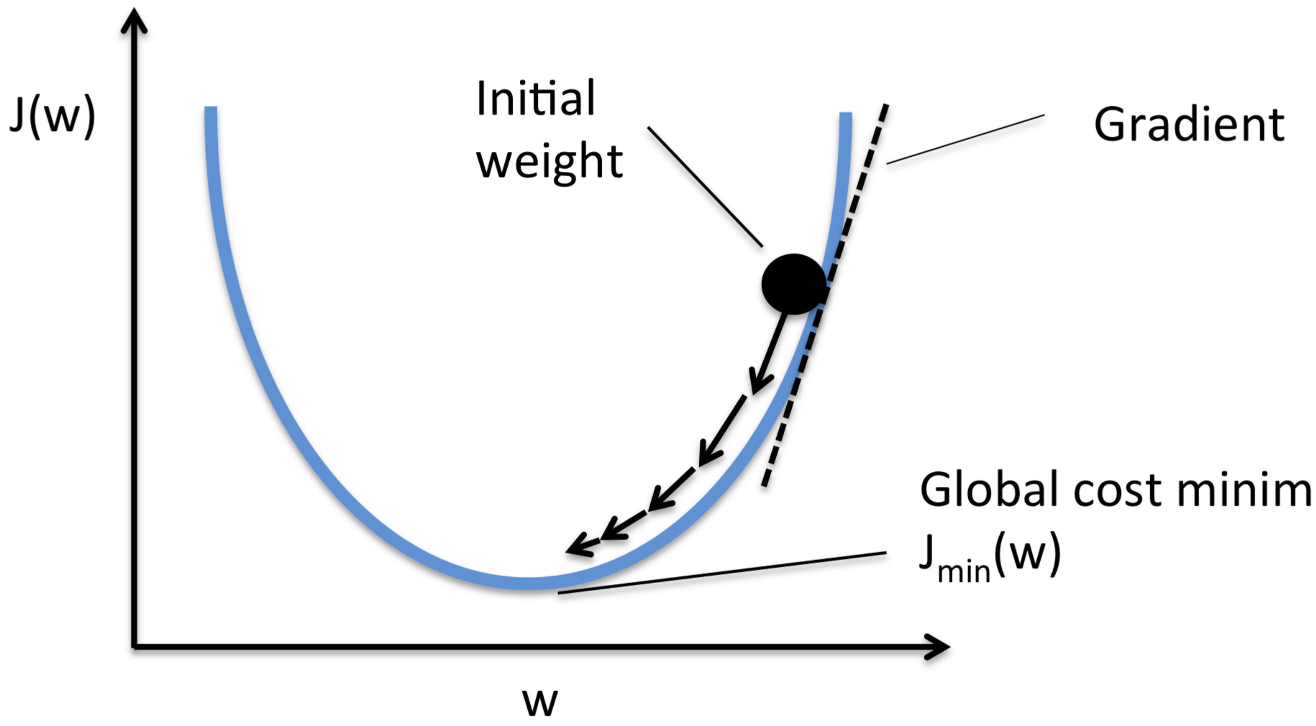

- Demo at http://cs231n.github.io/neural-networks-3/#update

# Train Faster: How to Update Using Gradient?

Parameters Gradient

- Vanilla Approach: `x += - learning_rate * dx`

Inefficient since steps get smaller as gradient gets smaller




http://cs231n.github.io/neural-networks-3/#update

Figure from: https://rasbt.github.io/mlxtend/user_guide/general_concepts/gradient-optimization/

# Train Faster: How to Update Using Gradient?

- Momentum optimization:
  - Analogy: roll a ball down a hill and it will pick up momentum

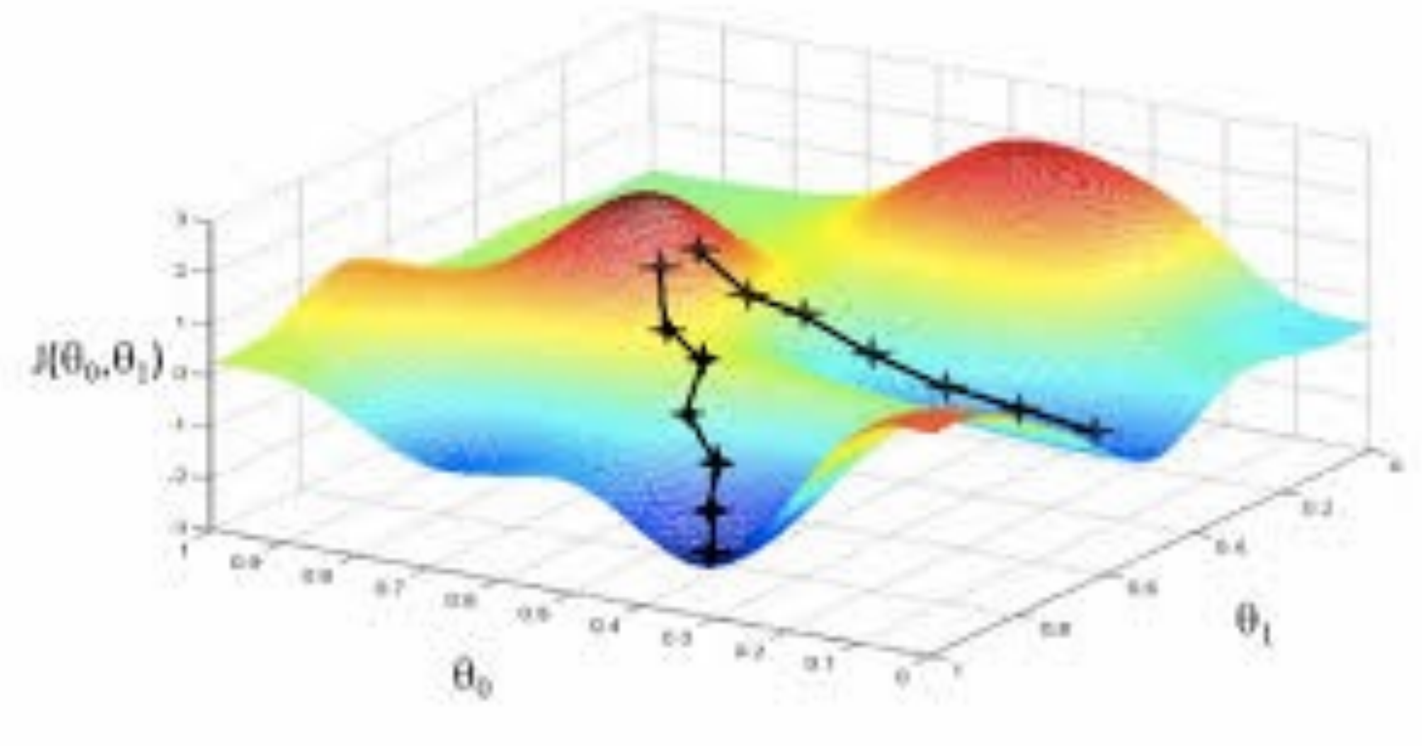



Figure from: https://medium.com/ai-society/hello-gradient-descent-ef74434bdfa5

# Train Faster: How to Update Using Gradient?

- Momentum optimization:
  - Analogy: roll a ball down a hill and it will pick up momentum

Like friction; values range from 0 to 1 with larger being greater friction

Velocity vector captures cumulative direction of previous gradients; initialized to 0

Gradient not used for speed but instead acceleration

```
v = mu * v - learning_rate * dx # integrate velocity
x += v # integrate position
```

- What are advantages and disadvantages?
  - Can roll past local minima ☺
  - It may roll past optimum and oscillate around it ☹
  - Another hyperparameter to tune: mu ☹

http://cs231n.github.io/neural-networks-3/#update

# Train Faster: How to Update Using Gradient?

- Step decay:
  - Reduce the learning rate by some factor every few epochs

- Exponential decay

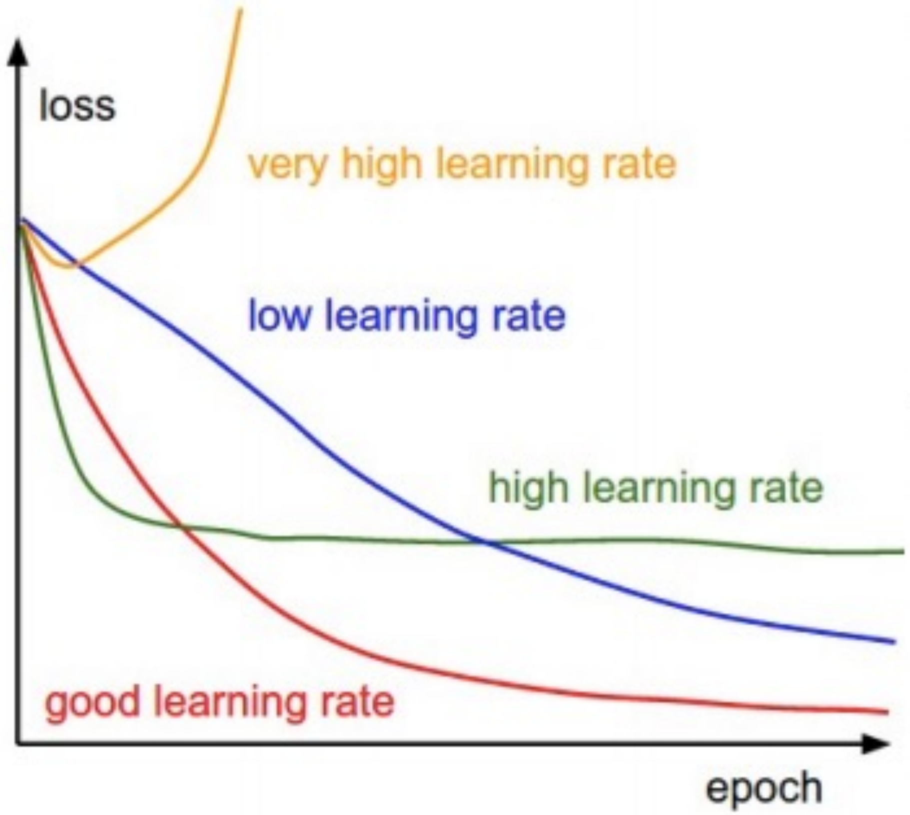
- 1/t decay

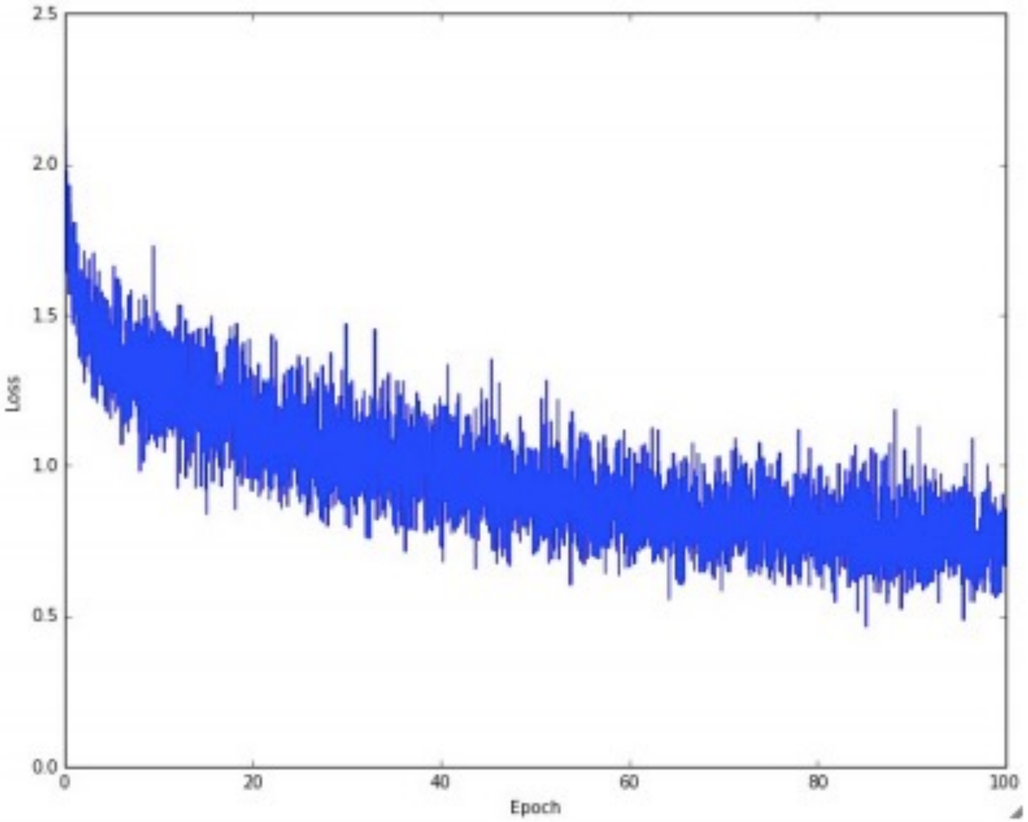
- Adapt learning rate per-parameter
- e.g., AdaGrad, RMSprop, and Adam (i.e., adaptive momentum – very popular in practice)

http://cs231n.github.io/neural-networks-3/#update

# Monitor Loss/Error During Training

- What should happen to the loss function value during training?

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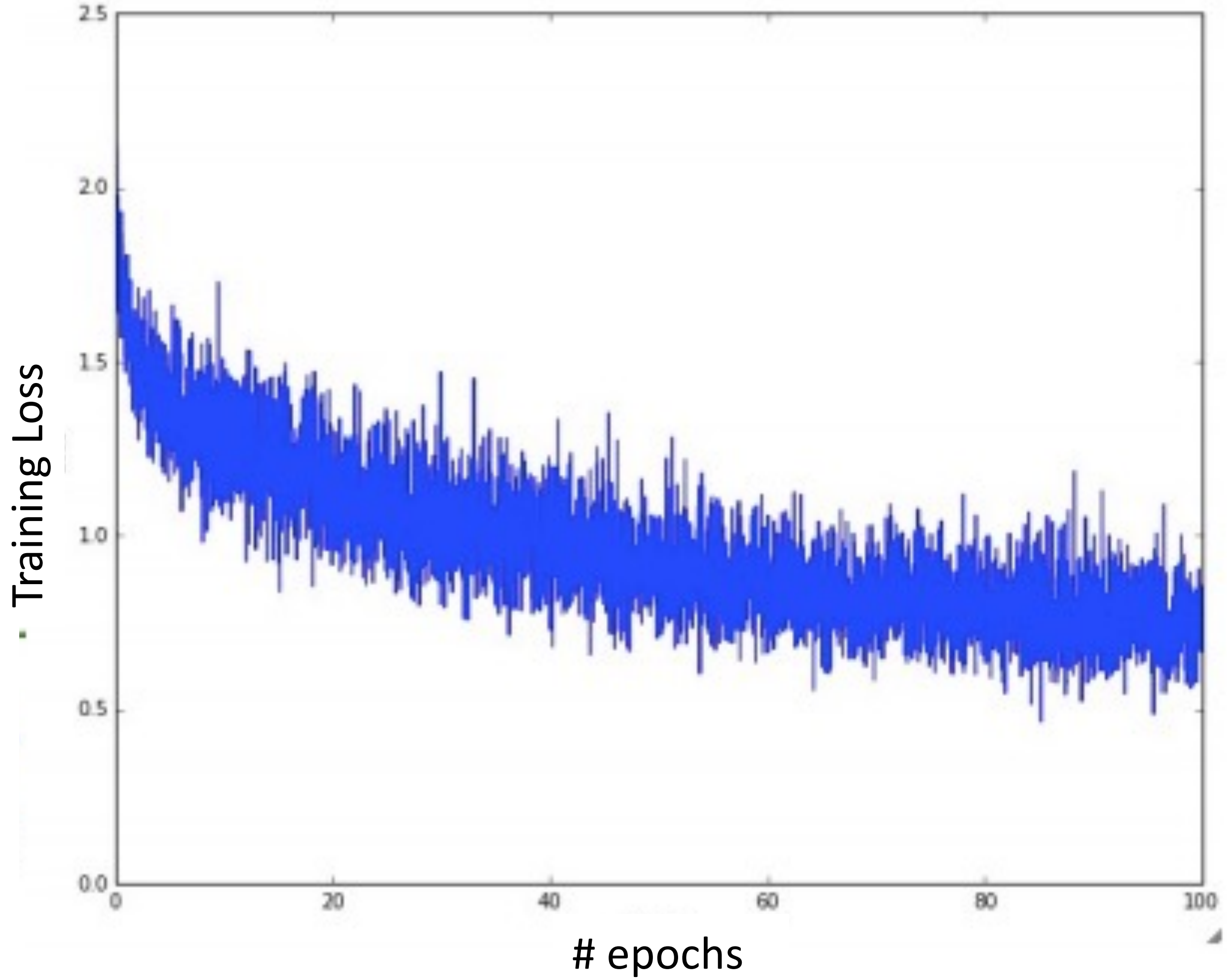
# Analysis: Why Might There Be Oscillations in the Learning Curve for the Training Loss?

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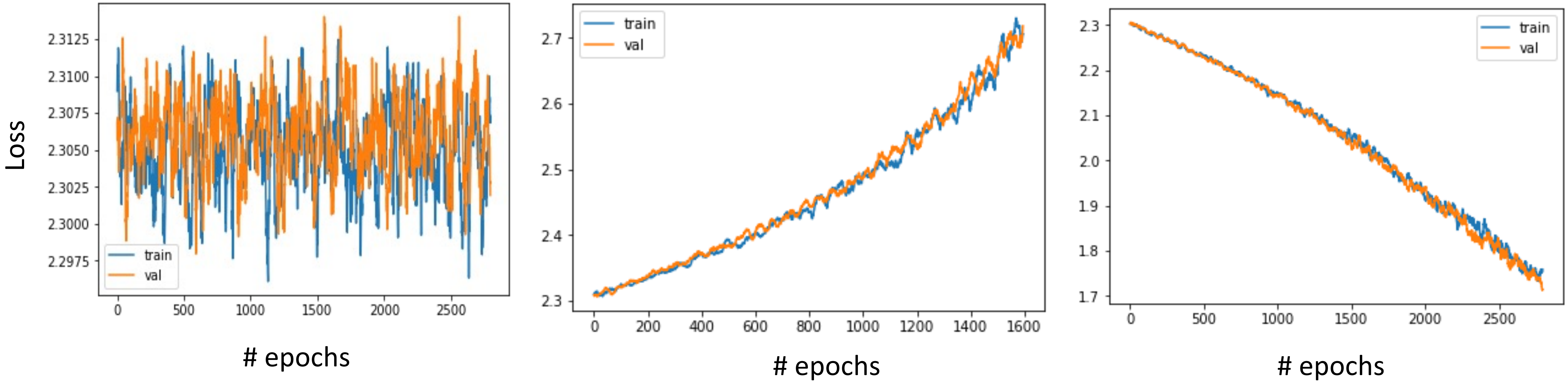
# Discussion: From These Learning Curves, What Do You Think Is Happening and What Might Be a Fix?

(a) (b) (c)



# Feeling Bewildered By Your Learning Curves?

You may feel better when looking at this link:

https://lossfunctions.tumblr.com/

# Today’s Topics

- Universal approximation theorem vs No Free Lunch theorem
- Selecting model capacity: avoid overfitting and underfitting
- Selecting model hyperparameters
- Learning efficiently: optimization methods
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The End