Neural Network Training

Deep Learning
CS 435/635

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AI Lab Coordinator @IIT Indore

Course Content

Module I: History of Deep Learning, Sigmoid Neurons, Perceptrons, and learning algorithms. Multilayer Perceptrons (MLPs), Representation Power of MLPs,.

Module II: Feedforward Neural Networks. Backpropagation. first and second-order training methods. **NN Training tricks, Regularization**

Module III: Introduction to Autoencoders and their characteristics, relation to PCA, Regularization in autoencoders, and Types of autoencoders.

Module IV: Architecture of Convolutional Neural Networks (CNN), types of CNNs.

Module V: Architecture of Recurrent Neural Networks (RNN), Backpropagation through time. Encoder-Decoder Models, Attention Mechanism. Advanced Topics: Transformers and BERT.

Acknowledgement

- Neural Networks and Deep Learning course by Danna Gurari University of Colorado Boulder

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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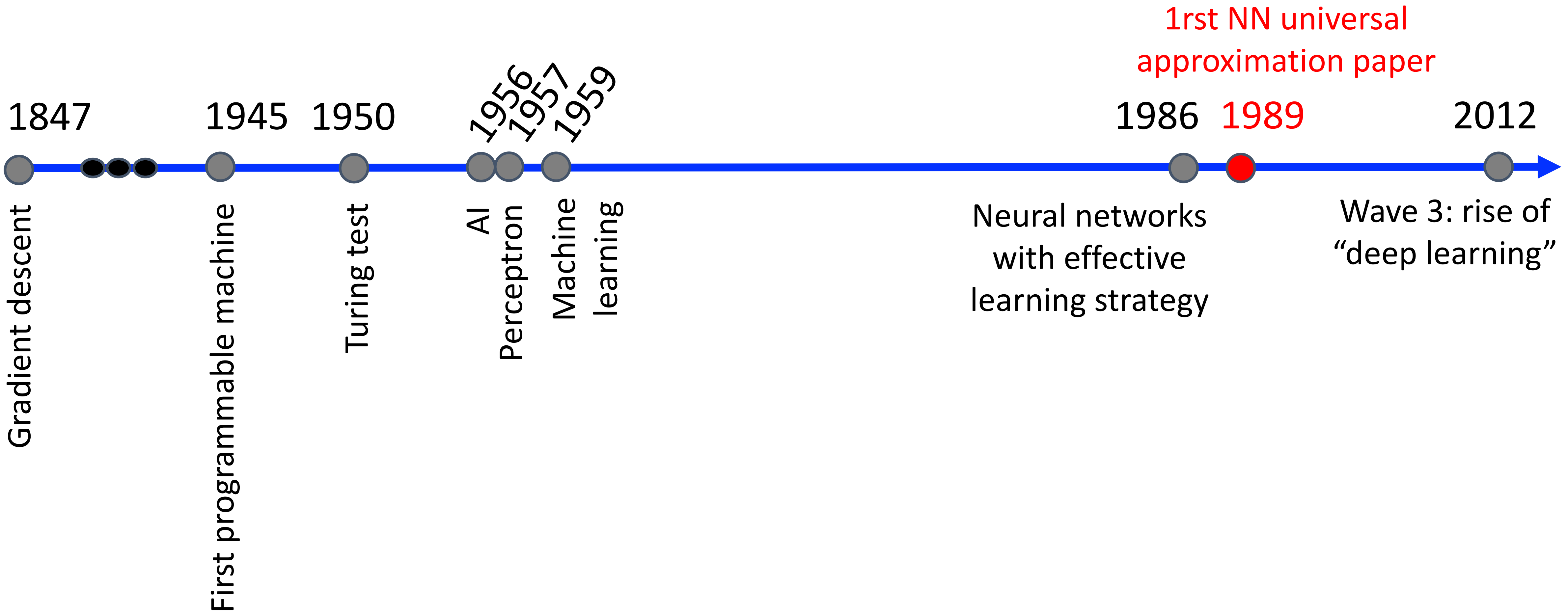
Historical Context: Universal Approximator

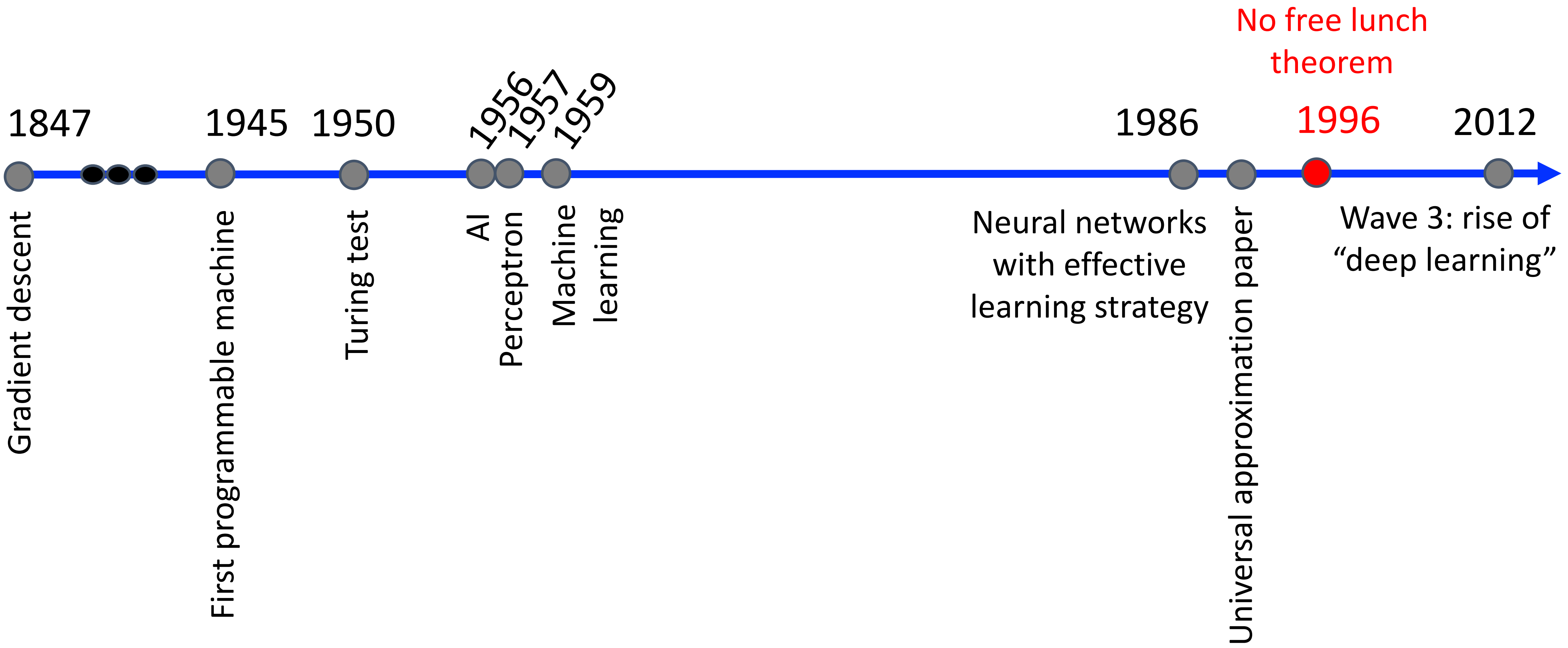


Hornik, Stinchcombe and White. Multilayer feedforward networks are universal approximators. Neural Networks, 1989

“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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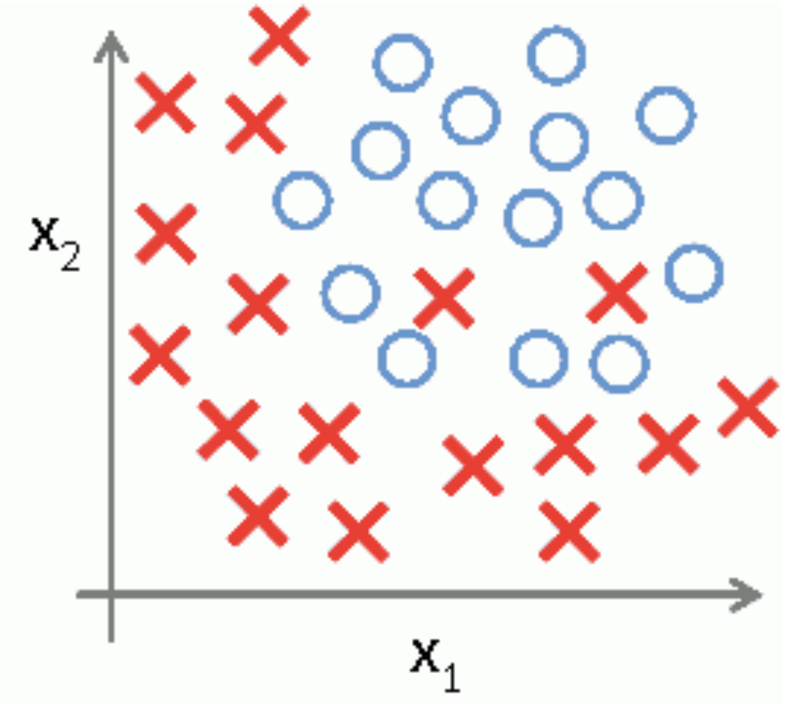
Recall: Class Exercise from Lecture 1

- 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?

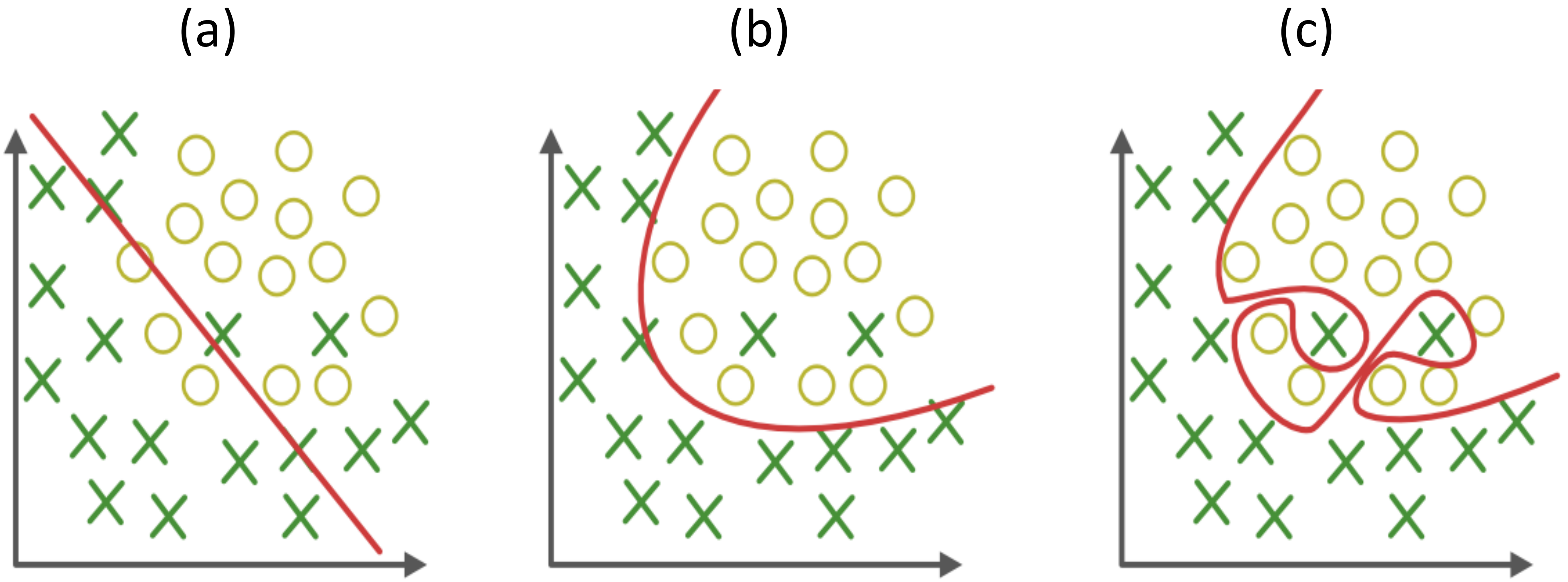


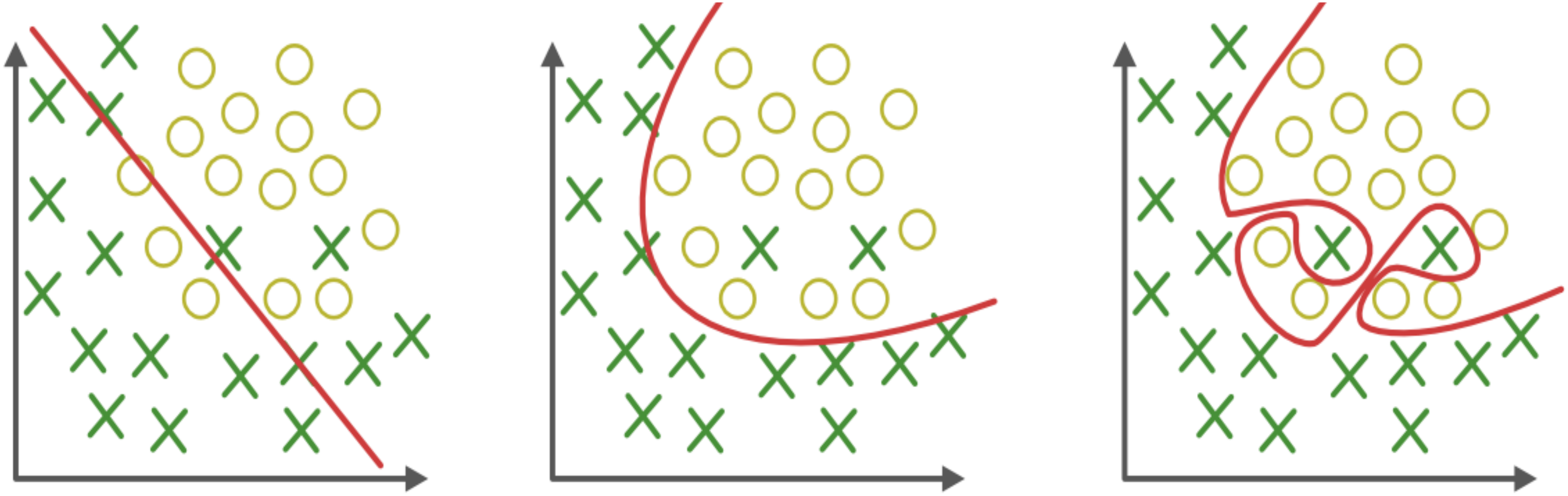
Figure source: https://towardsdatascience.com/underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6fe4a8a49dbf

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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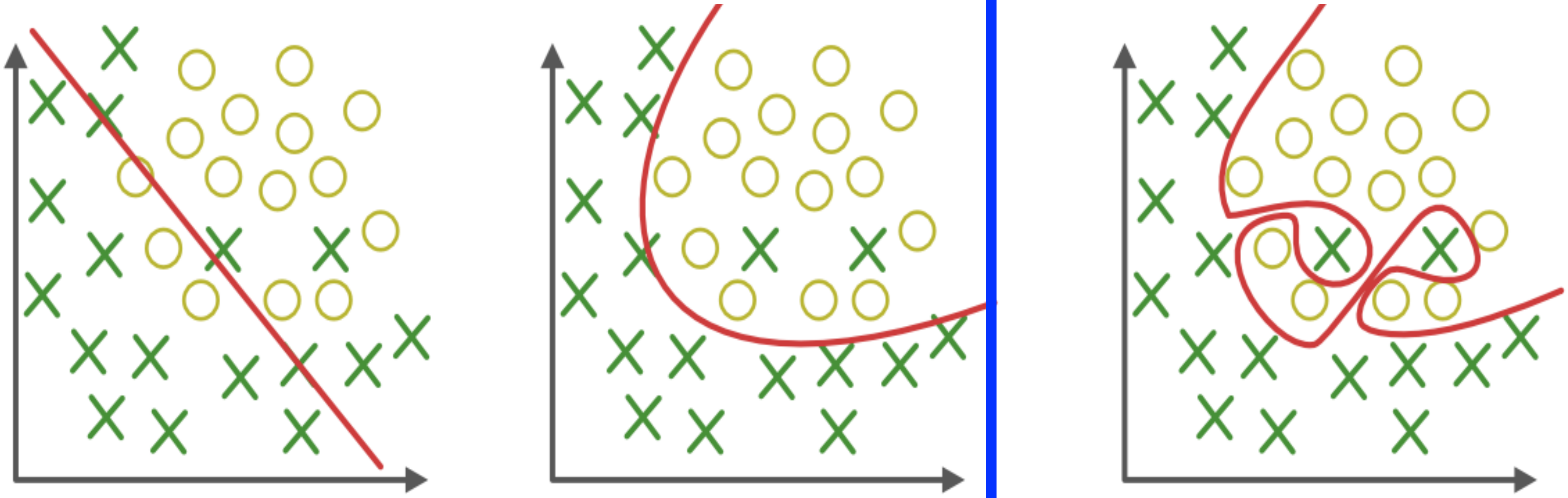
Model Capacity

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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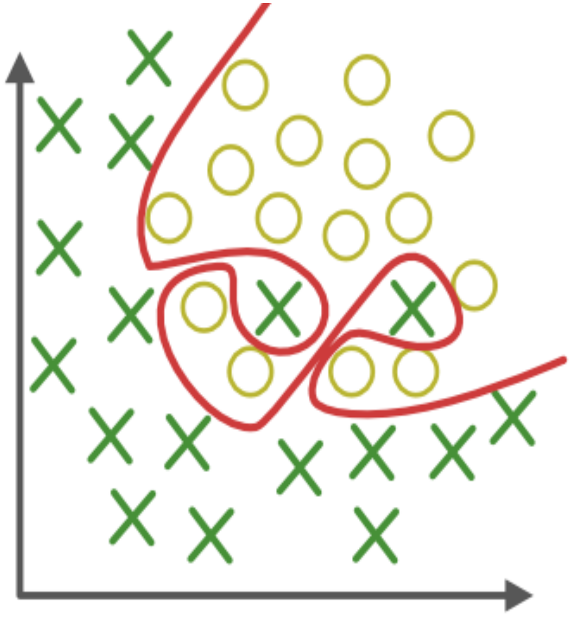
Model Capacity: Overfitting Problem

- 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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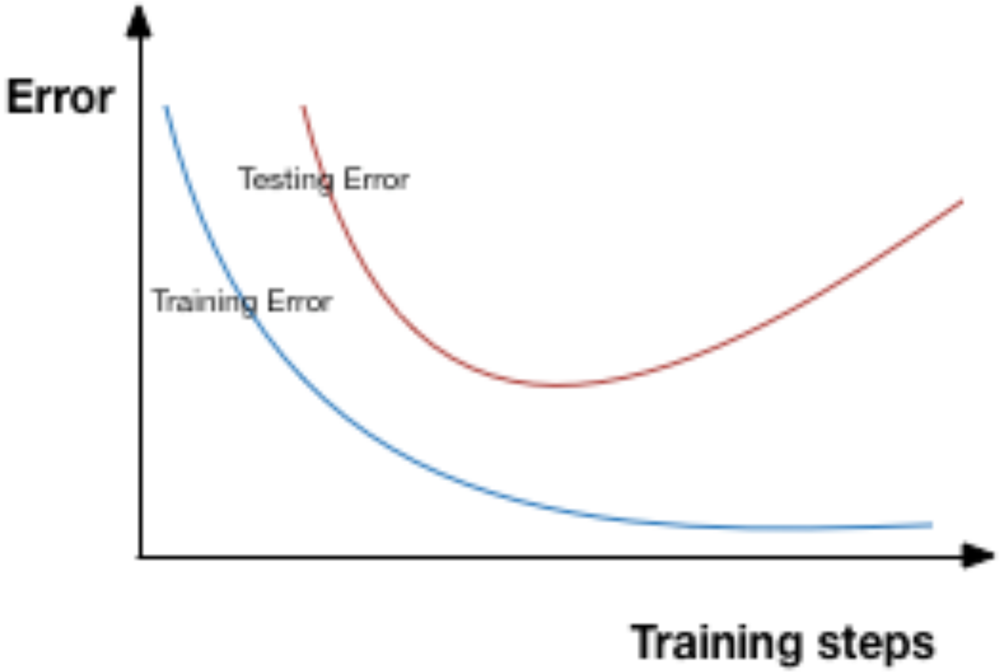
Model Capacity: Overfitting Remedy

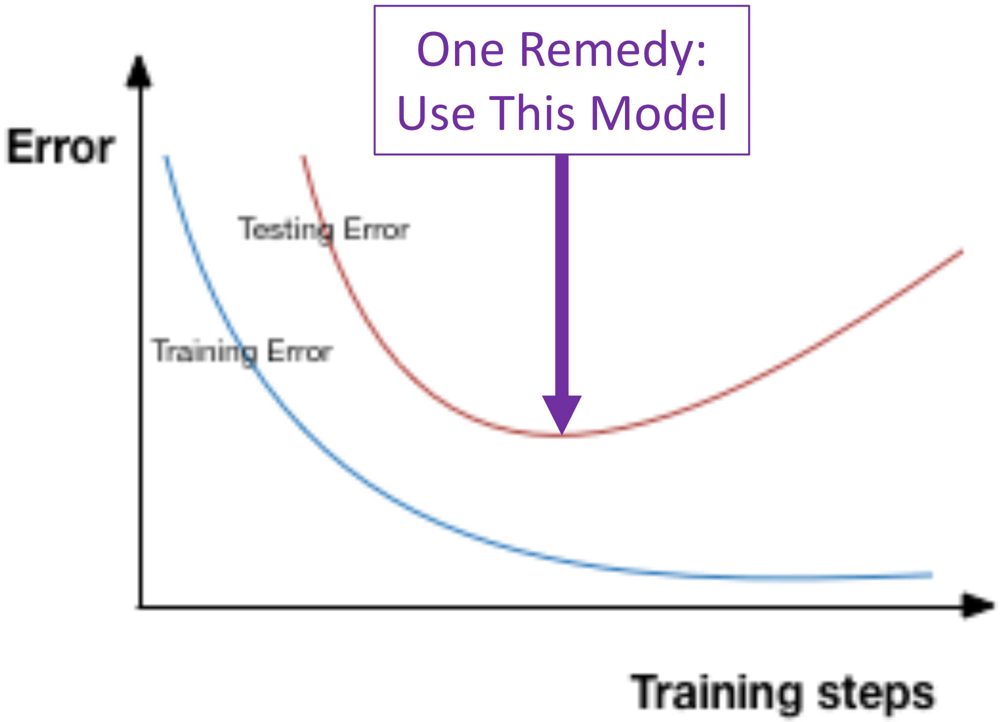


- To detect overfitting, analyze **learning curves** for models tested on training data and test data
  - What happens to training data error as number of training steps increases?
    - Error shrinks
  - What happens to test data error as number of training steps increases?
    - Error shrinks and then 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

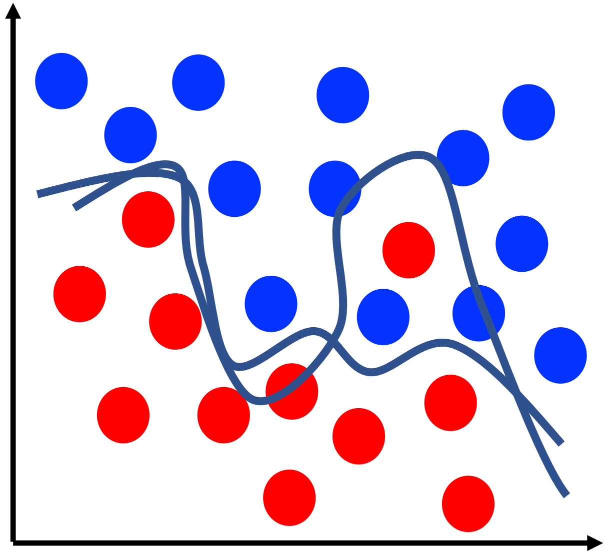
Image Source: https://chatbotslife.com/regularization-in-deep-learning-f649a45d6e0

Model Capacity: How to Avoid Overfitting?

Early stopping



Add training data



Many more techniques to be discussed in this course…

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

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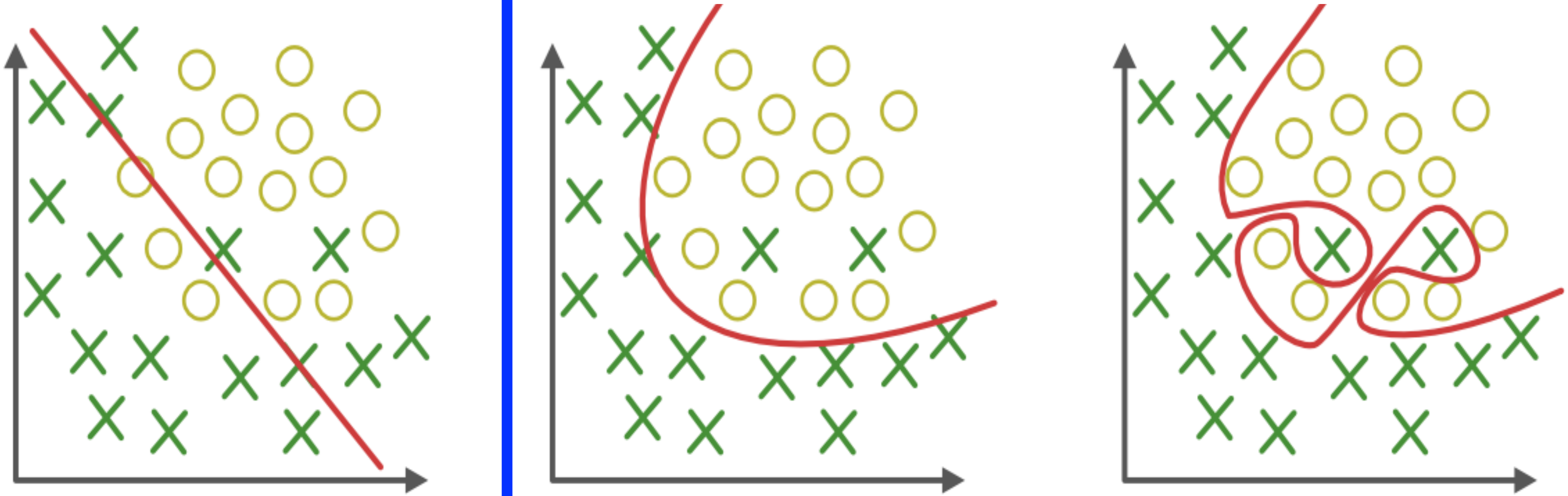

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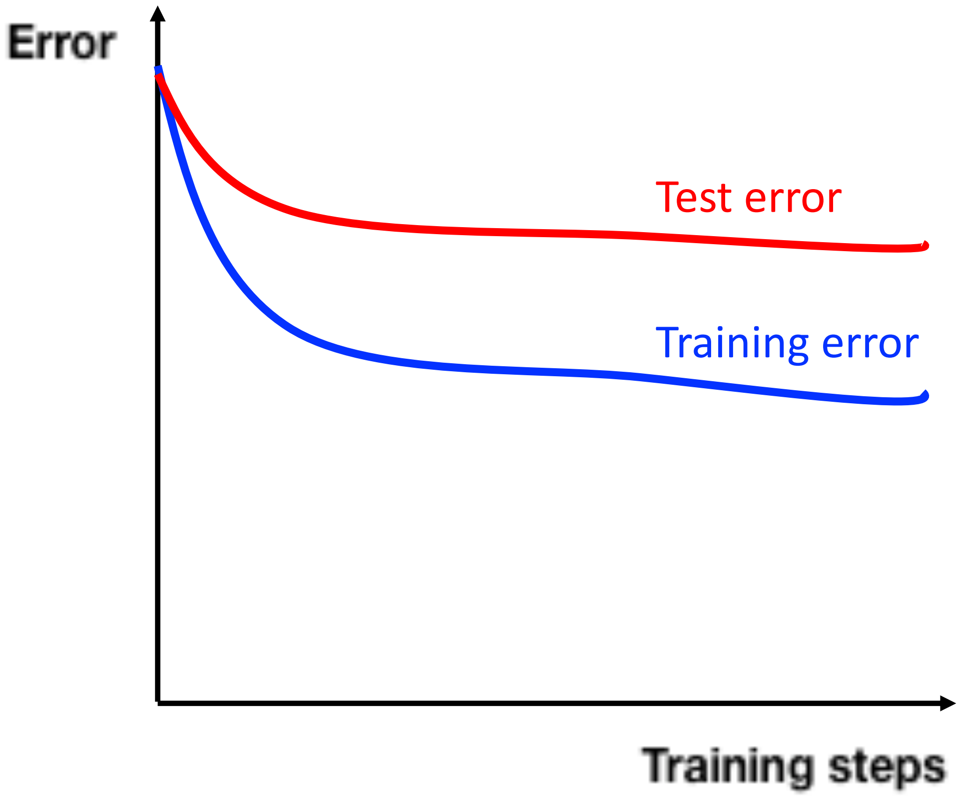
Model Capacity: Underfitting



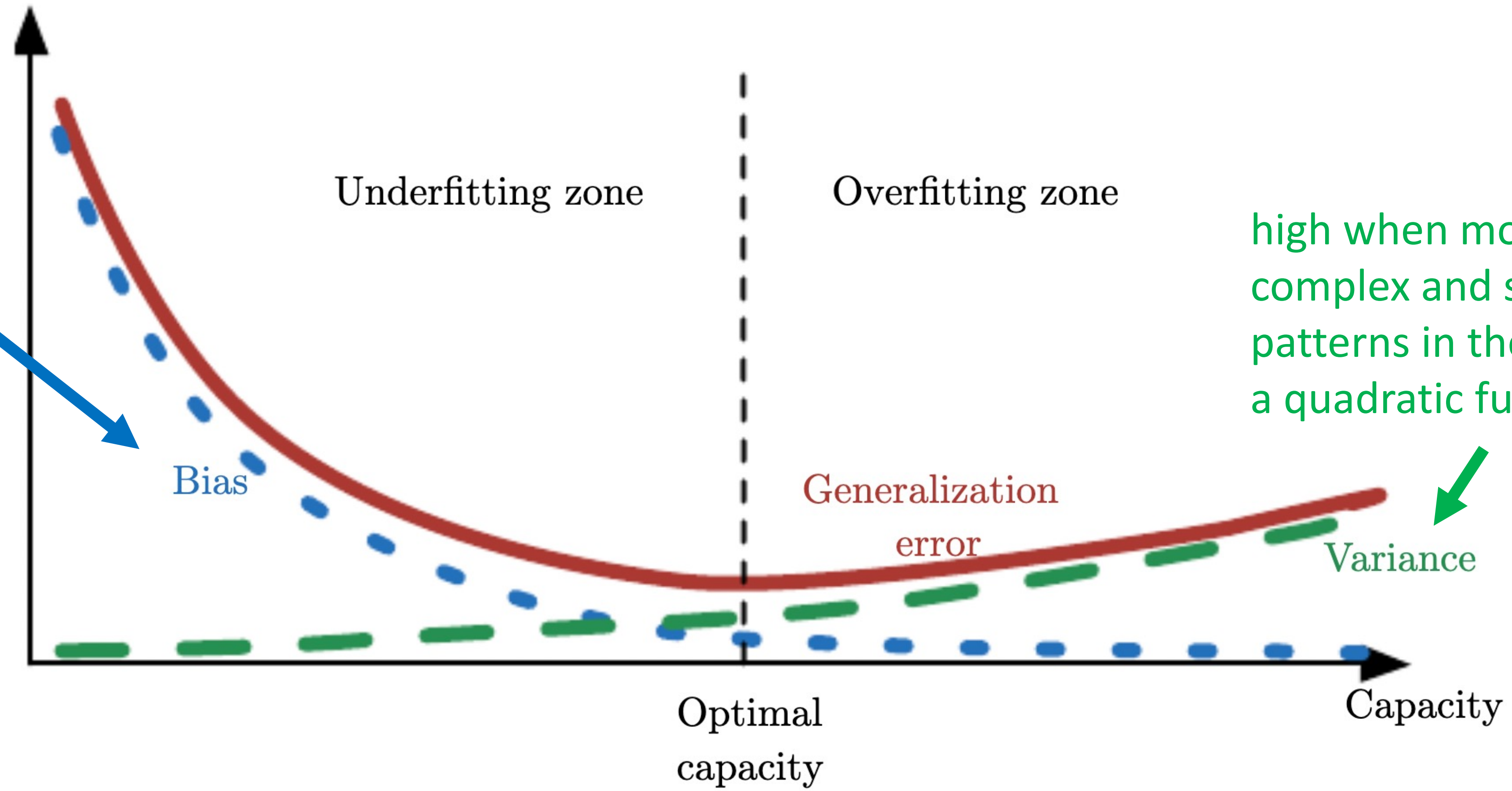
- To detect underfitting, analyze **learning curves** for models tested on training data
  - What happens to training data error as number of training steps increases?
    - Error remains high

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)

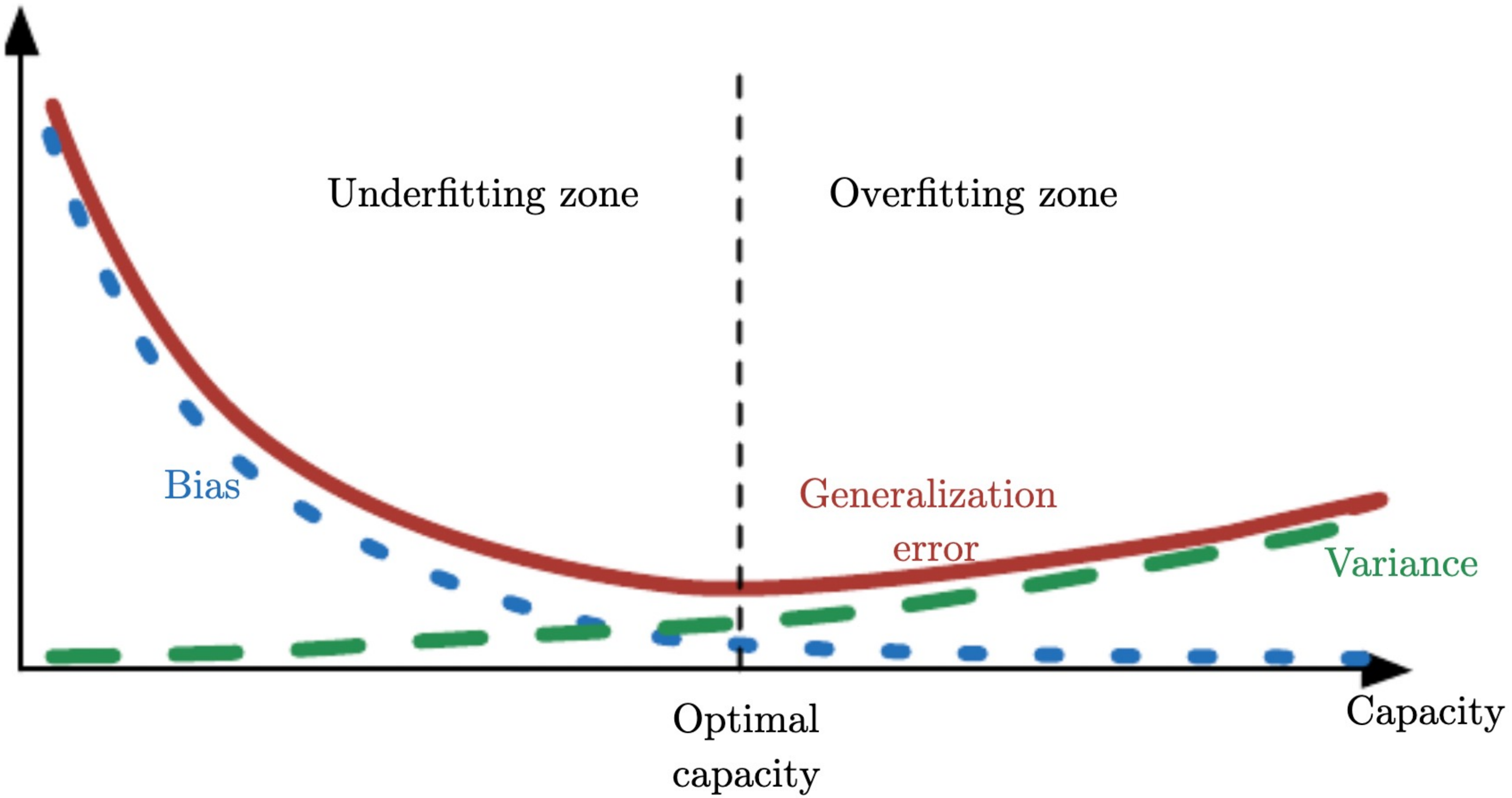


high when model is overly-complex and so misses simpler patterns in the data (e.g., does a quadratic function suffice?)

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 …

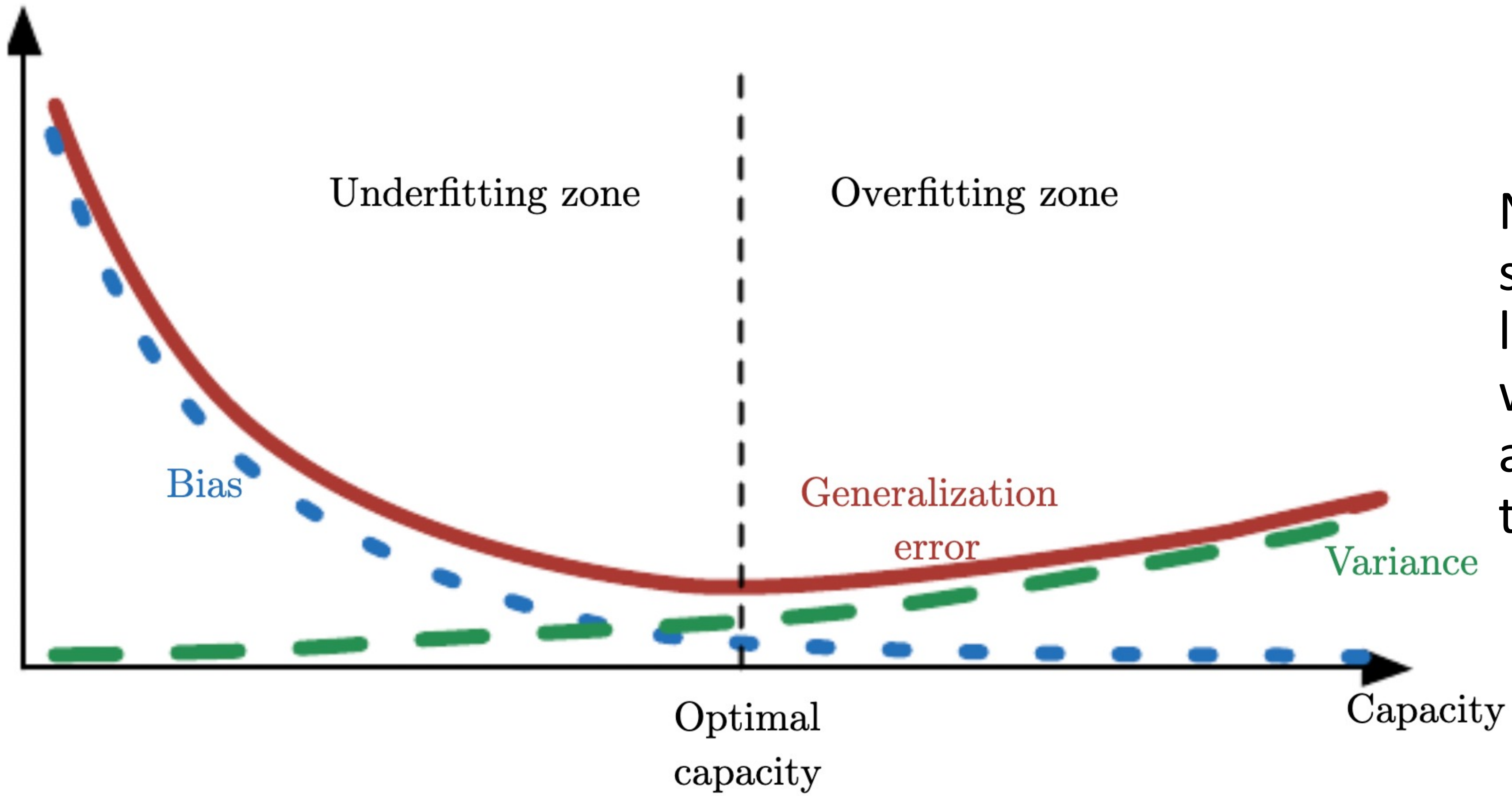
- High or low bias?
- High or low variance?

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.,

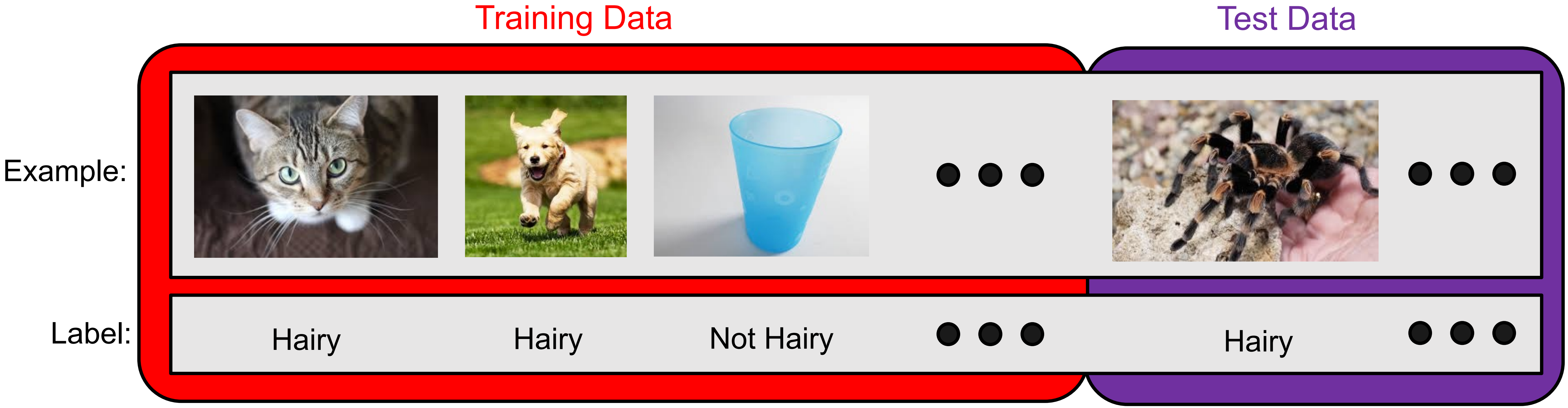
- Number of layers
- Number of units in each layer
- Activation function
- Batch size
- Learning rate
- …

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)

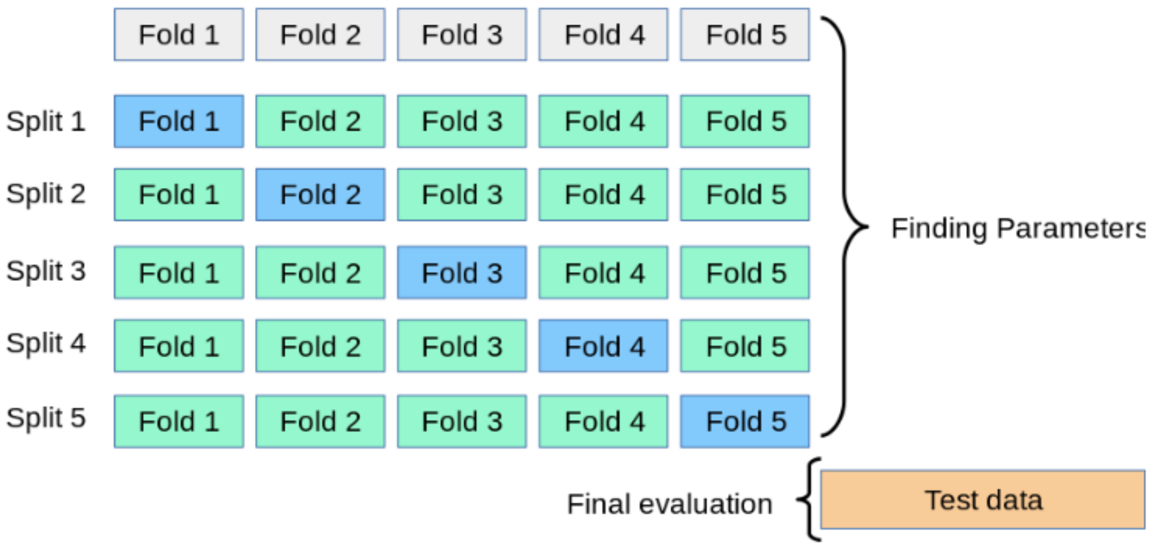


Key Challenge: how to design a model without repeatedly observing the test data (which leads to overfitting)?

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

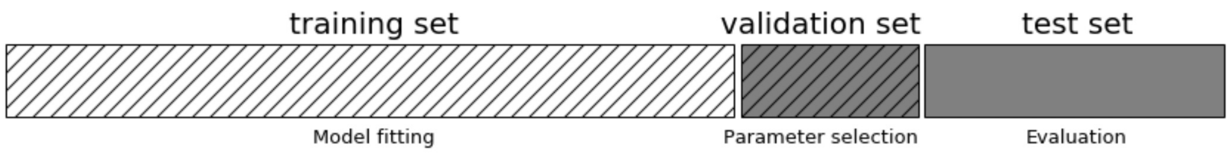
For statistically strong results:

Small training dataset: cross validation



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

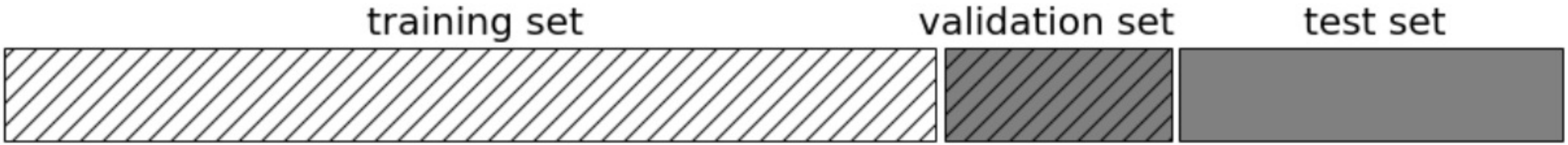
Else: train/validation split



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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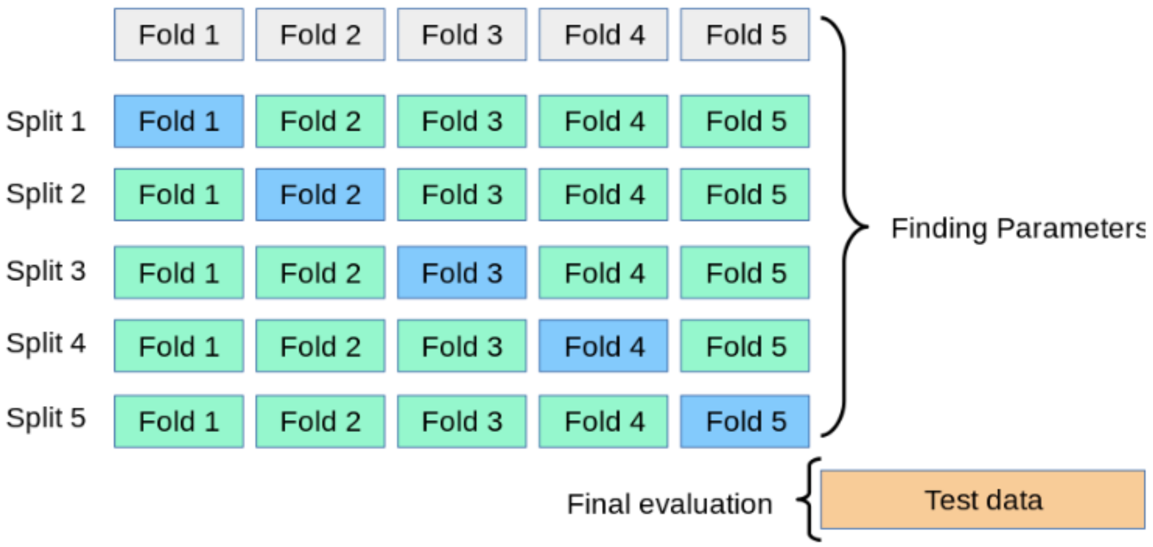

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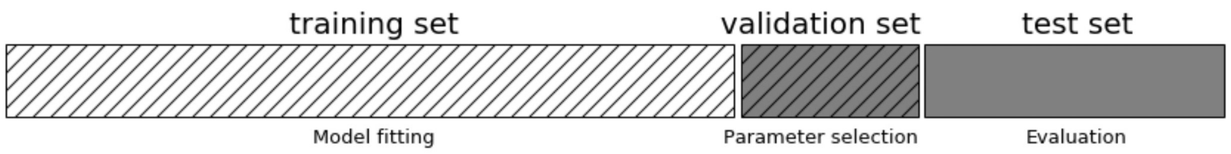

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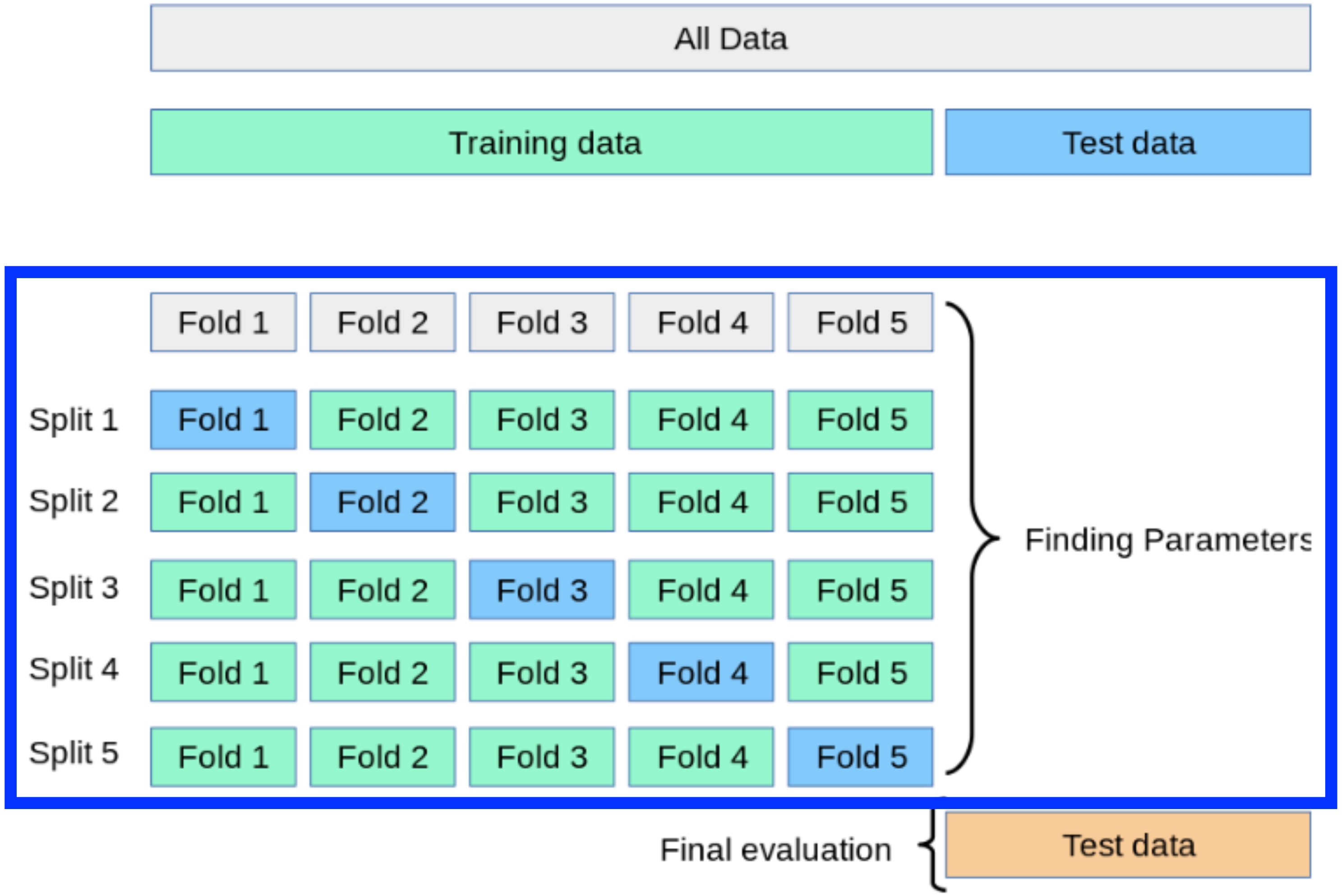
Cross-Validation: Limit Influence of Dataset Split



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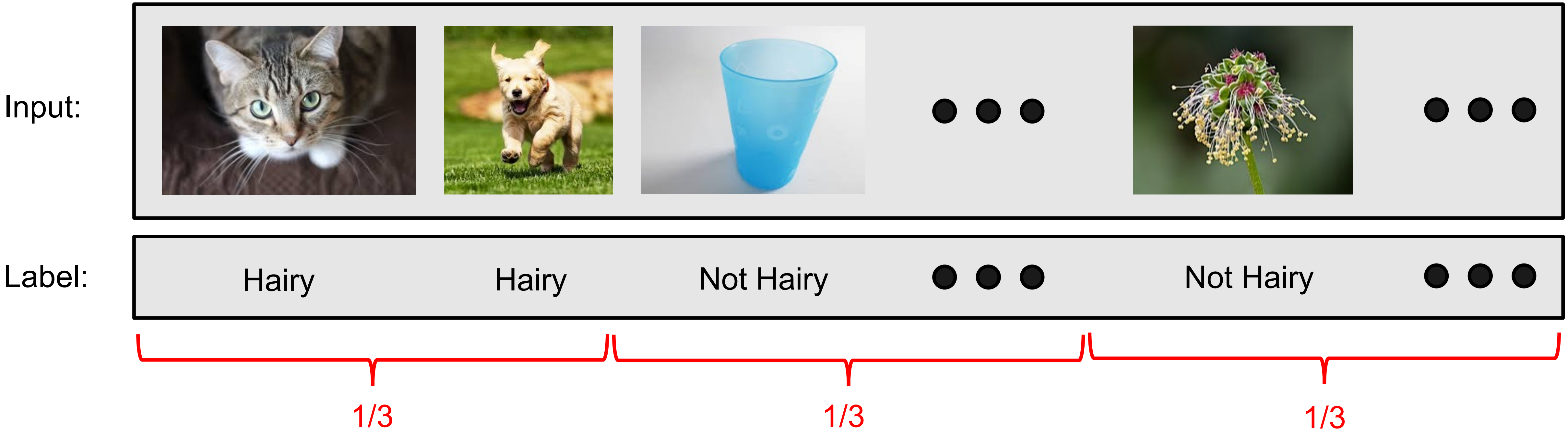
Cross-Validation: Limit Influence of Dataset Split

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



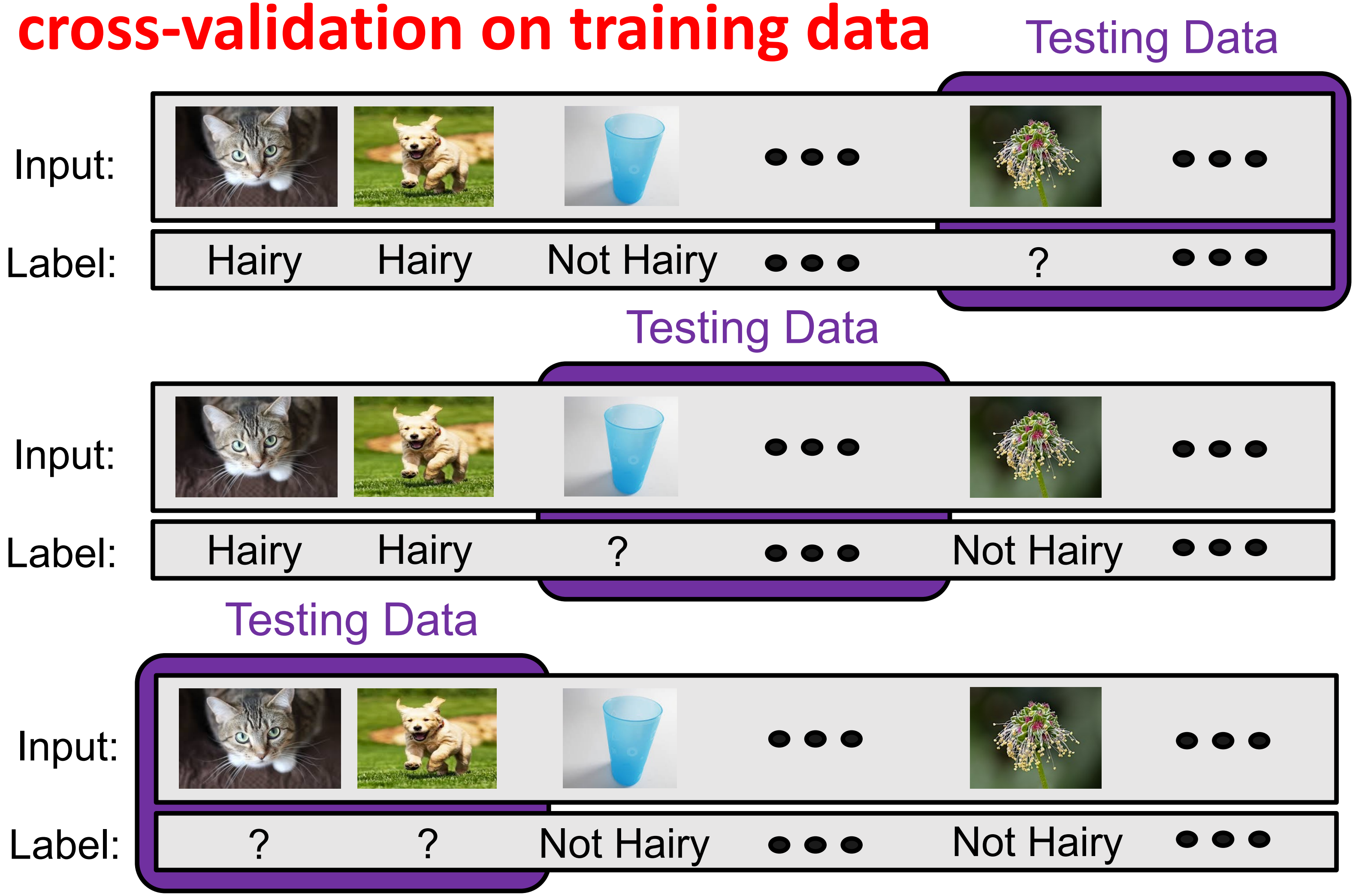
Cross-Validation: Limit Influence of Dataset Split

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

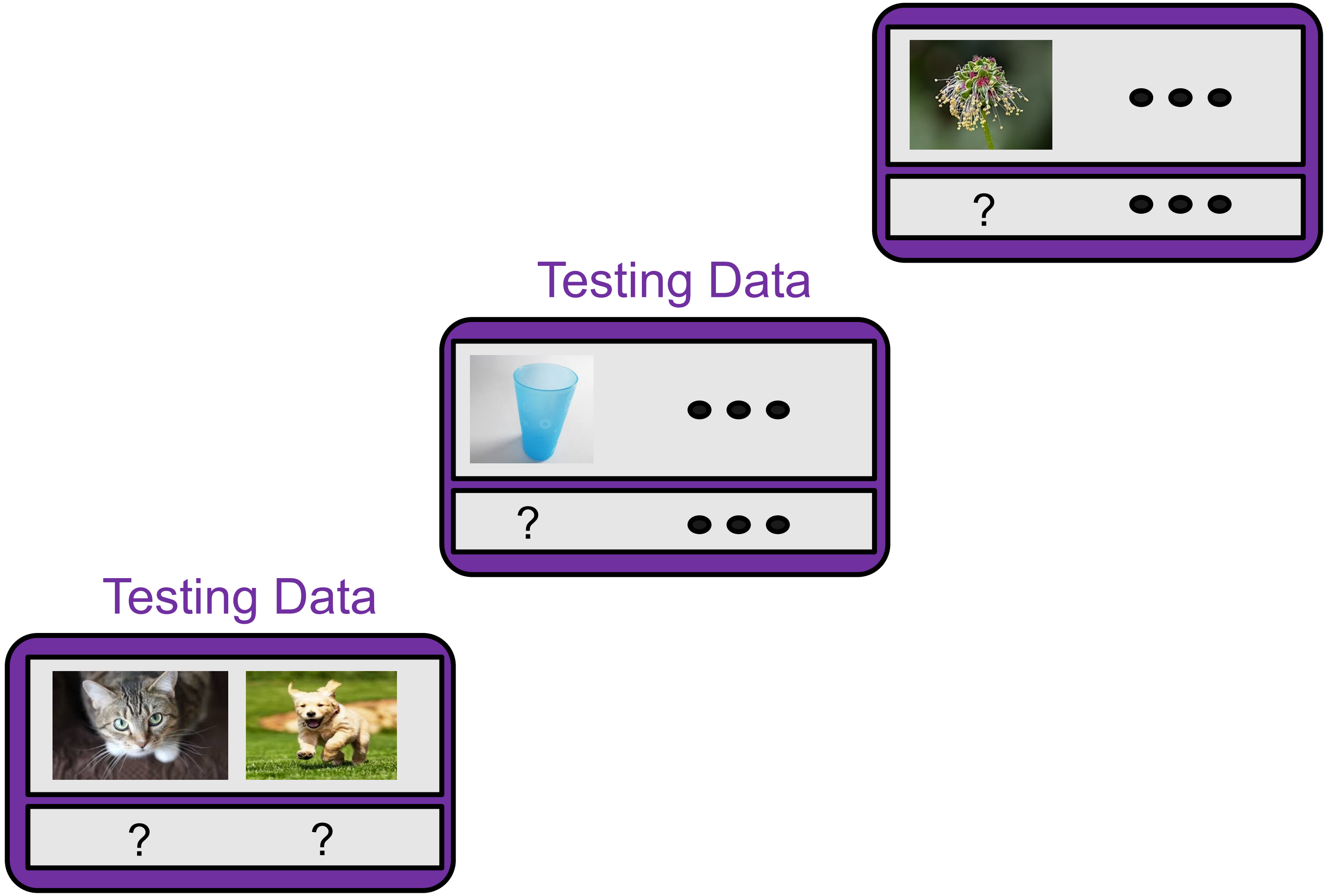


Cross-Validation: Limit Influence of Dataset Split

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

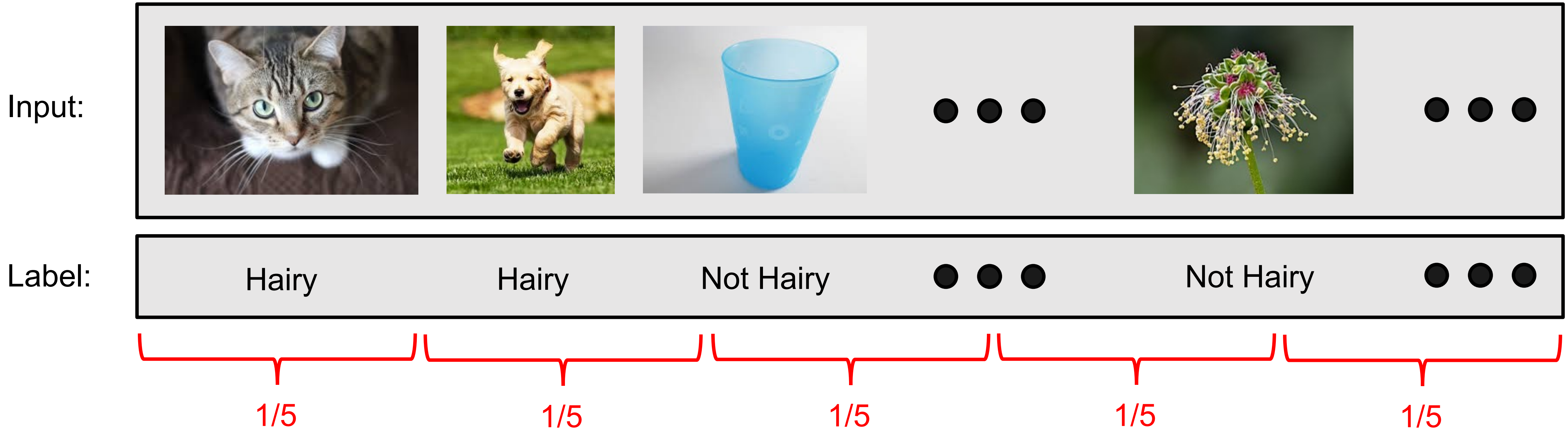
Model performance: performance across all folds of "test" data

Testing Data



Cross-Validation: Limit Influence of Dataset Split

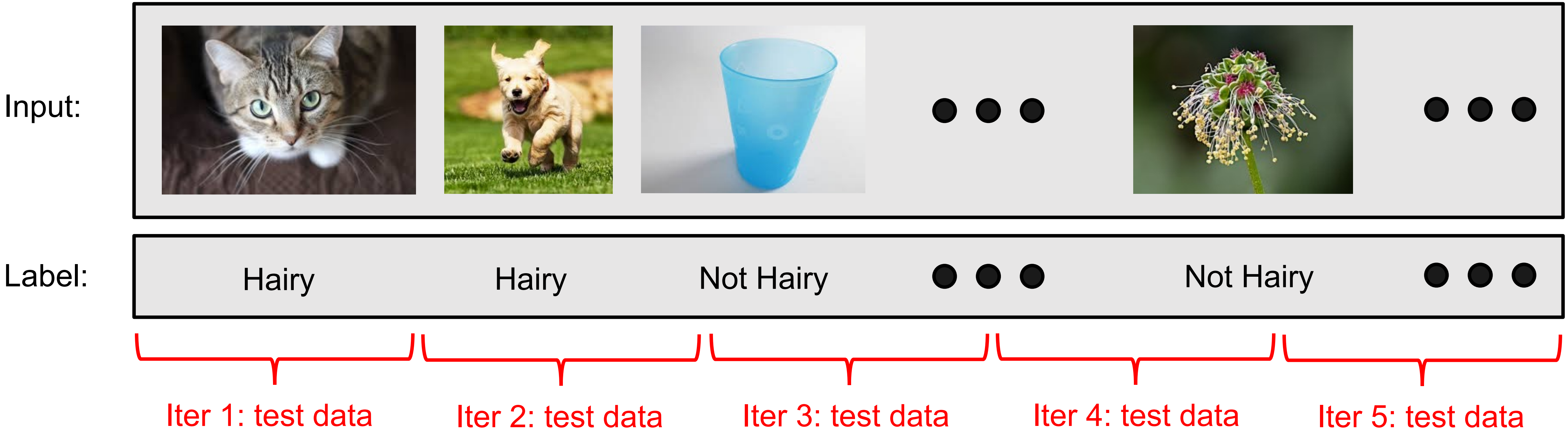
e.g., 5-fold cross-validation on training data



How many partitions of the data to create?

Cross-Validation: Limit Influence of Dataset Split

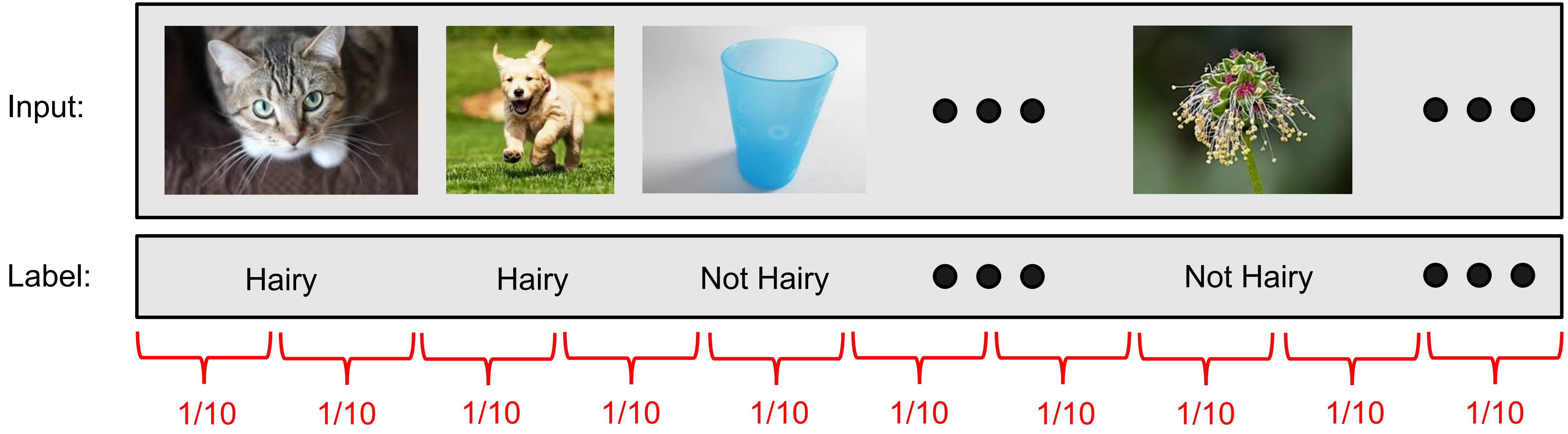
e.g., 5-fold cross-validation on training data



How many iterations of train & test to run?

Cross-Validation: Limit Influence of Dataset Split

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



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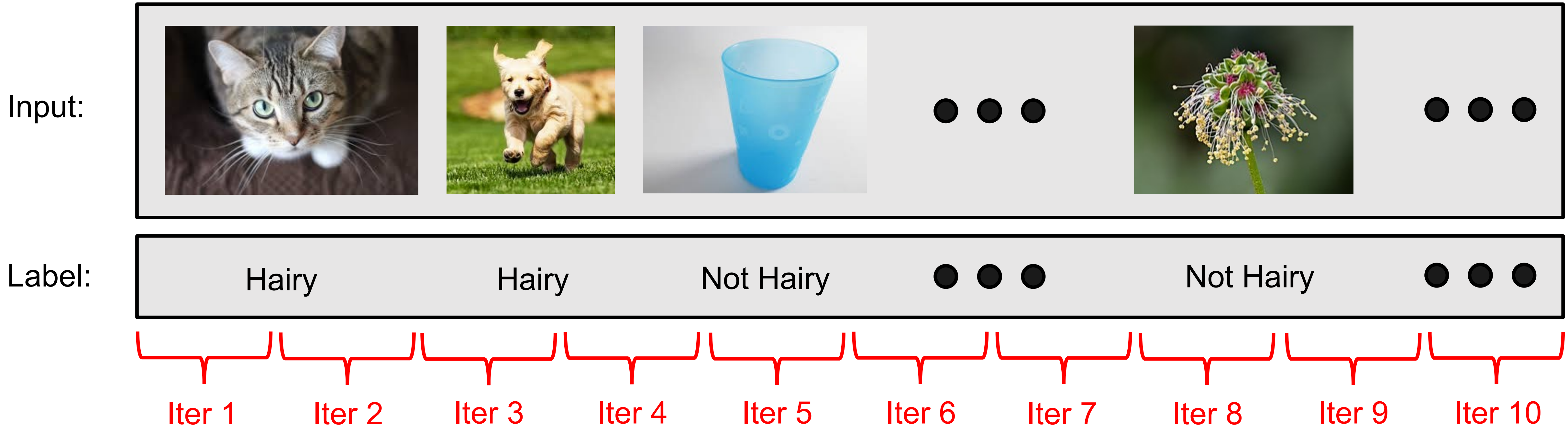


How many iterations of train & test to run?

Cross-Validation: Limit Influence of Dataset Split

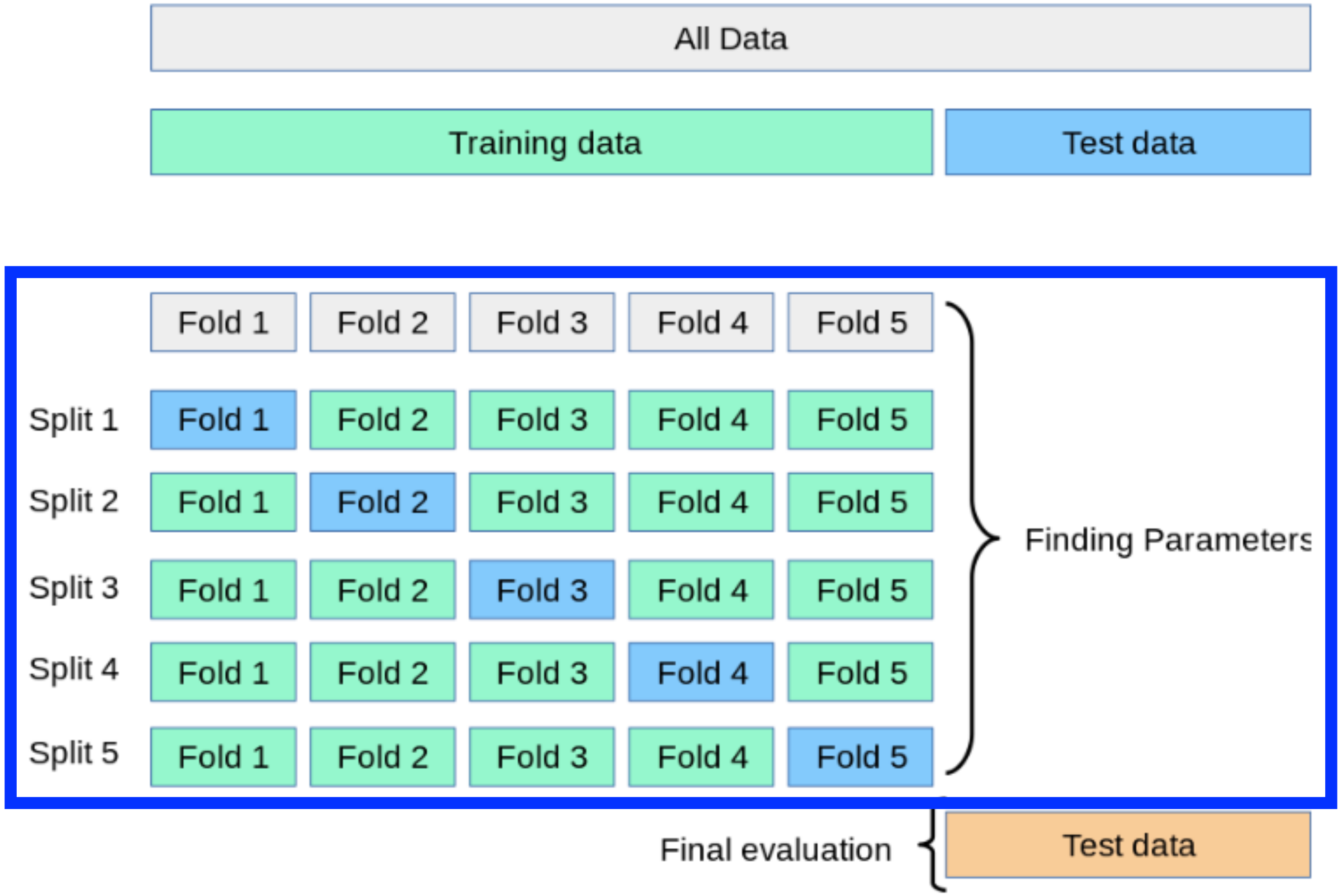
e.g., k-fold cross-validation on training data

Input:				● ● ●		● ● ●
Label:	Hairy	Hairy	Not Hairy	● ● ●	Not Hairy	● ● ●

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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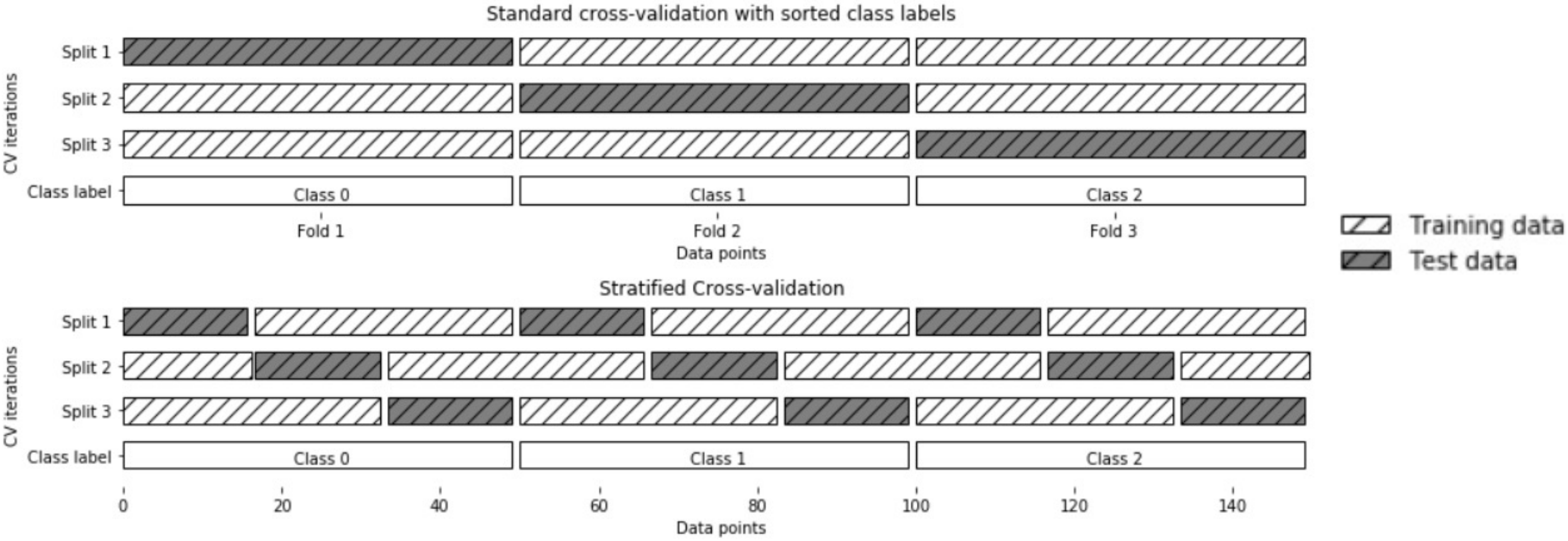
Stratified Dataset Splits

- 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:

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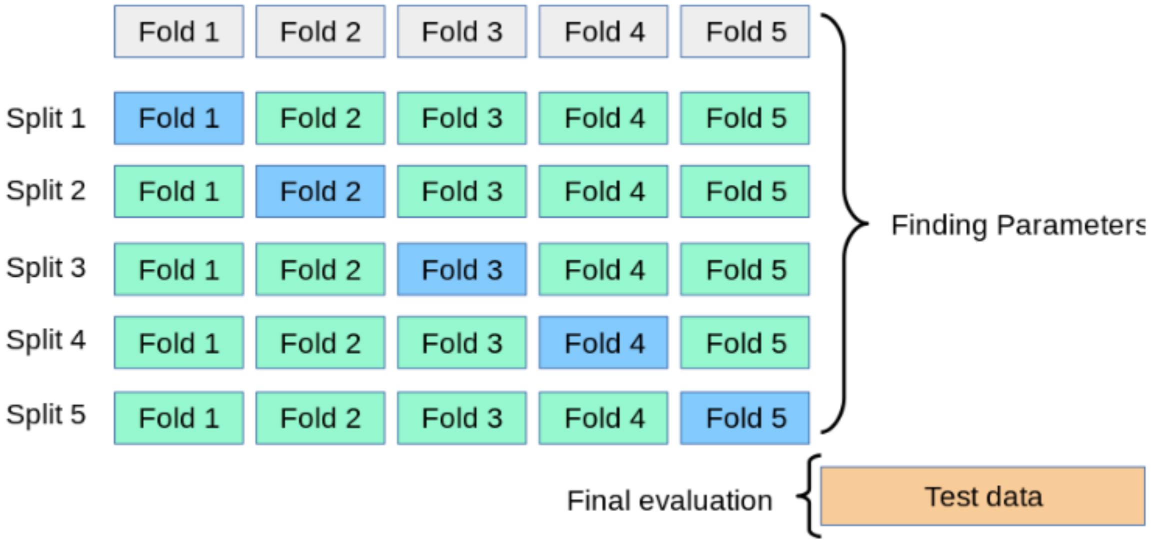

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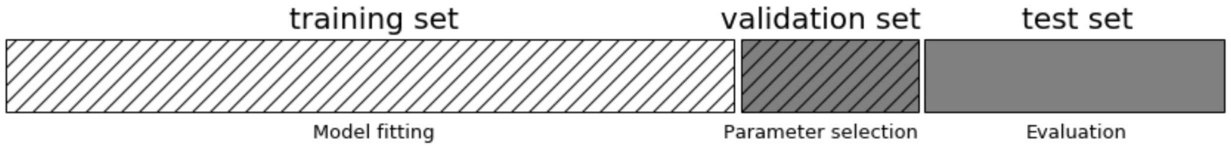

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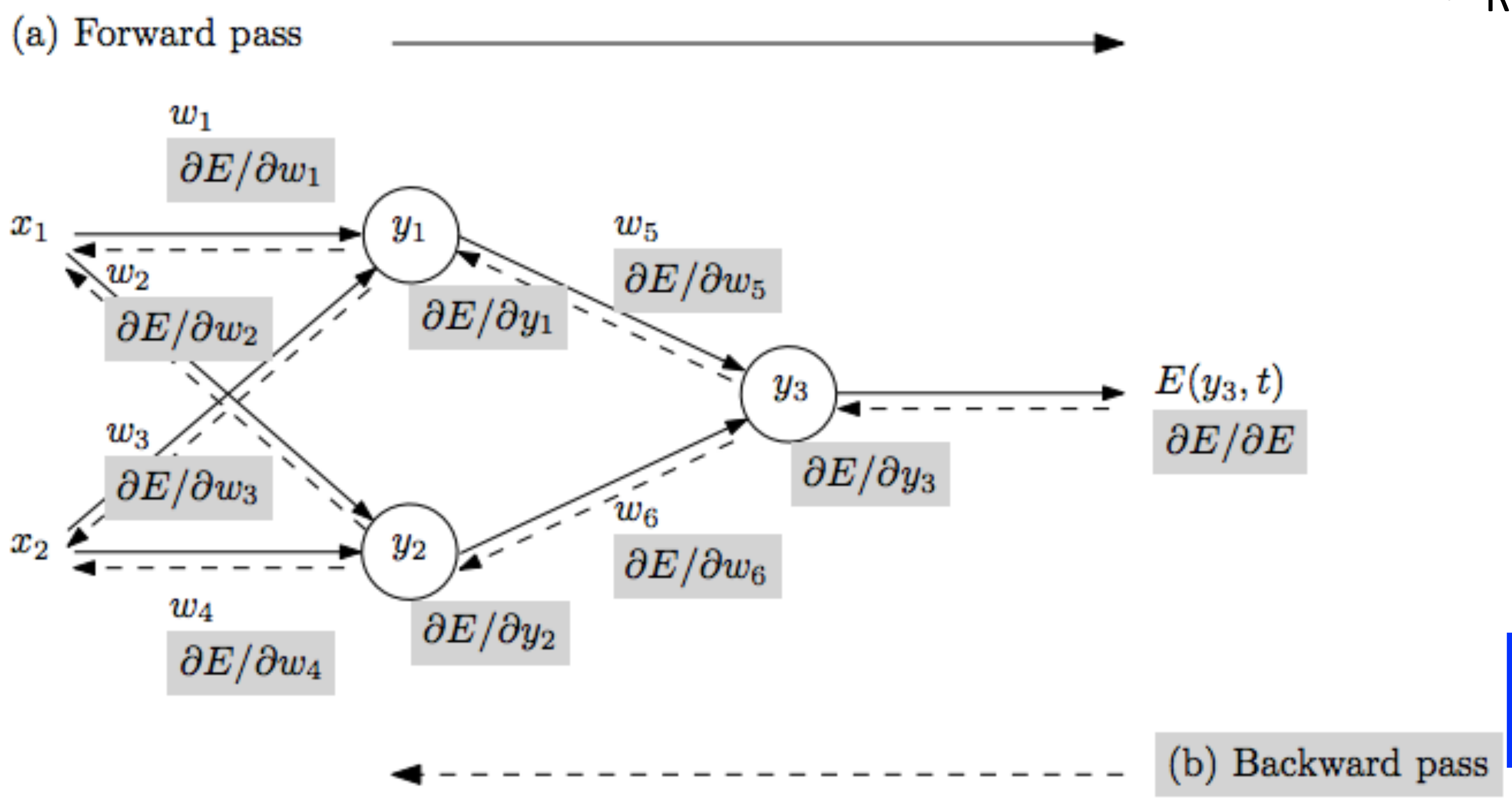
Challenge: Train Faster!!!

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

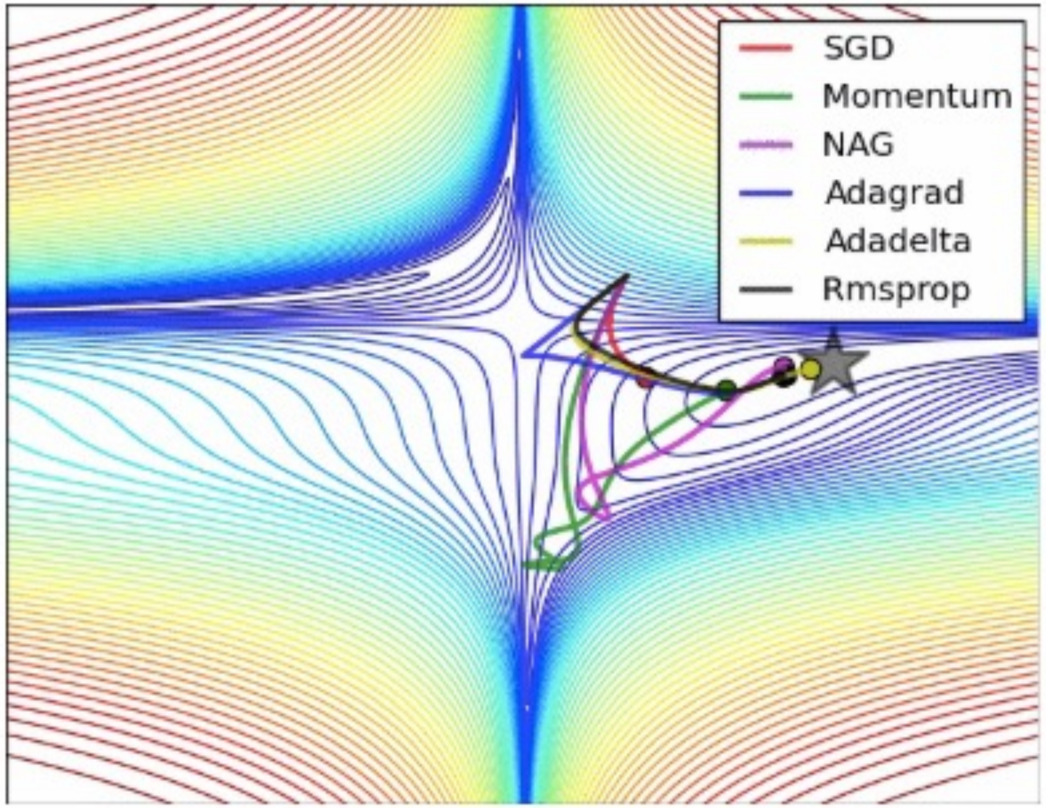
Recall: How Neural Networks Learn

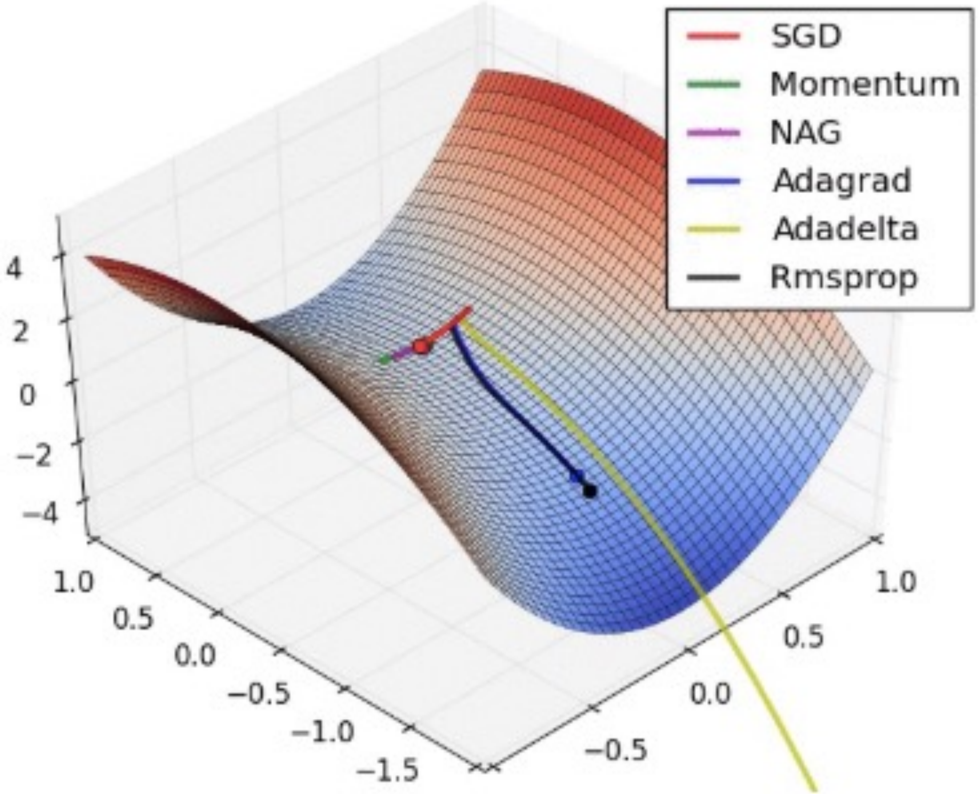


- Repeat until stopping criterion met:
  1. **Forward pass**: propagate training data through model to make prediction
  2. Quantify the dissatisfaction with a model's results on the training data
  3. **Backward pass**: using predicted output, calculate gradients backward to assign blame to each model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





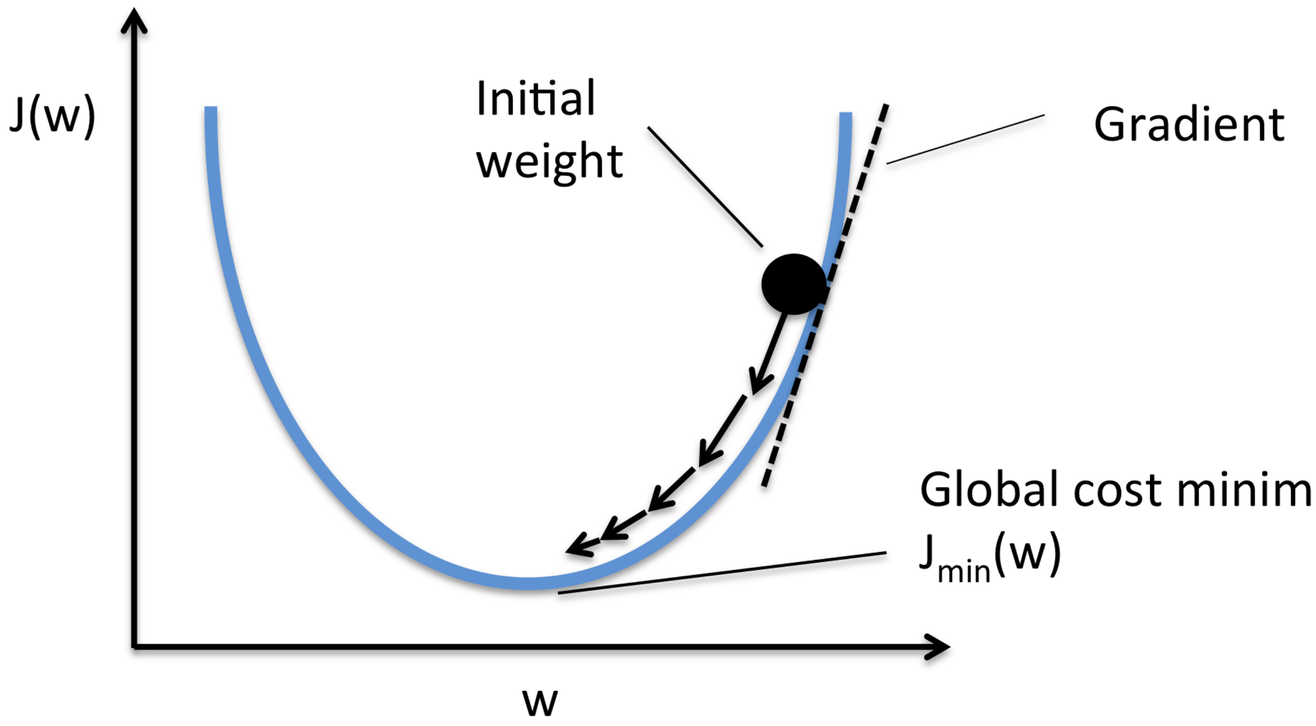
- Demo at http://cs231n.github.io/neural-networks-3/#update

Train Faster: How to Update Using Gradient?

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

Parameters (x) — Gradient (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

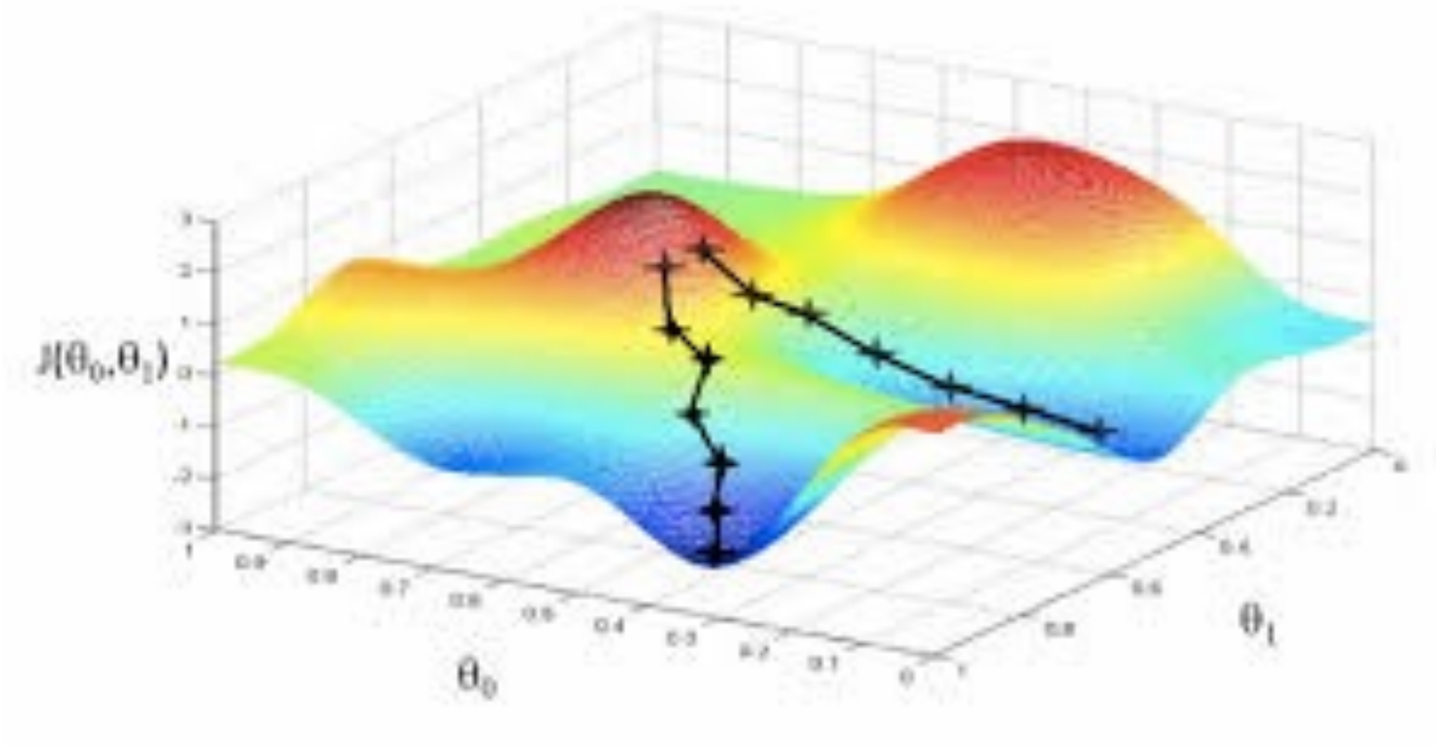


Figure from: https://medium.com/ai-society/hello-gradient-descent-ef74434bdfa5

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

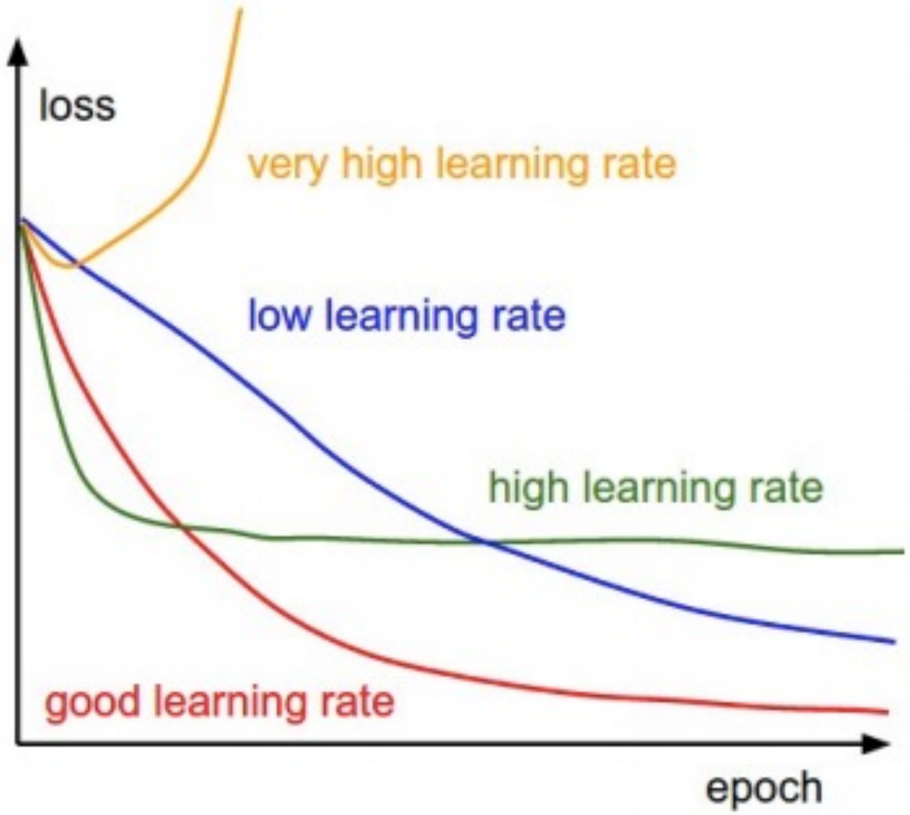
Train Faster: How to Update Using Gradient?

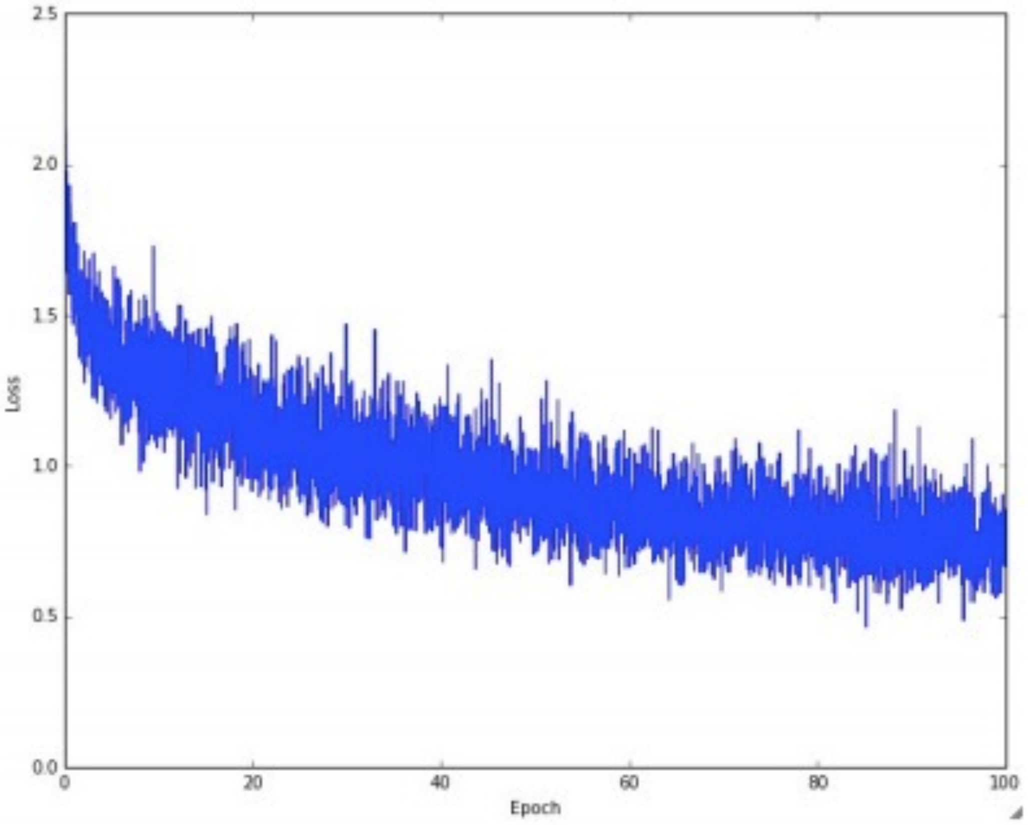
- Step decay:
  - Reduce the learning rate by some factor every few epochs
- Exponential decay
- 1/t decay
- Adapt learning rate per-parameter
- e.g., AdaGrad, RMSprop, and Adam (i.e., adaptive momentum – very popular in practice)

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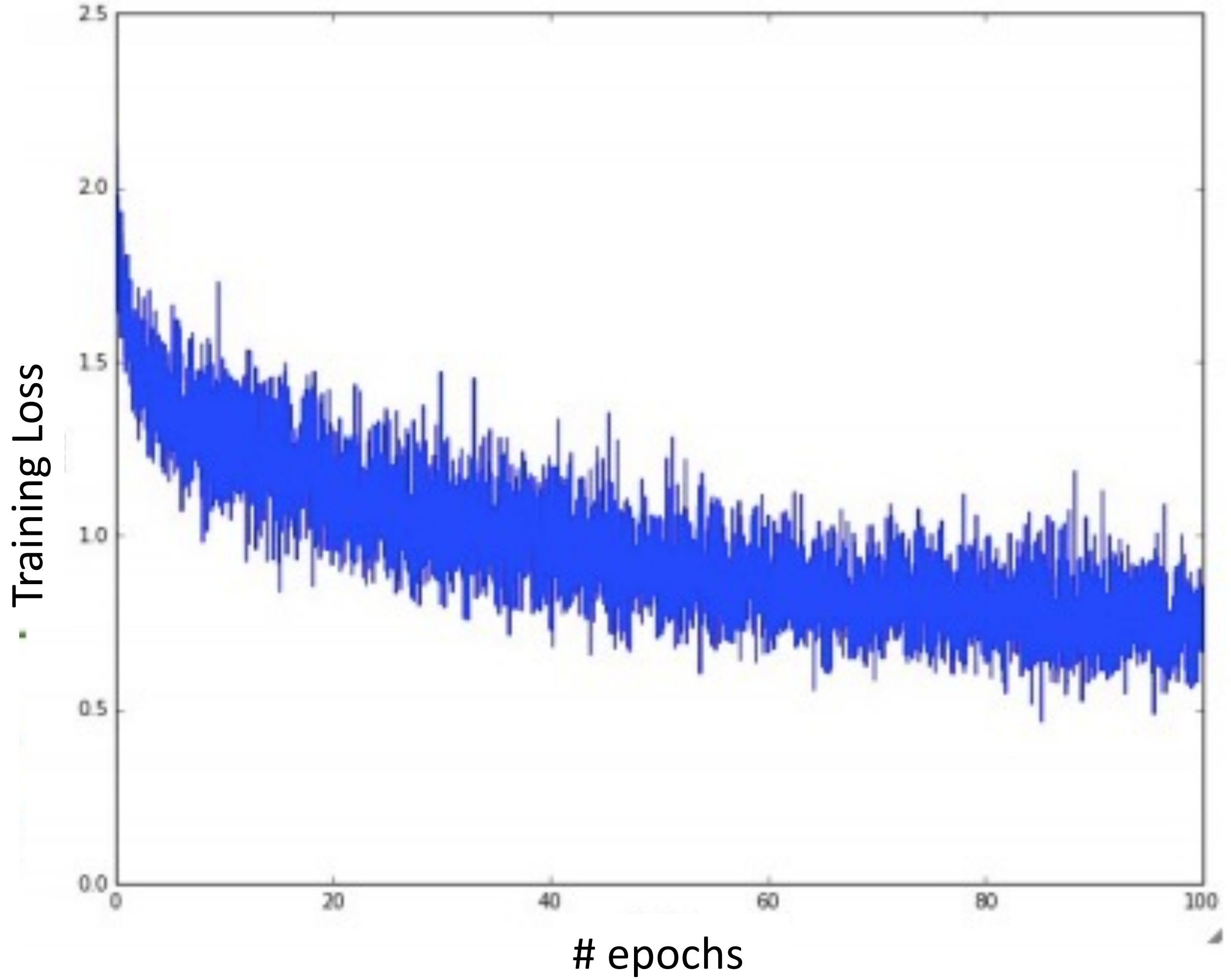
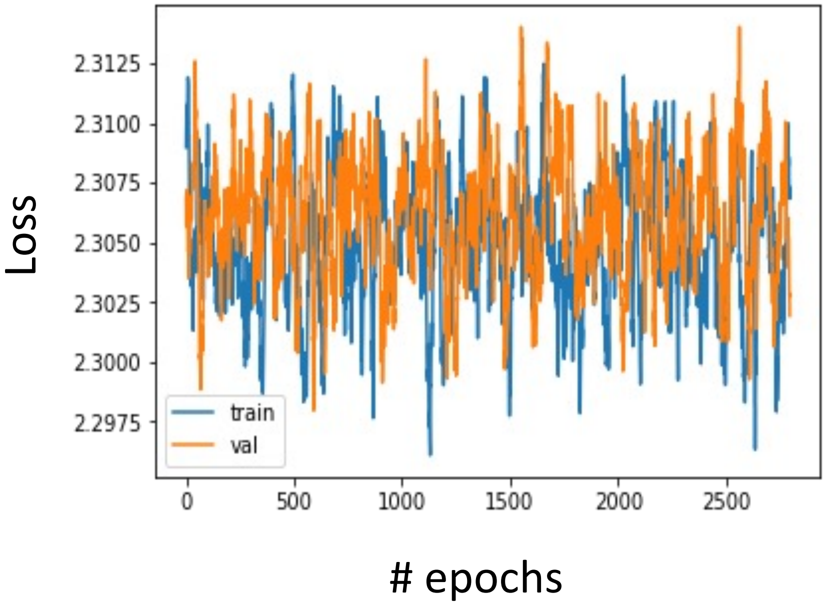
Analysis: Why Might There Be Oscillations in the Learning Curve for the Training Loss?



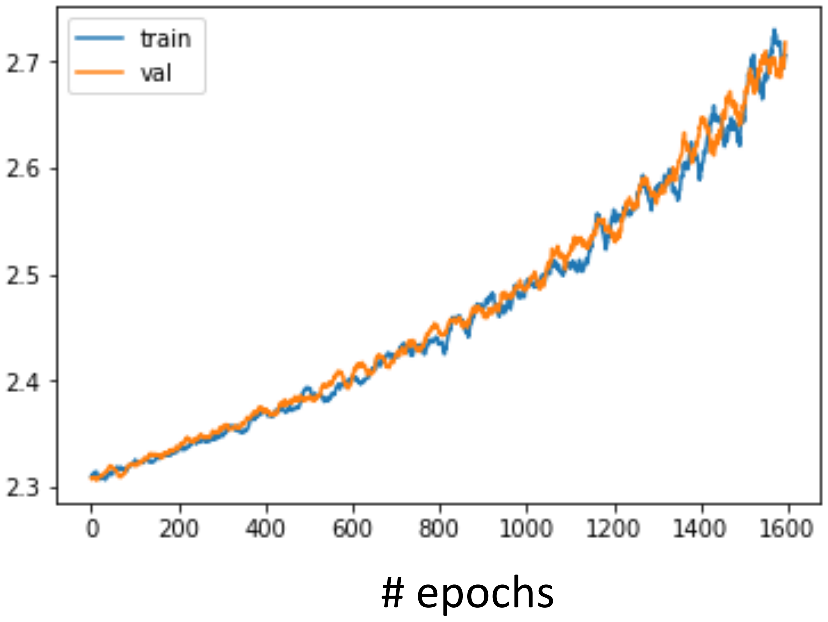
https://cs231n.github.io/neural-networks-3/#update

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

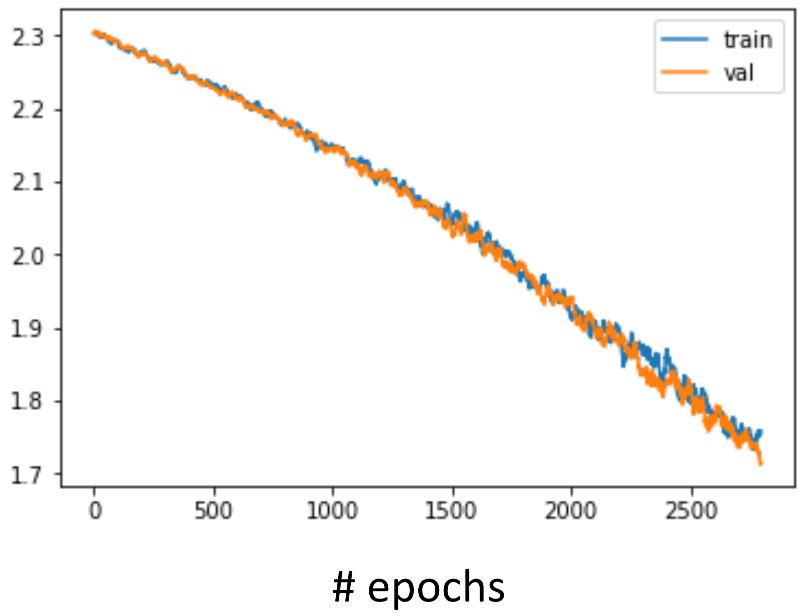
(a)



(b)



(c)



Feeling Bewildered By Your Learning Curves?

You may feel better when looking at this link:

https://lossfunctions.tumblr.com/

Today’s Topics

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- Selecting model capacity: avoid overfitting and underfitting
- Selecting model hyperparameters
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The End