CMP784

DEEP LEARNING

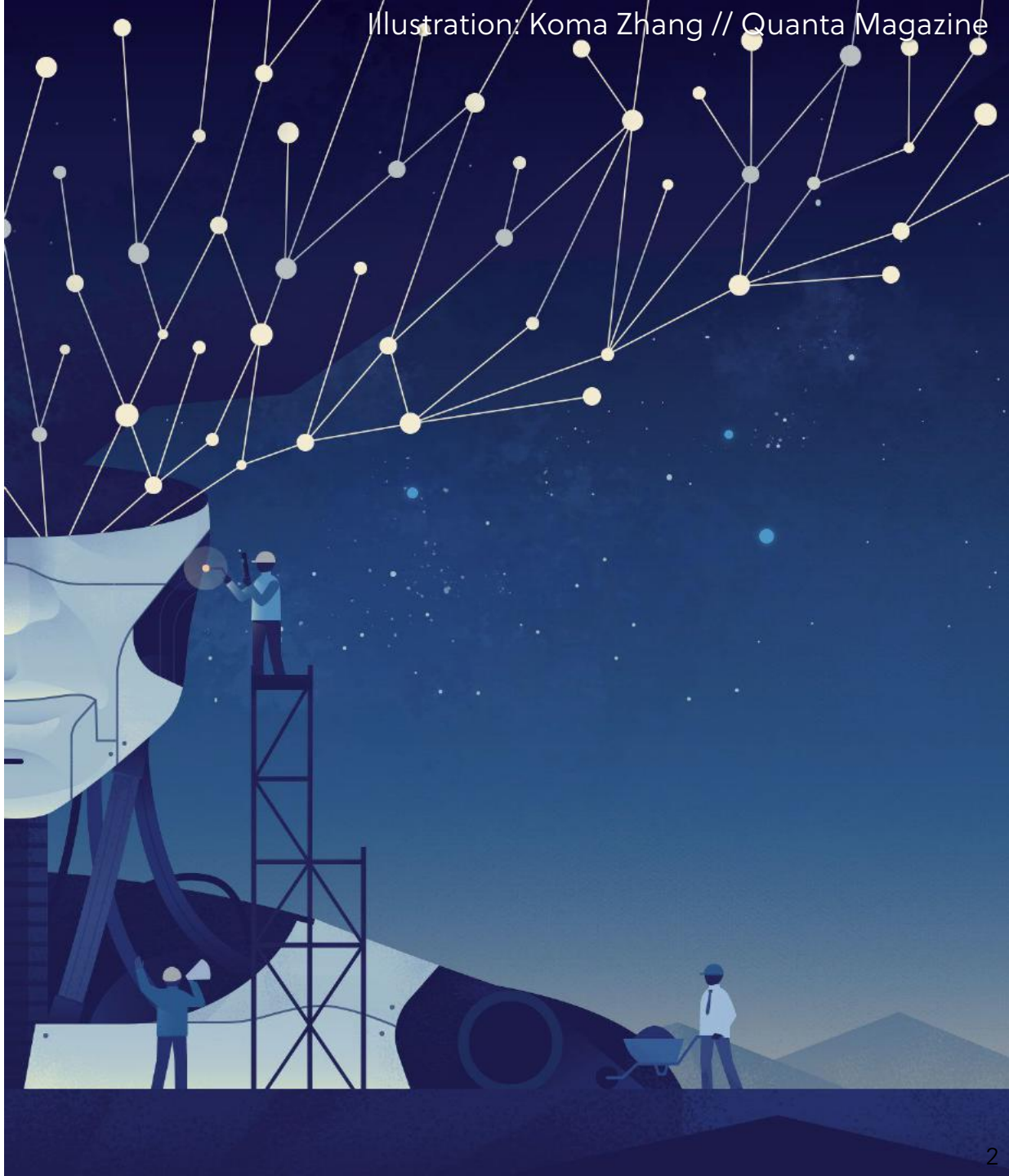
Lecture #2 – Machine Learning Overview

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Aykut Erdem // Hacettepe University // Spring 2020

Previously on CMP784

- what is deep learning
- a brief history of deep learning
- compositionality
- end-to-end learning
- distributed representations



Lecture overview

- what is learning?
- types of machine learning problems
- image classification
- linear regression
- generalization
- cross-validation
- maximum likelihood estimation

- **Disclaimer:** Much of the material and slides for this lecture were borrowed from

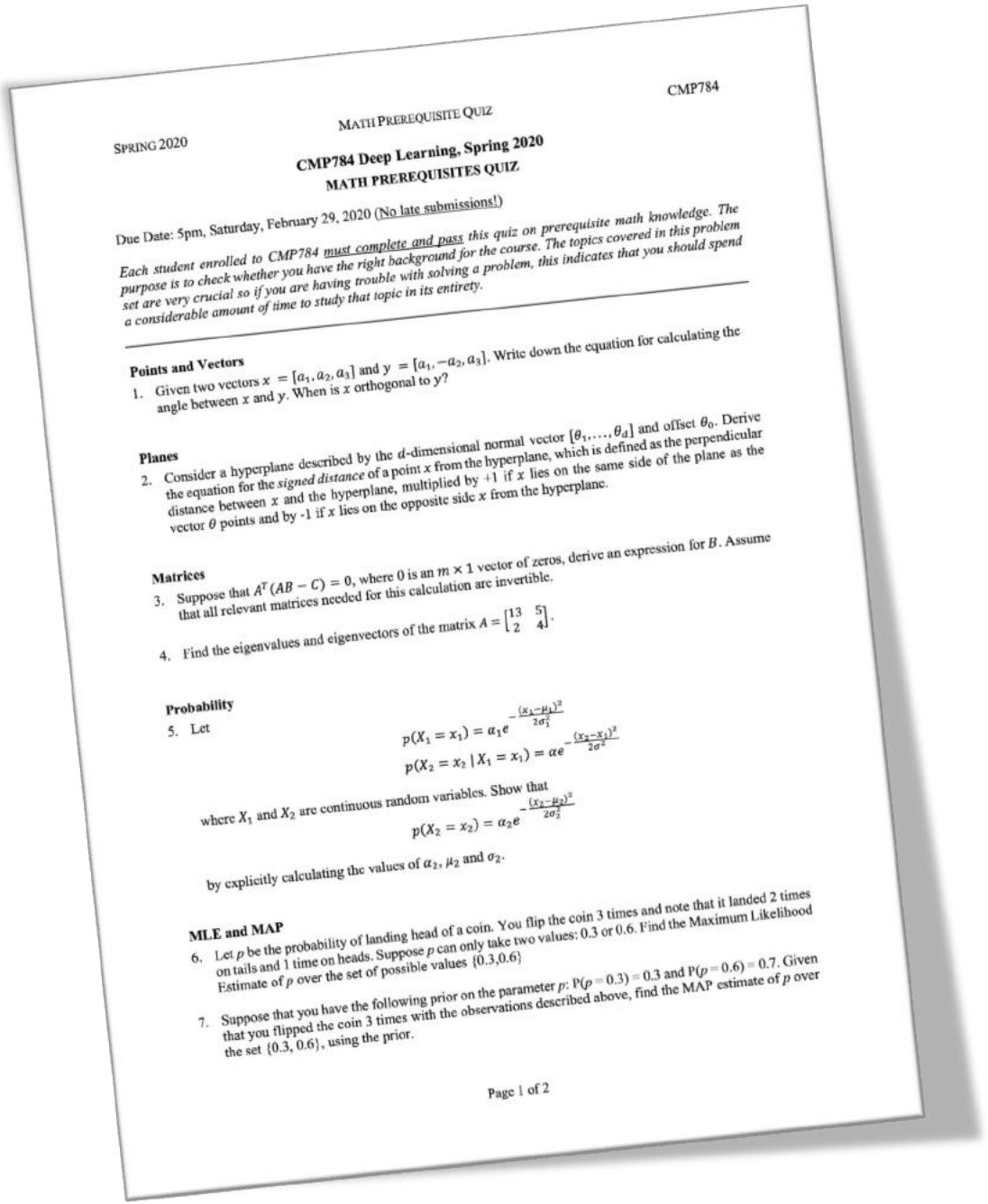
  —Bernhard Schölkopf's MLSS 2017 lecture,

  —Tommi Jaakkola's 6.867 class,

  —Fei-Fei Li, Andrej Karpathy and Justin Johnson's CS231n class

Pre-quiz

- Is there anyone who did not submit his/her quiz paper?
- If you failed to submit on time, contact me after the class.



SPRING 2020 MATH PREREQUISITE QUIZ CMP784

CMP784 Deep Learning, Spring 2020

MATH PREREQUISITES QUIZ

Due Date: 5pm, Saturday, February 29, 2020 (No late submissions!)

Each student enrolled to CMP784 must complete and pass this quiz on prerequisite math knowledge. The purpose is to check whether you have the right background for the course. The topics covered in this problem set are very crucial so if you are having trouble with solving a problem, this indicates that you should spend a considerable amount of time to study that topic in its entirety.

Points and Vectors

1. Given two vectors $x = [a_1, a_2, a_3]$ and $y = [a_1, -a_2, a_3]$. Write down the equation for calculating the angle between x and y. When is x orthogonal to y?

Planes

2. Consider a hyperplane described by the d-dimensional normal vector $[\theta_1, \ldots, \theta_d]$ and offset θ_0. Derive the equation for the *signed distance* of a point x from the hyperplane, which is defined as the perpendicular distance between x and the hyperplane, multiplied by +1 if x lies on the same side of the plane as the vector θ points and by -1 if x lies on the opposite side x from the hyperplane.

Matrices

3. Suppose that $A^T(AB - C) = 0$, where 0 is an $m \times 1$ vector of zeros, derive an expression for B. Assume that all relevant matrices needed for this calculation are invertible.

4. Find the eigenvalues and eigenvectors of the matrix $A = \begin{bmatrix} 13 & 5 \\ 2 & 4 \end{bmatrix}$.

Probability

5. Let

$$p(X_1 = x_1) = \alpha_1 e^{-\frac{(x_1-\mu_1)^2}{2\sigma_1^2}}$$

$$p(X_2 = x_2 \mid X_1 = x_1) = \alpha e^{-\frac{(x_2-x_1)^2}{2\sigma^2}}$$

where X_1 and X_2 are continuous random variables. Show that

$$p(X_2 = x_2) = \alpha_2 e^{-\frac{(x_2-\mu_2)^2}{2\sigma_2^2}}$$

by explicitly calculating the values of α_2, μ_2 and σ_2.

MLE and MAP

6. Let p be the probability of landing head of a coin. You flip the coin 3 times and note that it landed 2 times on tails and 1 time on heads. Suppose p can only take two values: 0.3 or 0.6. Find the Maximum Likelihood Estimate of p over the set of possible values {0.3,0.6}

7. Suppose that you have the following prior on the parameter p: P(p = 0.3) = 0.3 and P(p = 0.6) = 0.7. Given that you flipped the coin 3 times with the observations described above, find the MAP estimate of p over the set {0.3, 0.6}, using the prior.

Page 1 of 2

Good news, everyone!

- Practical 1 will be out next week
  - Multi-layer perceptrons
  - Word embeddings
  - Due March 26, 2020
  - Install TensorFlow to your machine to get ready!

More good news, everyone!

- Paper presentations will start in three weeks!
- Quizzes will also start at March 25th, 2020
  - 1 or 2 short answer questions about the paper (10 mins long)

Paper presentations

- Choose your paper
  - 8 papers
  - 30 students
- Choose your role
  - **Overview** (1 student)
  - **Strengths** (1 student)
  - **Weaknesses** (1 student)

Spring 2020
CMP784: Deep Learning

Instructor: Aykut Erdem

PAPER LIST

March 25: Training Deep Neural Networks
The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks
Jonathan Frankle, Michael Carbin. ICLR 2019.

April 1: Convolutional Neural Networks
Panoptic Feature Pyramid Networks
Alexander Kirillov, Ross Girshick, Kaiming He, Piotr Dollár. CVPR 2019.

April 8: Understanding and Visualizing CNNs
A Tour of Convolutional Networks Guided by Linear Interpreters
Pablo Navarrete Michelini, Hanwen Liu, Yunhua Lu, Xingqun Jiang. ICCV 2019.

April 15: Recurrent Neural Networks
Mogrifier LSTM
Gábor Melis, Tom Koisk, Phil Blunsom. ICLR 2020.

April 29: Attention and Memory
Reformer: The Efficient Transformer
Nikita Kitaev, Lukasz Kaiser, Anselm Levskaya. ICLR 2020.

May 6: Autoencoders and Autoregressive Models
Scaling Autoregressive Video Models
Dirk Weissenborn, Oscar Tckstrm, Jakob Uszkoreit. ICLR 2020.

May 13: Generative Adversarial Networks
Analyzing and Improving the Image Quality of StyleGAN
Tero Karras, Samuli Laine, Miika Aittala, Janne Hellsten, Jaakko Lehtinen and Timo Aila. Preprint, 2019.

May 20: Variational Autoencoders
From Variational to Deterministic Autoencoders
Partha Ghosh, Mehdi S. M. Sajjadi, Antonio Vergari, Michael Black, Bernhard Scholkopf. ICLR 2020.

Overview of the paper

- Roughly 14 mins long

Problem statement and motivation Clear definition of the problem, why it is interesting and important
High-level overview of the paper Main contributions
Key technical ideas Overview of the approach, related work
Experimental set-up Datasets, evaluation metrics, applications
Overall effectiveness of slide text/visuals Good balance of text and figures
Overall effectiveness of the presentation Good oral skills, ability to answer follow-on questions, good leading of the class discussions
Time Effective usage of time (~14 minutes long)

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Strengths of the paper

- Roughly 8 mins long

Summary of the paper One slide summary of the proposed approach
Connections with other work How the method relates to other approaches
Strengths of the approach Discuss the novelty of the approach, how it improves the existing work
Strengths of the evaluation protocol Discuss the baselines and the ablation procedure
Overall effectiveness of slide text/visuals Good balance of text and figures
Overall effectiveness of the presentation Good oral skills, ability to answer follow-on questions, good leading of the class discussions
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Weaknesses of the paper

- Roughly 8 mins long

Summary of the paper One slide summary of the proposed approach
Weaknesses of the approach Describe some cases in which you expect the approach performs poorly
Weaknesses of the evaluation protocol Describe how the evaluation could be improved
Future direction Open research questions, possible improvements over the approach
Overall effectiveness of slide text/visuals Good balance of text and figures
Overall effectiveness of the presentation Good oral skills, ability to answer follow-on questions, good leading of the class discussions
Time Effective usage of time (~8 minutes long)

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More on paper presentations

- Discuss your slides with me 3-4 days prior to your presentation
- Submit your final slides by the night before the class
- You are allowed to reuse the material already exist on the web

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CMP784: Deep Learning

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What is learning?

Two definitions of learning

- “Learning is the acquisition of knowledge about the world.“
  Kupfermann (1985)

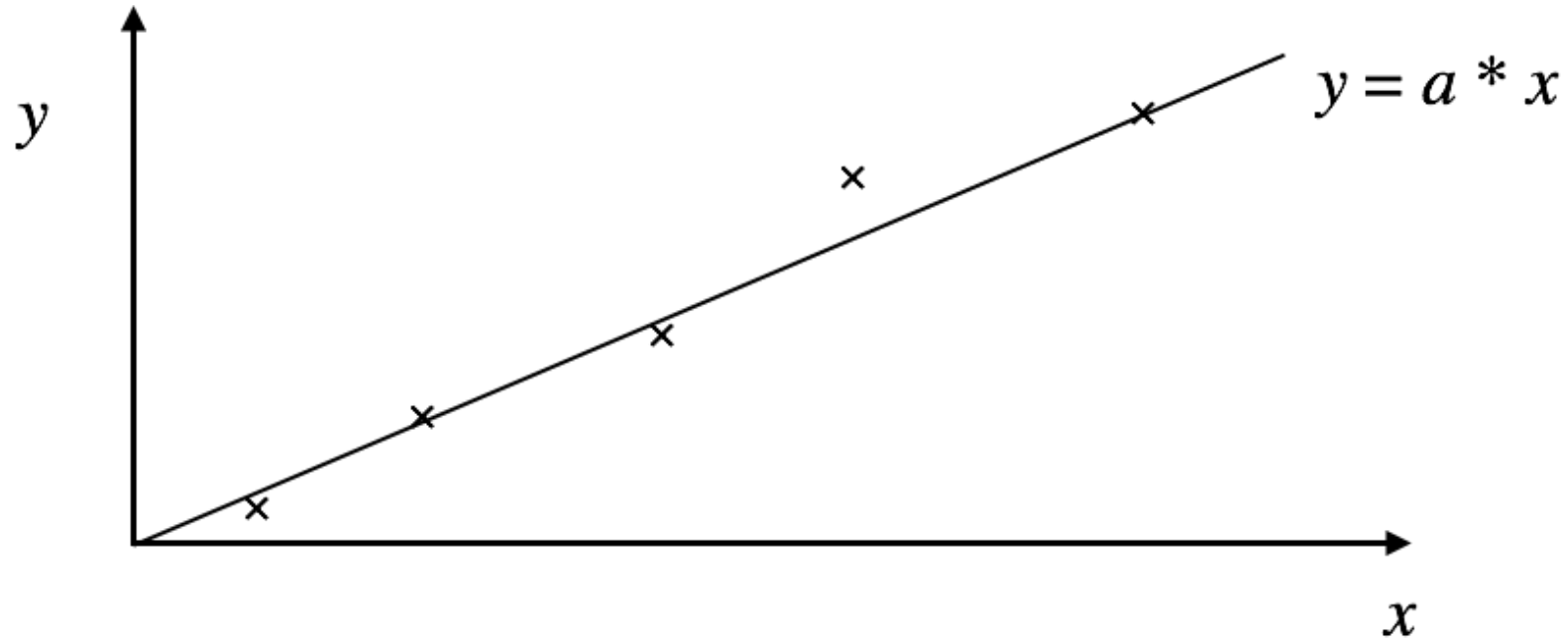
- “Learning is an adaptive change in behavior caused by experience.“
  Shepherd (1988)

Empirical Inference

- Drawing conclusions from empirical data (observations, measurements)
- Example 1: scientific inference

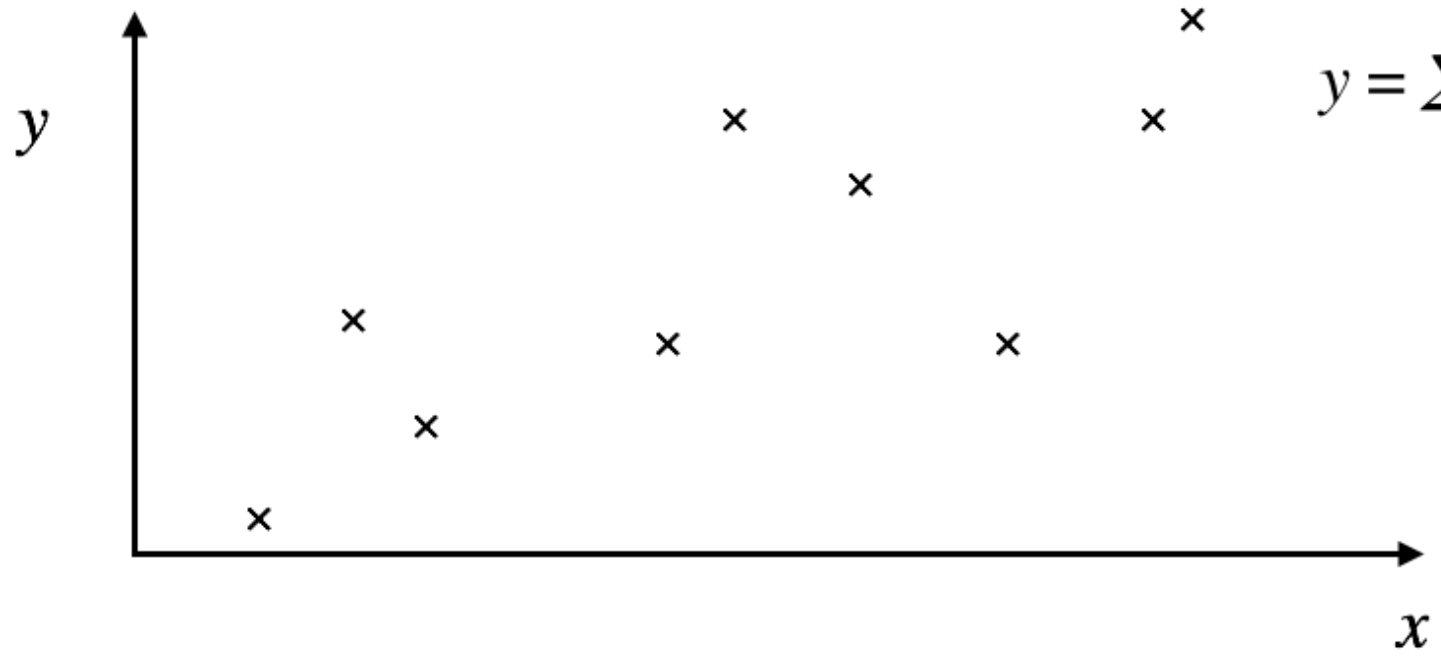
Empirical Inference

- Drawing conclusions from empirical data (observations, measurements)
- Example 1: scientific inference



Empirical Inference

- Drawing conclusions from empirical data (observations, measurements)
- Example 1: scientific inference

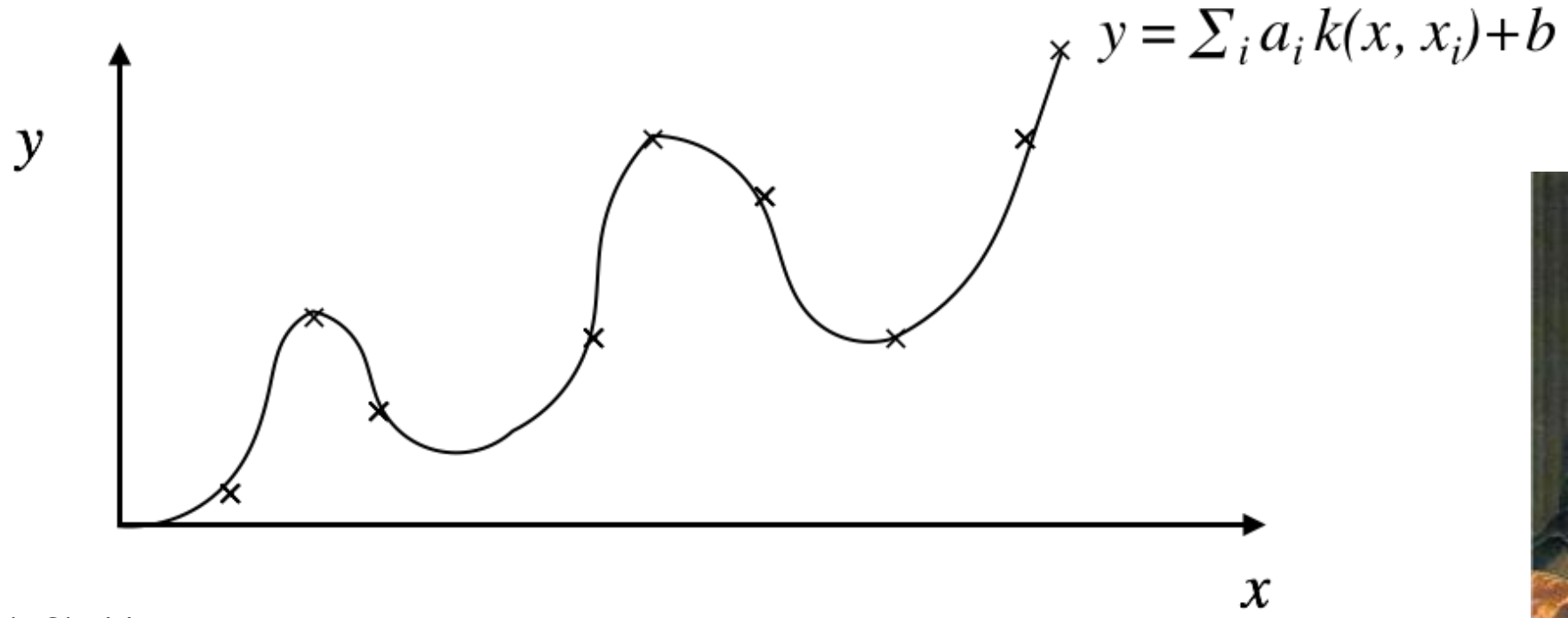


$$y = \sum_i a_i k(x, x_i) + b$$

Leibniz, Weyl, Chaitin

Empirical Inference

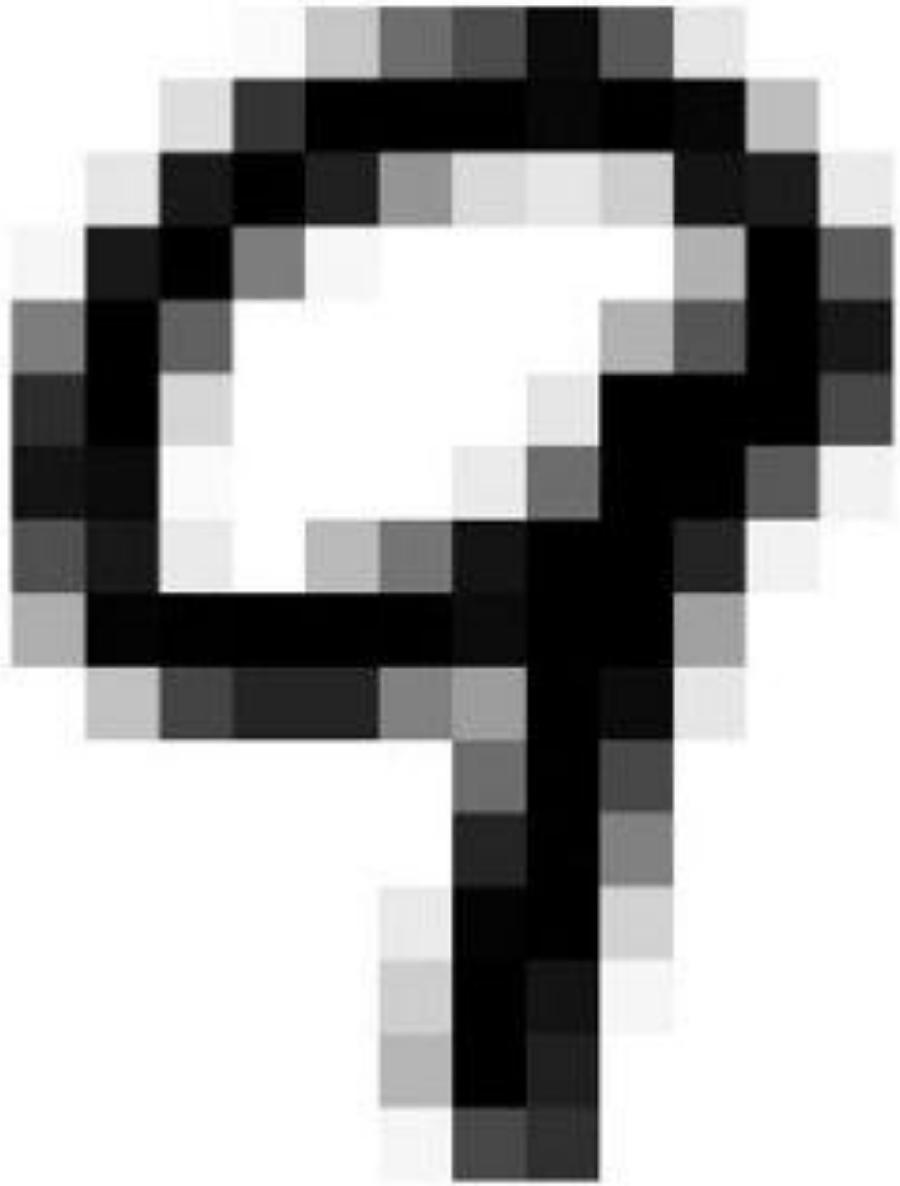
- Drawing conclusions from empirical data (observations, measurements)
- Example 1: scientific inference



Leibniz, Weyl, Chaitin

Empirical Inference

- Example 2: perception



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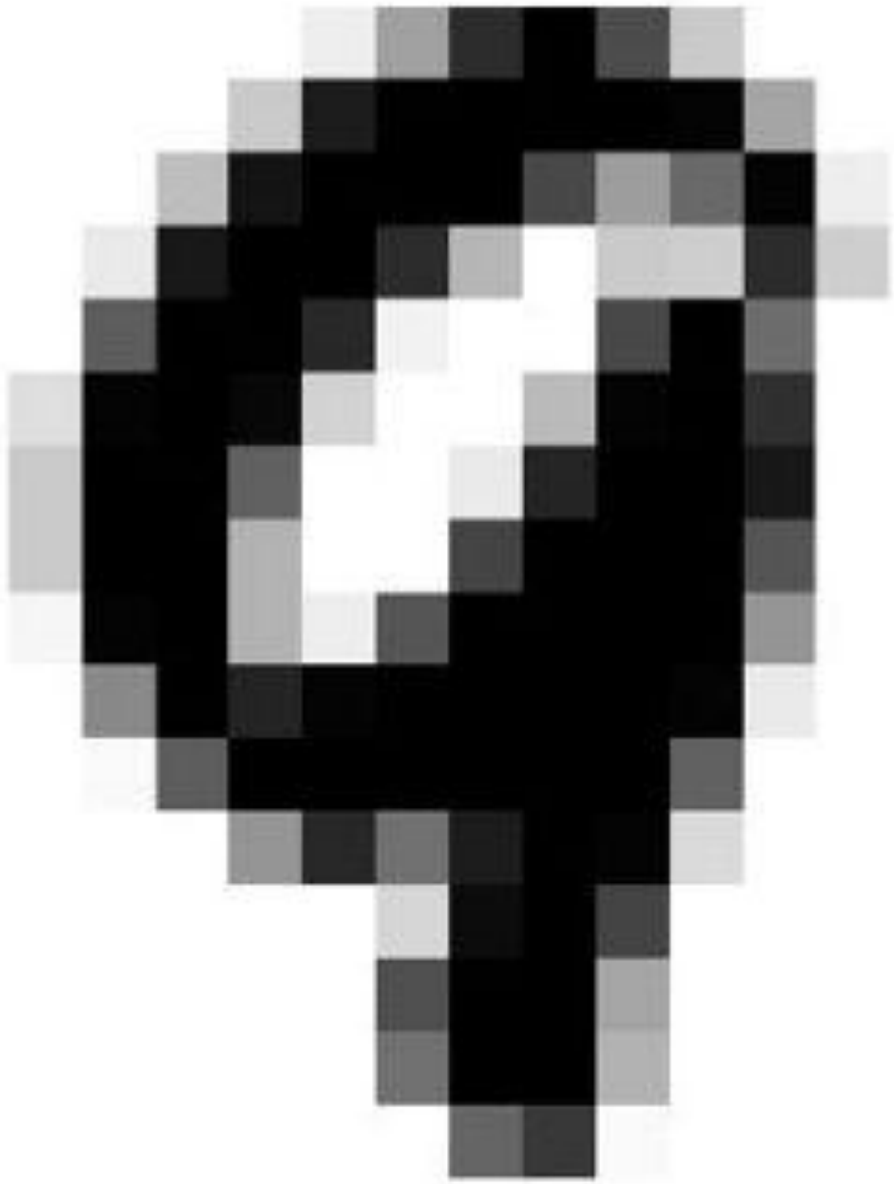

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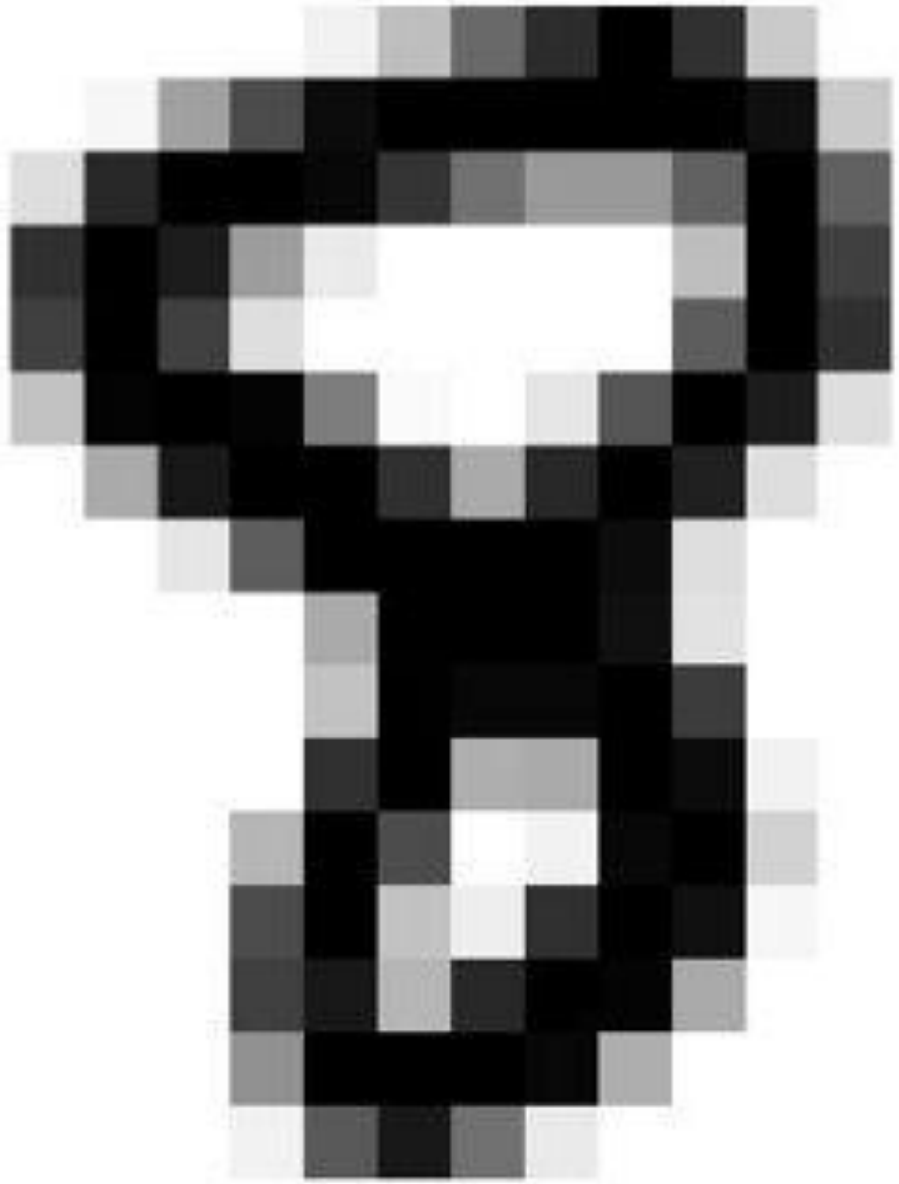

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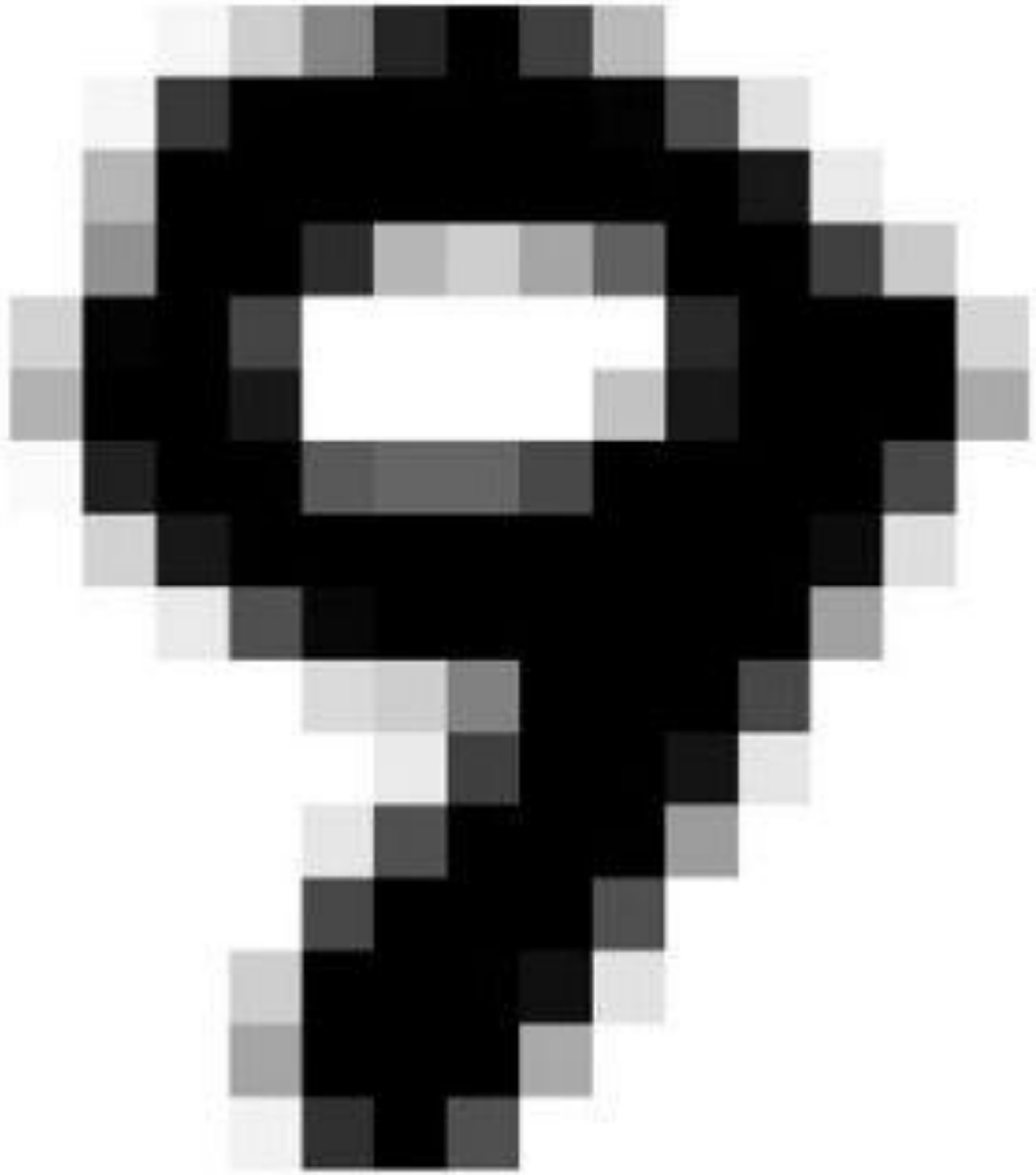

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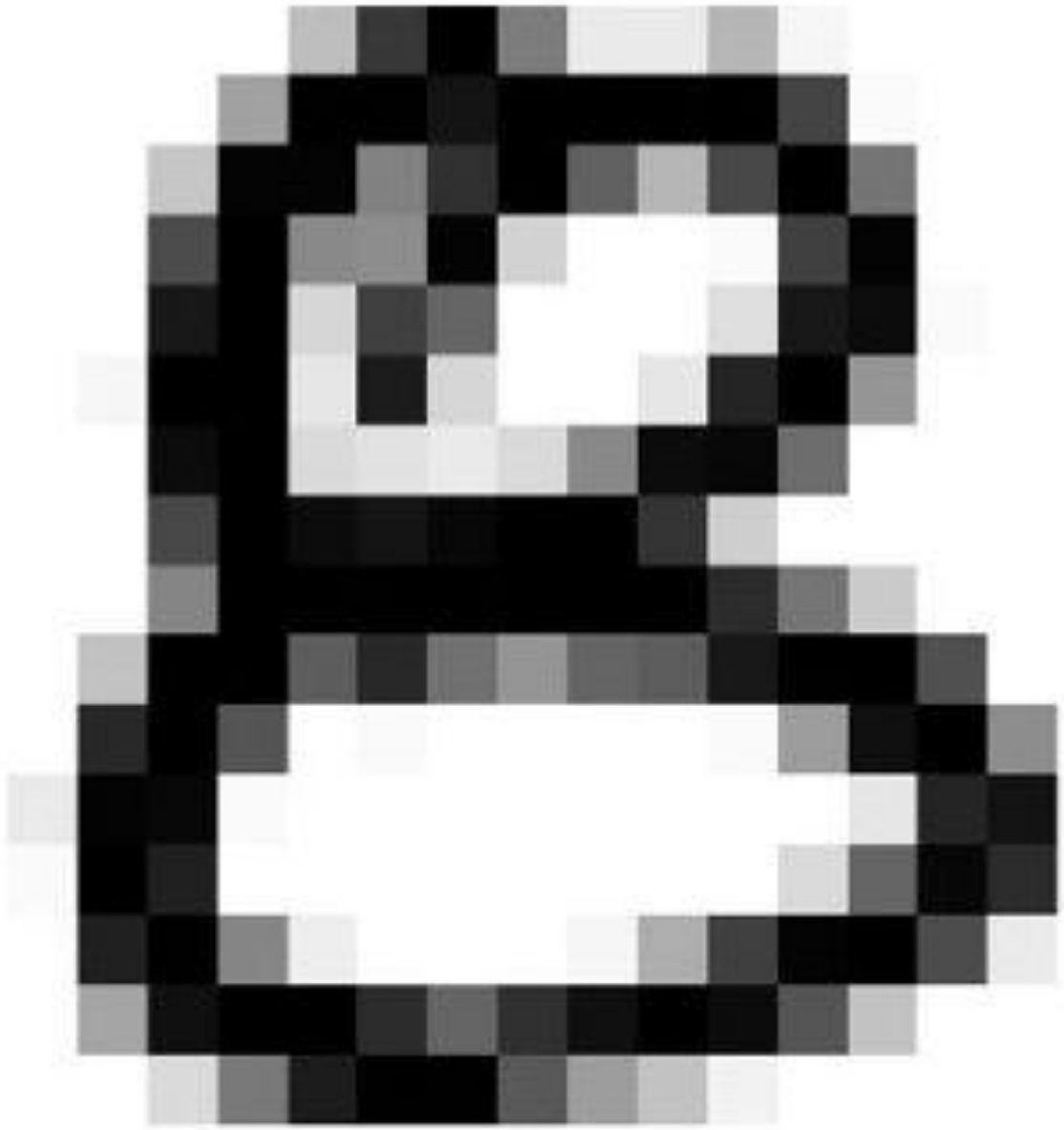

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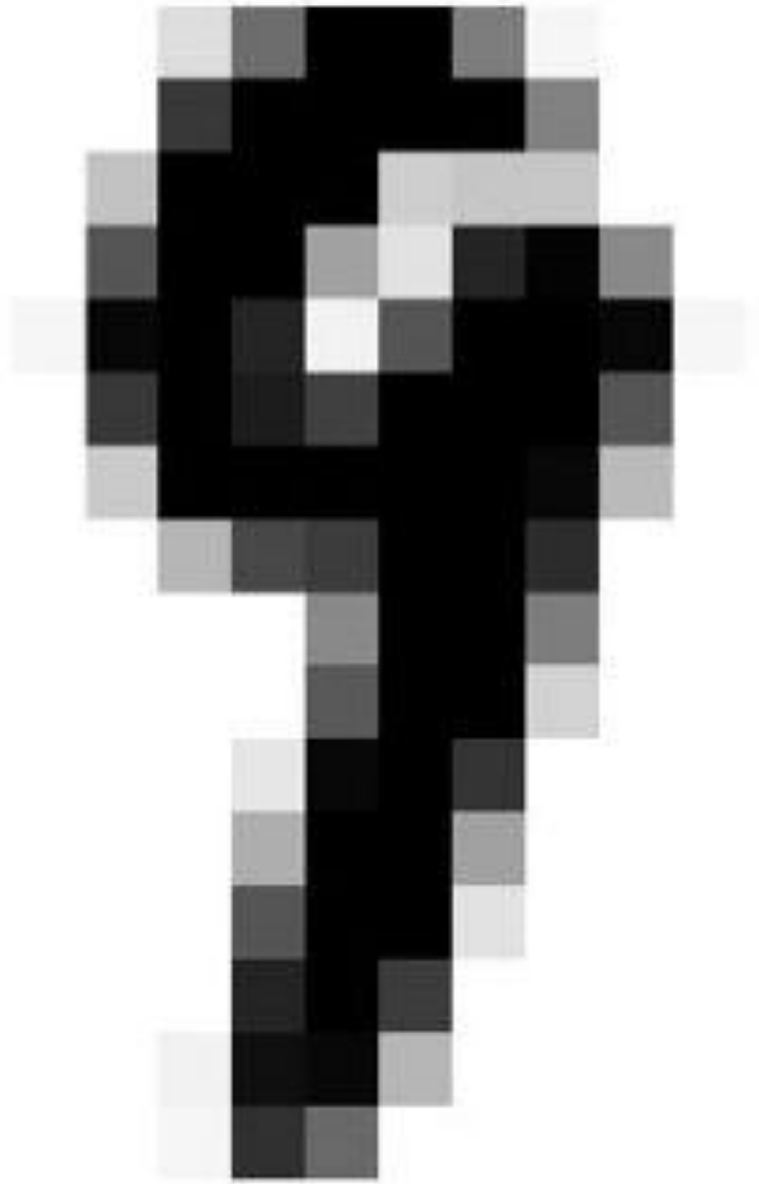

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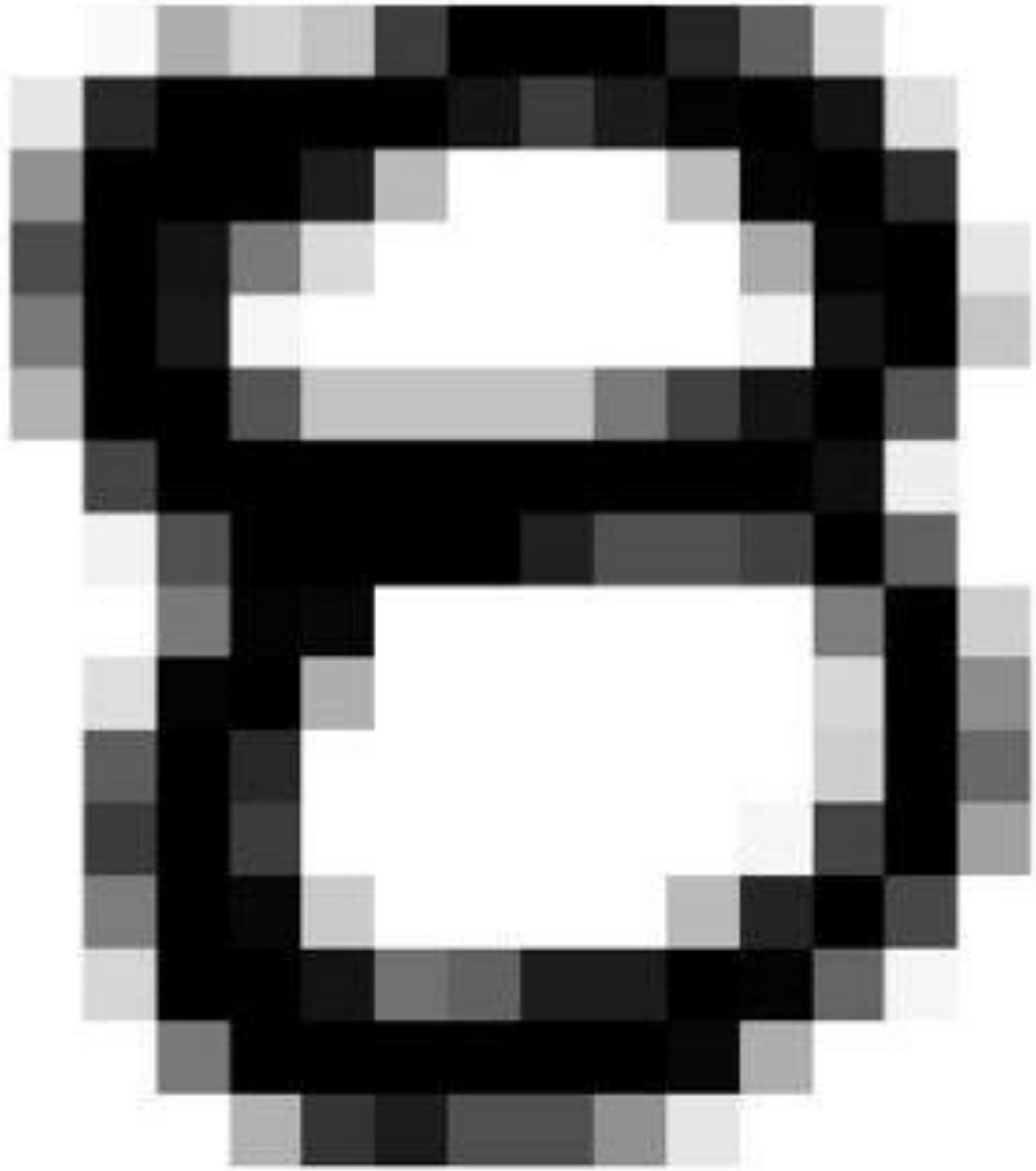

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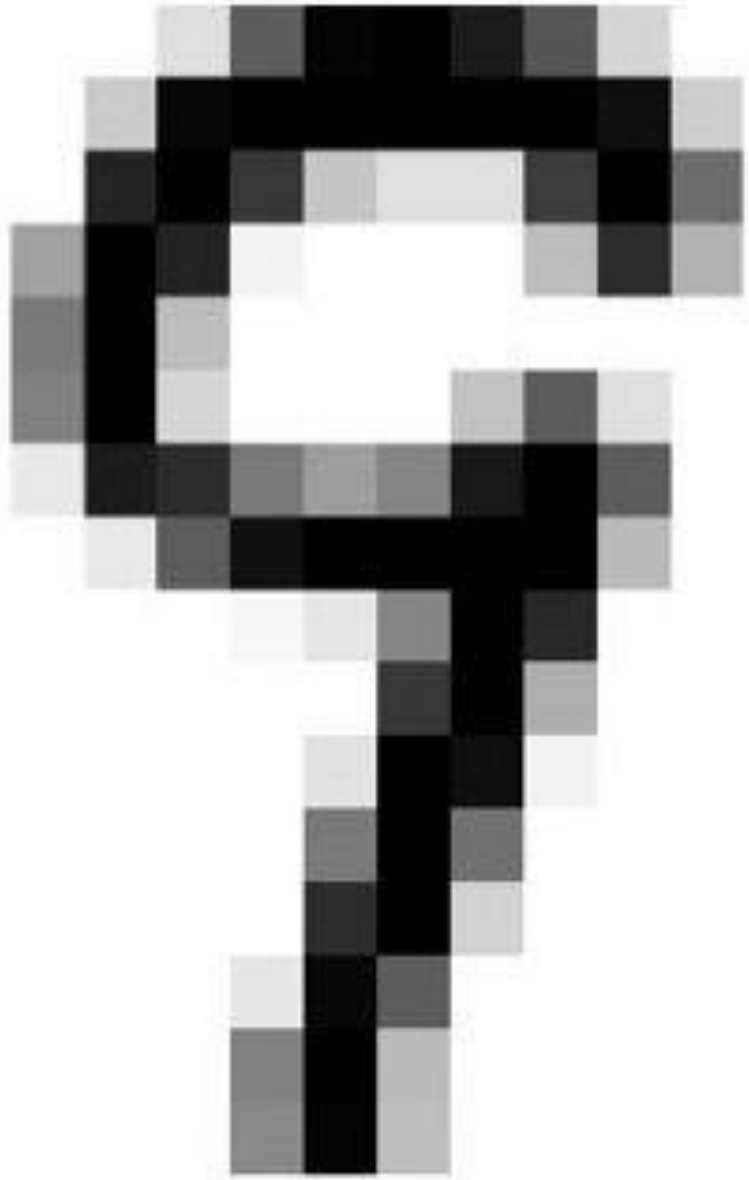

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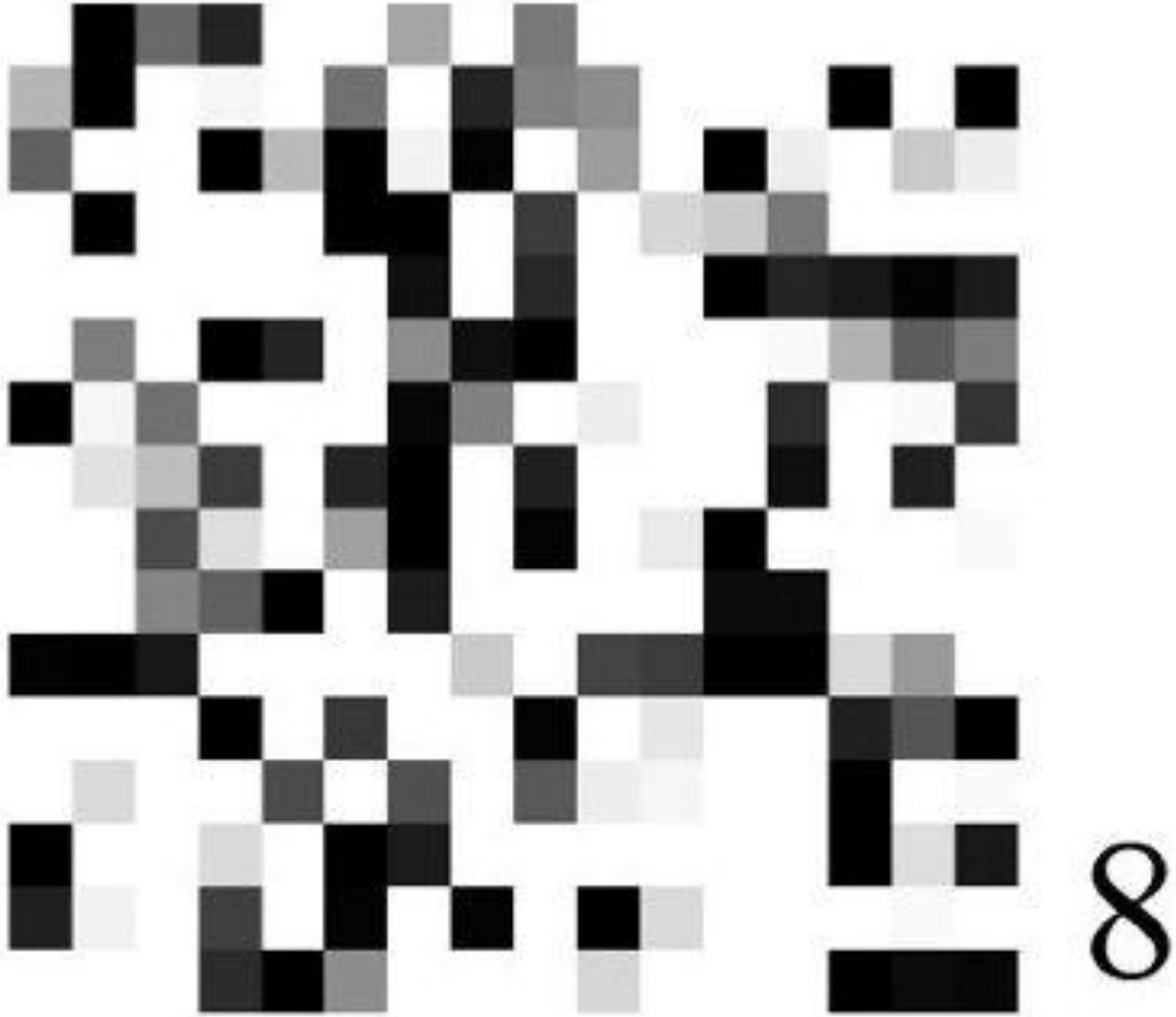


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The choice of representation may determine whether the learning task is very easy or very difficult!

Generalization

- *observe* 1, 2, 4, 7, …
- What's next?

+1 +2 +3

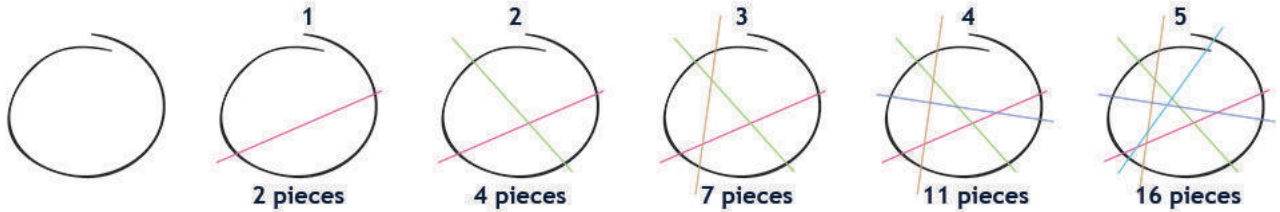


Image credit: mathspice.com

- 1,2,4,7,11,16,…: $a_{n+1} = a_n + n$ ("lazy caterer's sequence")
- 1,2,4,7,12,20,…: $a_{n+2} = a_{n+1} + a_n + 1$
- 1,2,4,7,13,24,…: "Tribonacci"-sequence
- 1,2,4,7,14,28 : divisors of 28
- 1,2,4,7,1,1,5,… : decimal expansions of π=3.14159… and e=2.718… interleaved *(thanks to O. Bousquet)*

- don't need e: 1247 appears at position 16992 in π
- The On-Line Encyclopedia of Integer Sequences: > 600 hits…

Generalization, II

- Question: which continuation is correct ("generalizes")?
- *Answer?* There's no way to tell *("induction problem")*

- Question of statistical learning theory: how to come up with a law that generalizes *("demarcation problem")*

Types of ML problems

Types of machine learning problems

Based on the information available:

- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Reinforcement learning

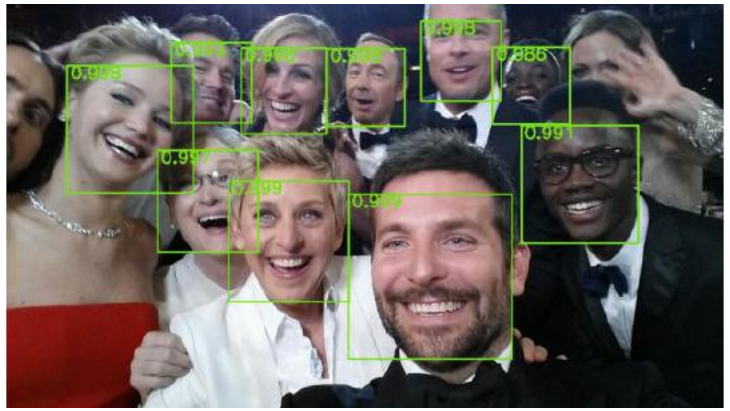
Supervised learning

- **Input:** $\{(\mathbf{x}, y)\}$

- **Task:** Predict target y from input $\mathbf{x}$
  - **Classification:** Discrete output
  - **Regression:** Real-valued output

→ cat

Image classification

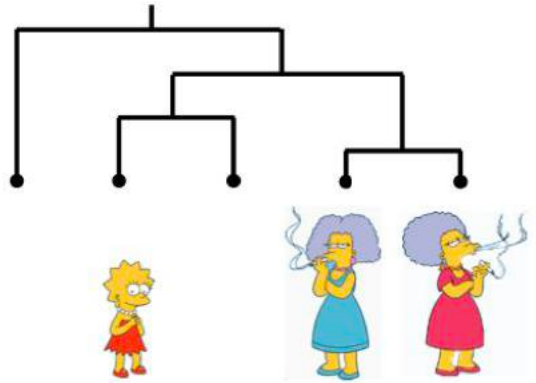


Face detection

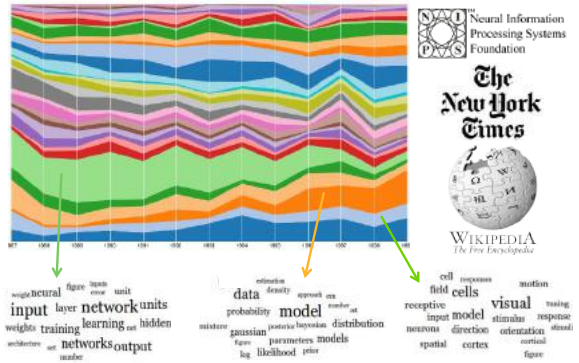
Unsupervised learning

- **Input:** $\{\mathbf{x}\}$

- **Task:** Reveal structure in the observed data
  - **Clustering:** Partition data into groups
  - **Feature extraction:** Learning meaningful features automatically
  - **Dimensionality reduction:** Learning a lower-dimensional representation of input



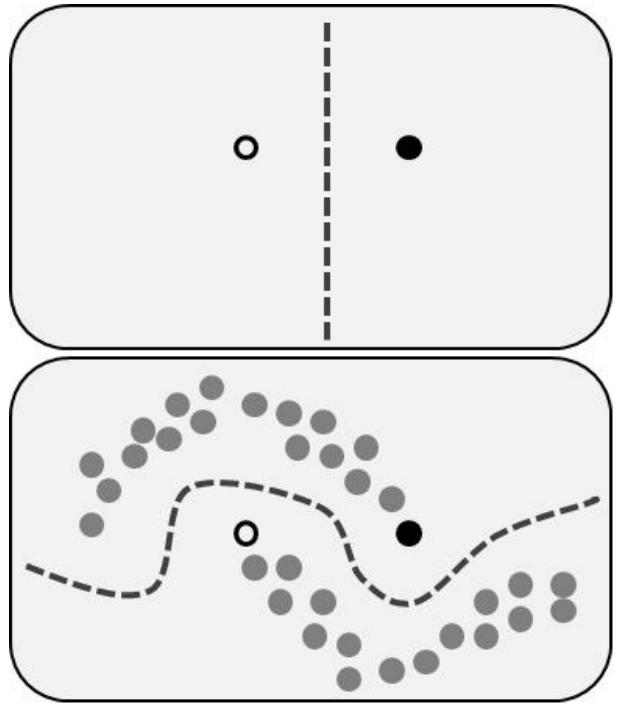
Agglomerative clustering



Topic modeling

Anomaly detection

Semi-supervised learning



- **Input:**

  Few labeled examples $\{(\mathbf{x}, y)\}$

  Many unlabeled examples $\{\mathbf{x}\}$

- **Task:** Predict target y from input $\mathbf{x}$
  - **Classification:** Discrete output
  - **Regression:** Real-valued output

interactive segmentation

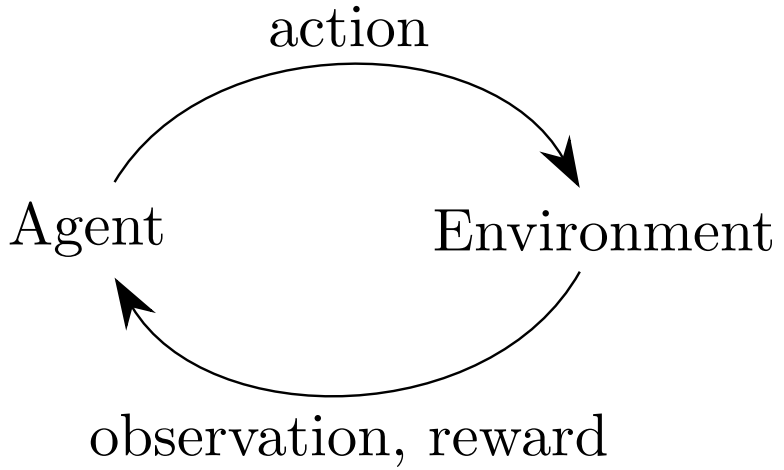
Try to improve predictions based on examples by making use of the additional "unlabeled" examples

Image credit: Wikipedia

Reinforcement learning

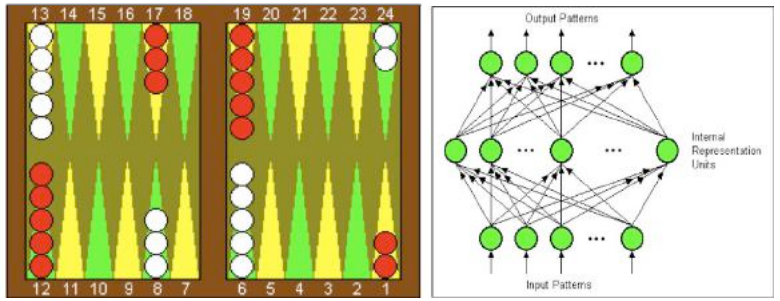
- **Input:**

  Interaction with an environment; the agent receives a numerical reward signal



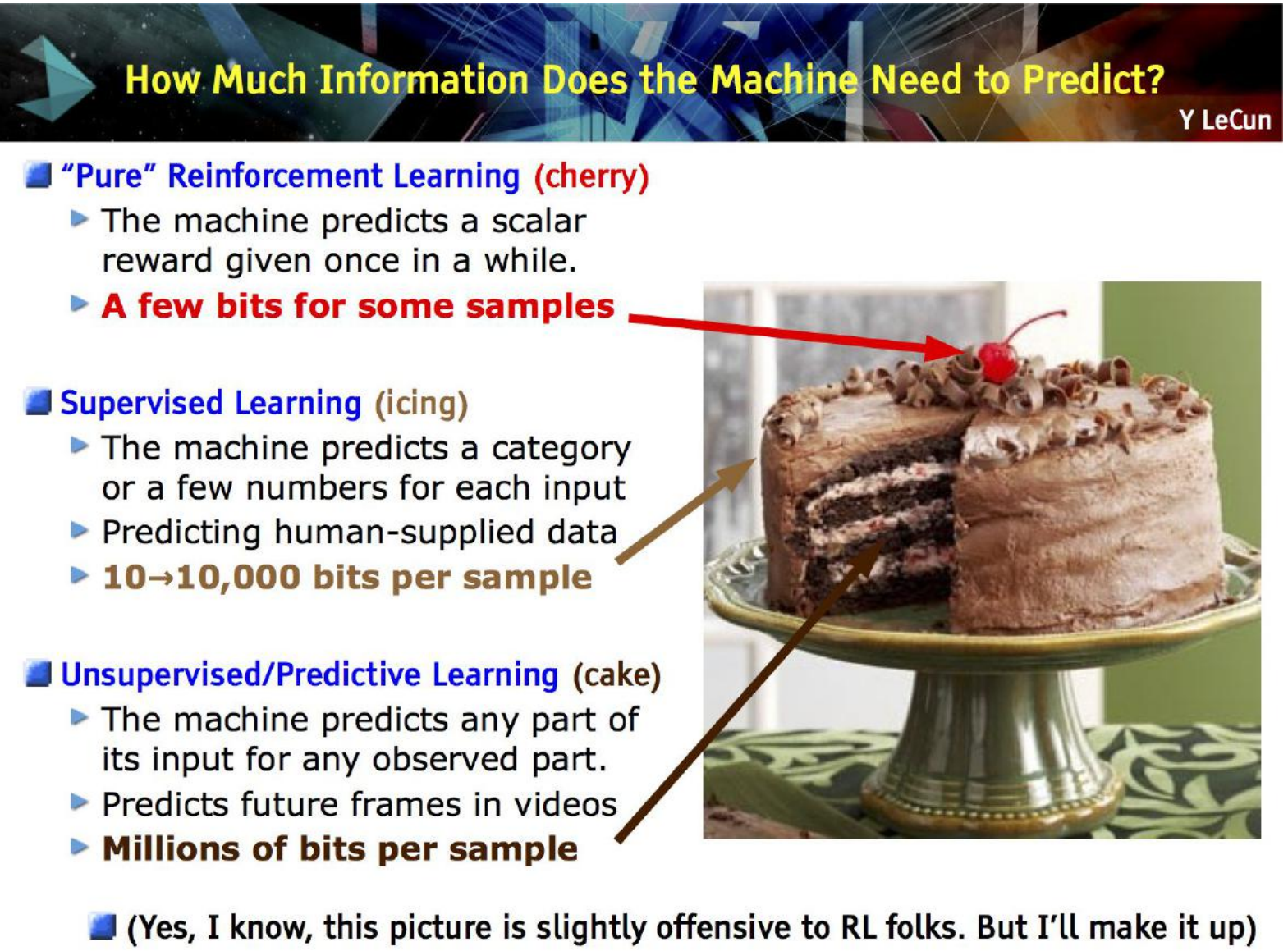
- **Task:** A way of behaving that is very rewarding in the long run

- Goal is to estimate and maximize the long-term cumulative reward



TD-Gammon (Tesauro, 1990-1995)

Types of machine learning problems



"If intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake. We know how to make the icing and the cherry, but we don't know how to make the cake."

– Yann LeCun
NIPS 2016 Keynote

Image classification

— non-parametric vs. parametric models
— nearest neighbor classifier
— hyperparameter
— cross-validation

Image Classification: a core task in Computer Vision

(assume given set of discrete labels)
{dog, cat, truck, plane, ...}

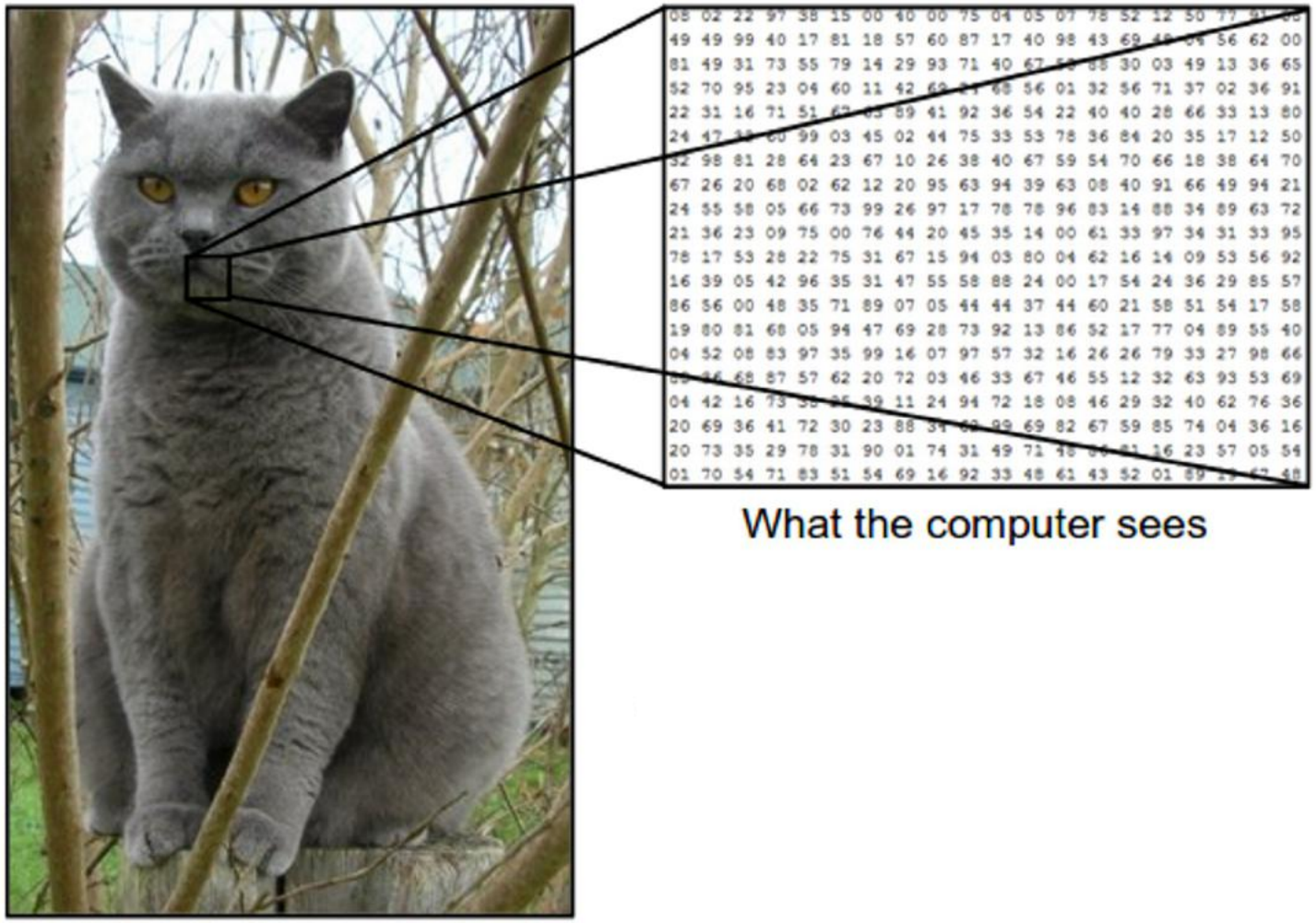
cat

The problem: **semantic gap**

Images are represented as 3D arrays of numbers, with integers between [0, 255].

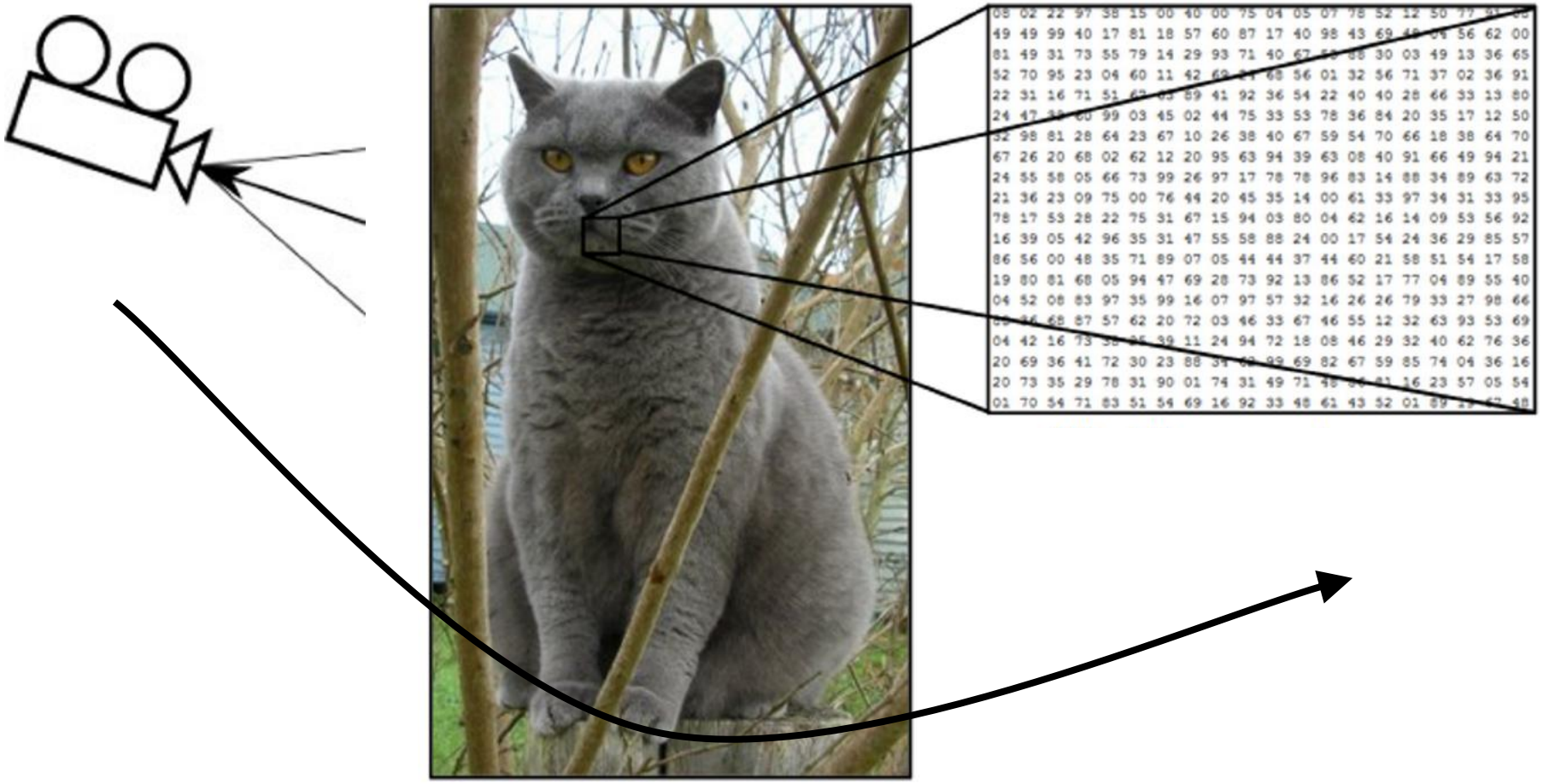
e.g.
300 x 100 x 3

(3 for 3 color channels RGB)



What the computer sees

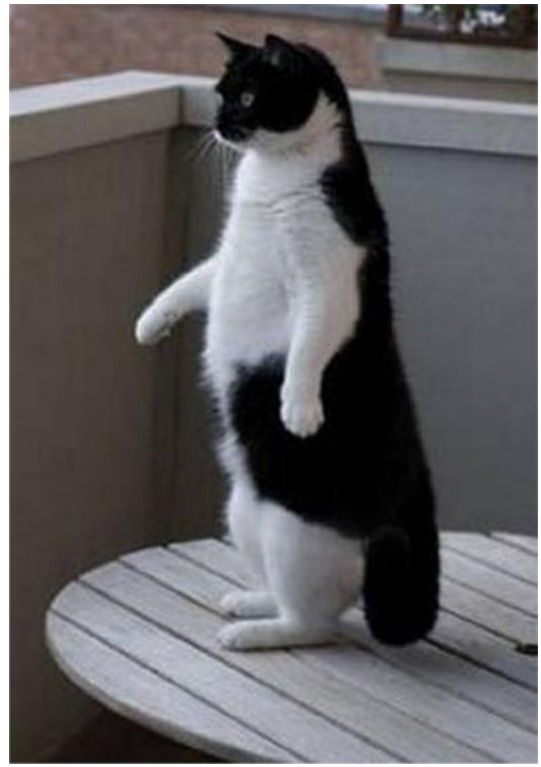
Challenges: Viewpoint Variation



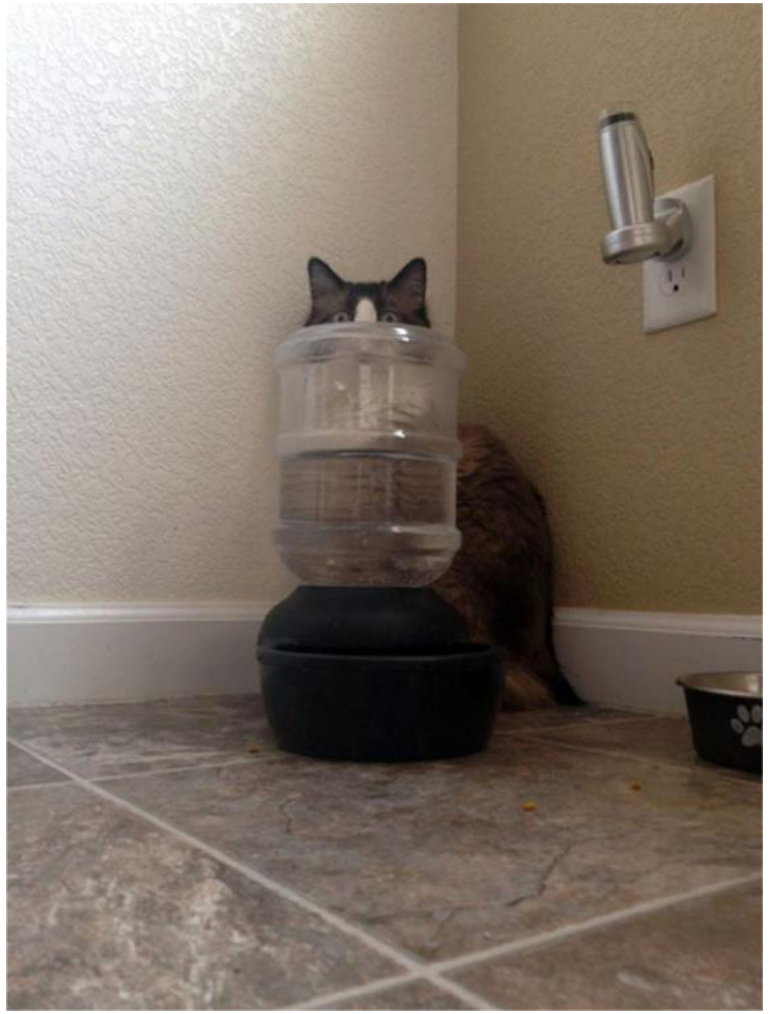
Challenges: Illumination

Challenges: Deformation



Challenges: Occlusion



Challenges: Background clutter

Challenges: Intraclass variation

An image classifier

```
def predict(image):
    # ????
    return class_label
```

Unlike e.g. sorting a list of numbers,

no obvious way to hard-code the algorithm for recognizing a cat, or other classes.

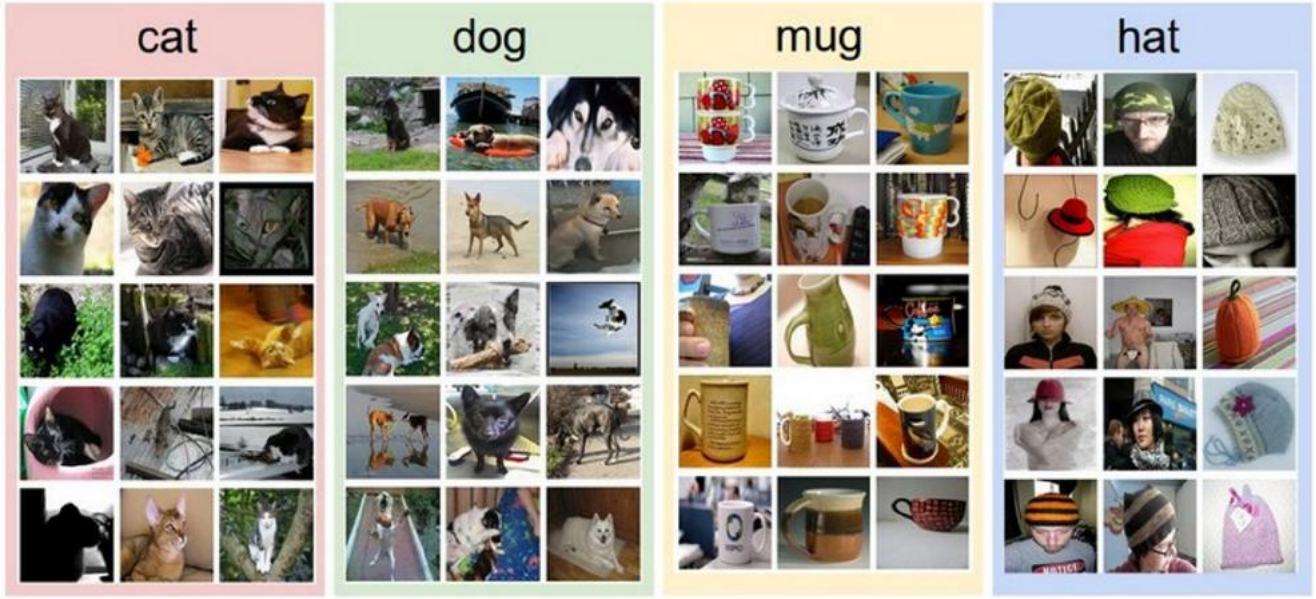
Data-driven approach:

1. Collect a dataset of images and labels
2. Use Machine Learning to train an image classifier
3. Evaluate the classifier on a withheld set of test images

```
def train(train_images, train_labels):
  # build a model for images -> labels...
  return model

def predict(model, test_images):
  # predict test_labels using the model...
  return test_labels
```

Example training set



First classifier: Nearest Neighbor Classifier

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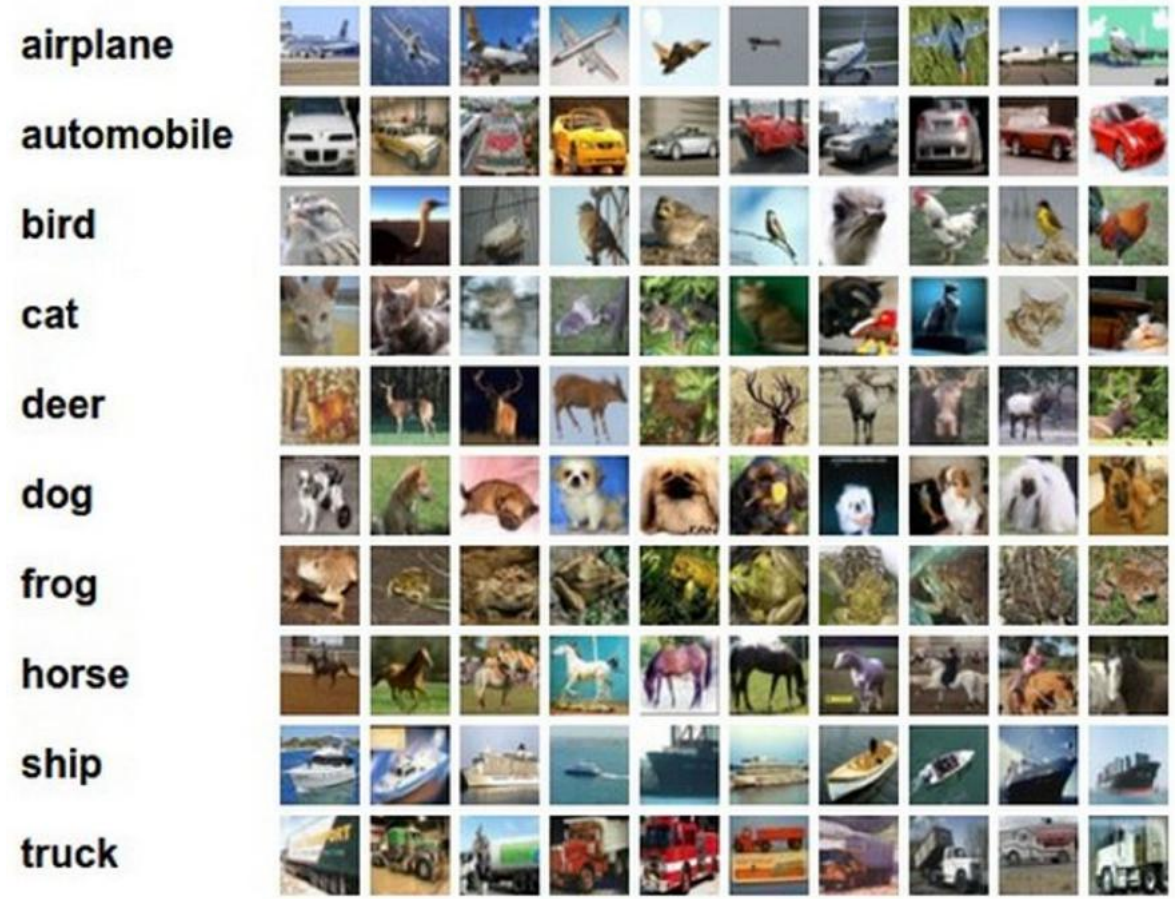
```

Remember all training images and their labels

Predict the label of the most similar training image

Example dataset: **CIFAR-10**
10 labels
50,000 training images, each image is tiny: 32x32
10,000 test images.



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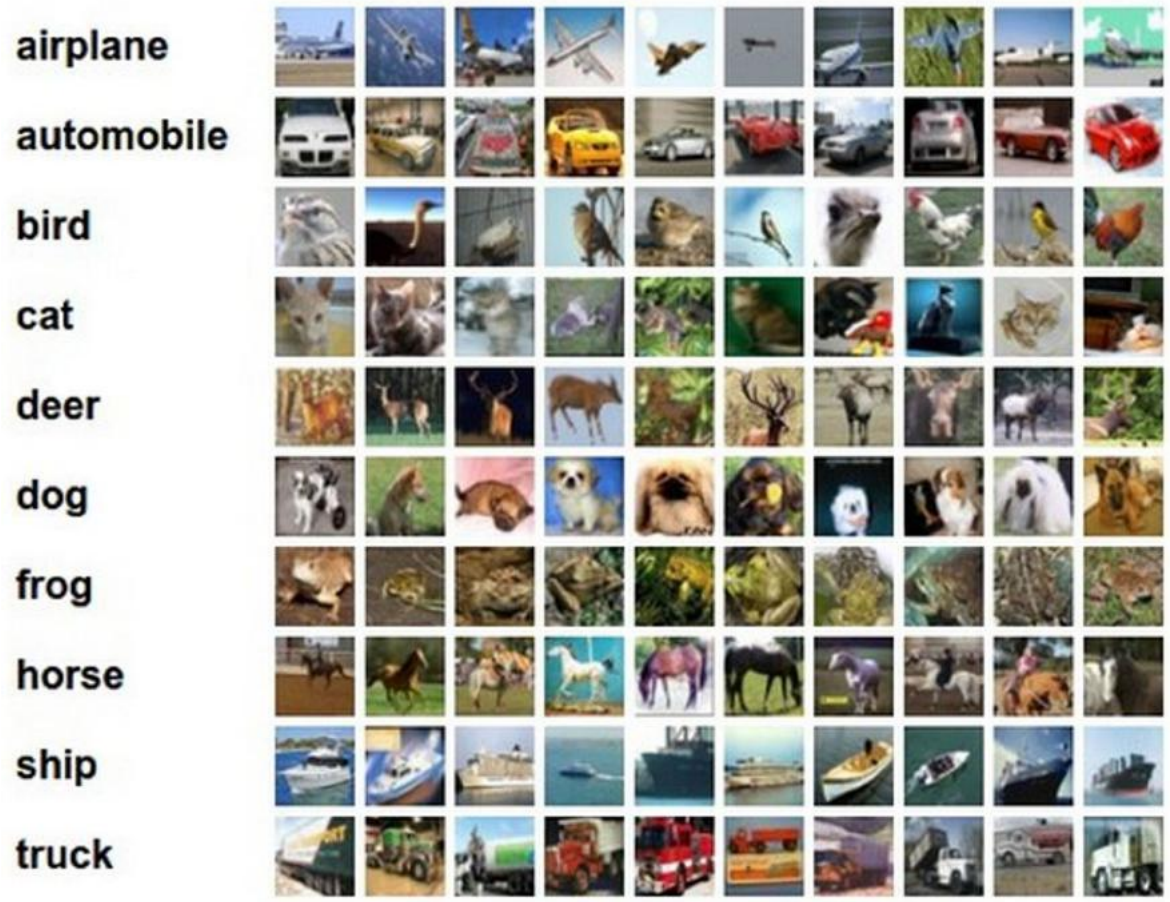
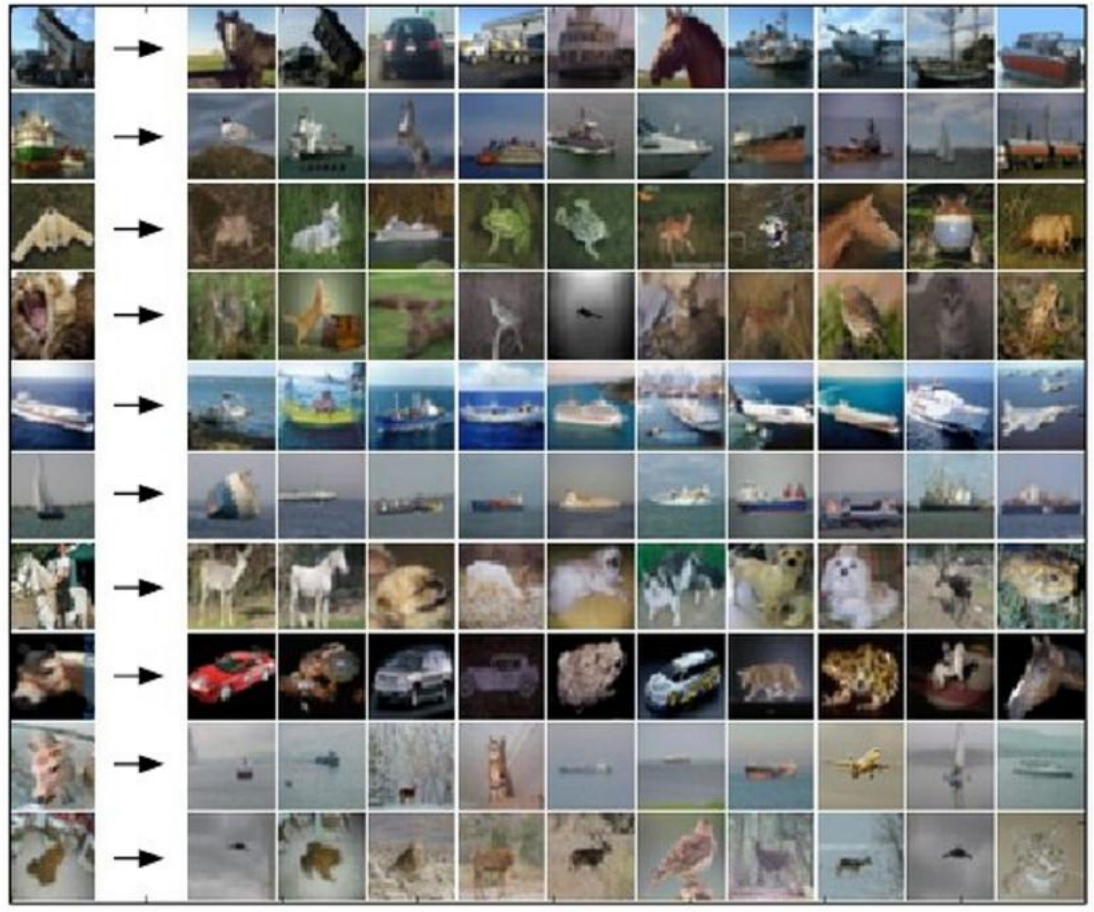
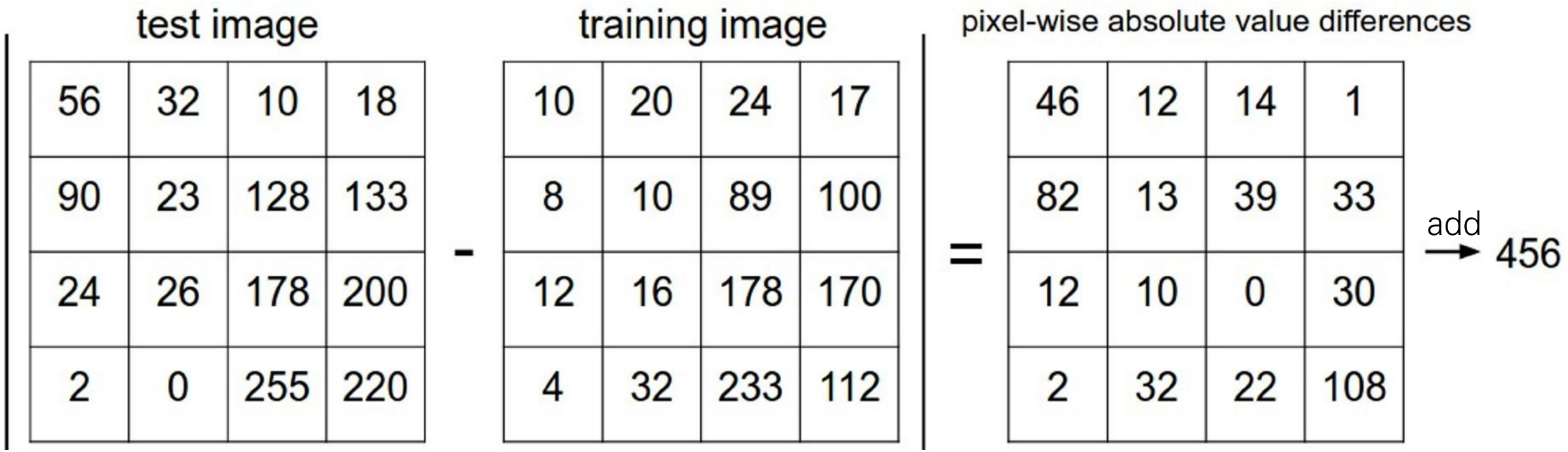


For every test image (first column), examples of nearest neighbors in rows



How do we compare the images? What is the **distance metric**?

L1 distance: $d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$



Nearest Neighbor classifier

```python
import numpy as np

class NearestNeighbor:
  def __init__(self):
    pass

  def train(self, X, y):
    """ X is N x D where each row is an example. Y is 1-dimension of size N """
    # the nearest neighbor classifier simply remembers all the training data
    self.Xtr = X
    self.ytr = y

  def predict(self, X):
    """ X is N x D where each row is an example we wish to predict label for """
    num_test = X.shape[0]
    # lets make sure that the output type matches the input type
    Ypred = np.zeros(num_test, dtype = self.ytr.dtype)

    # loop over all test rows
    for i in xrange(num_test):
      # find the nearest training image to the i'th test image
      # using the L1 distance (sum of absolute value differences)
      distances = np.sum(np.abs(self.Xtr - X[i,:]), axis = 1)
      min_index = np.argmin(distances) # get the index with smallest distance
      Ypred[i] = self.ytr[min_index] # predict the label of the nearest example

    return Ypred
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remember the training data

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```

for every test image:

- find nearest train image with L1 distance
- predict the label of nearest training image

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Nearest Neighbor classifier

Q: how does the classification speed depend on the size of the training data?

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```

Nearest Neighbor classifier

Q: how does the classification speed depend on the size of the training data? **linearly :(**

This is **backwards**:

- test time performance is usually much more important in practice.
- CNNs flip this: expensive training, cheap test evaluation

Aside: Approximate Nearest Neighbor

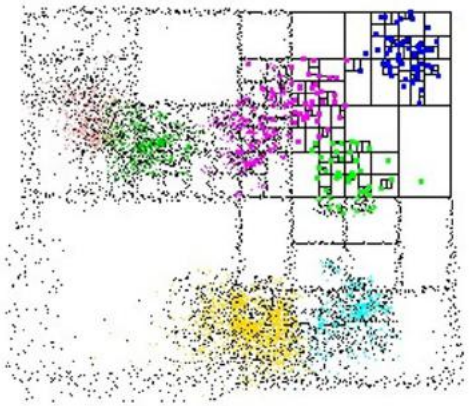
find approximate nearest neighbors quickly

ANN: A Library for Approximate Nearest Neighbor Searching

David M. Mount and Sunil Arya

Version 1.1.2

Release Date: Jan 27, 2010



What is ANN?

ANN is a library written in C++, which supports data structures and algorithms for both exact and approximate nearest neighbor searching in arbitrarily high dimensions.

In the nearest neighbor problem a set of data points in d-dimensional space is given. These points are preprocessed into a data structure, so that given any query point q, the nearest or generally k nearest points of P to q can be reported efficiently. The distance between two points can be defined in many ways. ANN assumes that distances are measured using any class of distance functions called Minkowski metrics. These include the well known Euclidean distance, Manhattan distance, and max distance.

Based on our own experience, ANN performs quite efficiently for point sets ranging in size from thousands to hundreds of thousands, and in dimensions as high as 20. (For applications in significantly higher dimensions, the results are rather spotty, but you might try it anyway.)

The library implements a number of different data structures, based on kd-trees and box-decomposition trees, and employs a couple of different search strategies.

The library also comes with test programs for measuring the quality of performance of ANN on any particular data sets, as well as programs for visualizing the structure of the geometric data structures.

FLANN - Fast Library for Approximate Nearest Neighbors

- Home
- News
- Publications
- Download
- Changelog
- Repository

What is FLANN?

FLANN is a library for performing fast approximate nearest neighbor searches in high dimensional spaces. It contains a collection of algorithms we found to work best for nearest neighbor search and a system for automatically choosing the best algorithm and optimum parameters depending on the dataset.

FLANN is written in C++ and contains bindings for the following languages: C, MATLAB and Python.

News

- (14 December 2012) Version 1.8.0 is out bringing incremental addition/removal of points to/from indexes
- (20 December 2011) Version 1.7.0 is out bringing two new index types and several other improvements.
- You can find binary installers for FLANN on the Point Cloud Library project page. Thanks to the PCL developers!
- Mac OS X users can install flann though MacPorts (thanks to Mark Moll for maintaining the Portfile)
- New release introducing an easier way to use custom distances, kd-tree implementation optimized for low dimensionality search and experimental MPI support
- New release introducing new C++ templated API, thread-safe search, save/load of indexes and more.
- The FLANN license was changed from LGPL to BSD.

How fast is it?

In our experiments we have found FLANN to be about one order of magnitude faster on many datasets (in query time), than previously available approximate nearest neighbor search software.

Publications

More information and experimental results can be found in the following papers:

- Marius Muja and David G. Lowe: **"Scalable Nearest Neighbor Algorithms for High Dimensional Data"**. Pattern Analysis and Machine Intelligence (PAMI), Vol. 36, 2014. [PDF] [BibTeX]
- Marius Muja and David G. Lowe: **"Fast Matching of Binary Features"**. Conference on Computer and Robot Vision (CRV) 2012. [PDF] [BibTeX]
- Marius Muja and David G. Lowe, **"Fast Approximate Nearest Neighbors with Automatic Algorithm Configuration"**, in International Conference on Computer Vision Theory and Applications (VISAPP'09), 2009 [PDF] [BibTeX]

The choice of distance is a **hyperparameter** common choices:

L1 (Manhattan) distance

$$d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$$

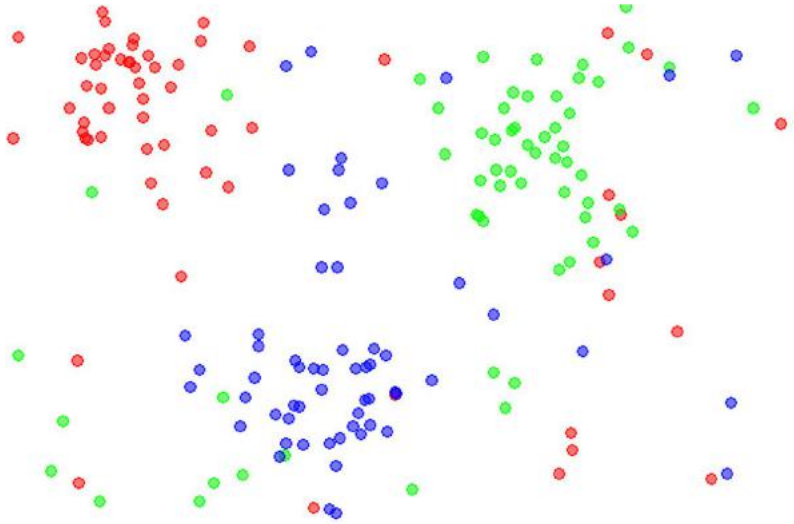
L2 (Euclidean) distance

$$d_2(I_1, I_2) = \sqrt{\sum_p (I_1^p - I_2^p)^2}$$

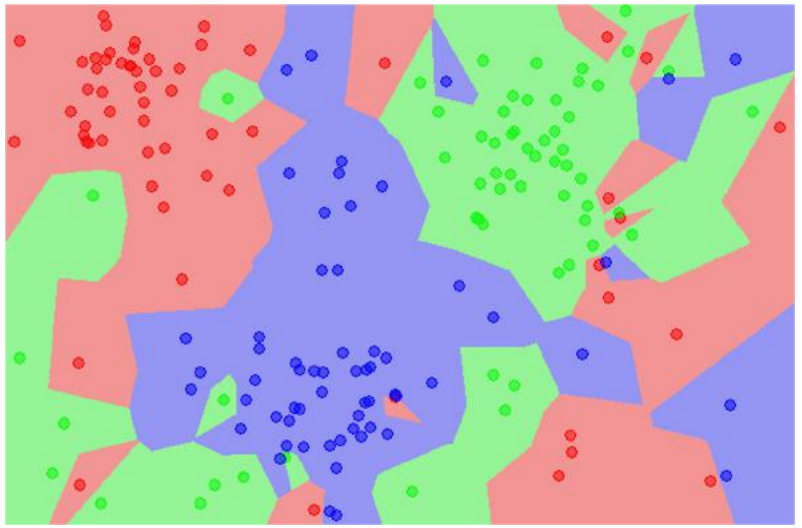
k-Nearest Neighbor

find the k nearest images, have them vote on the label

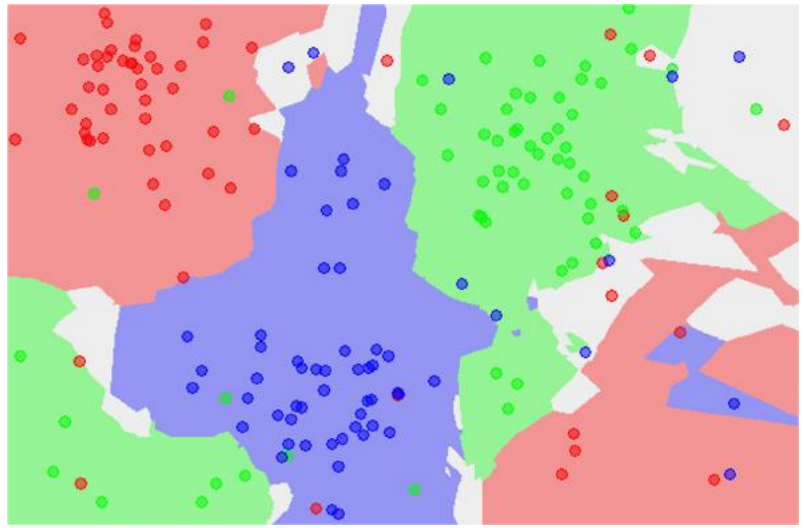
the data



NN classifier



5-NN classifier



http://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm

Example dataset: **CIFAR-10**
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50,000 training images
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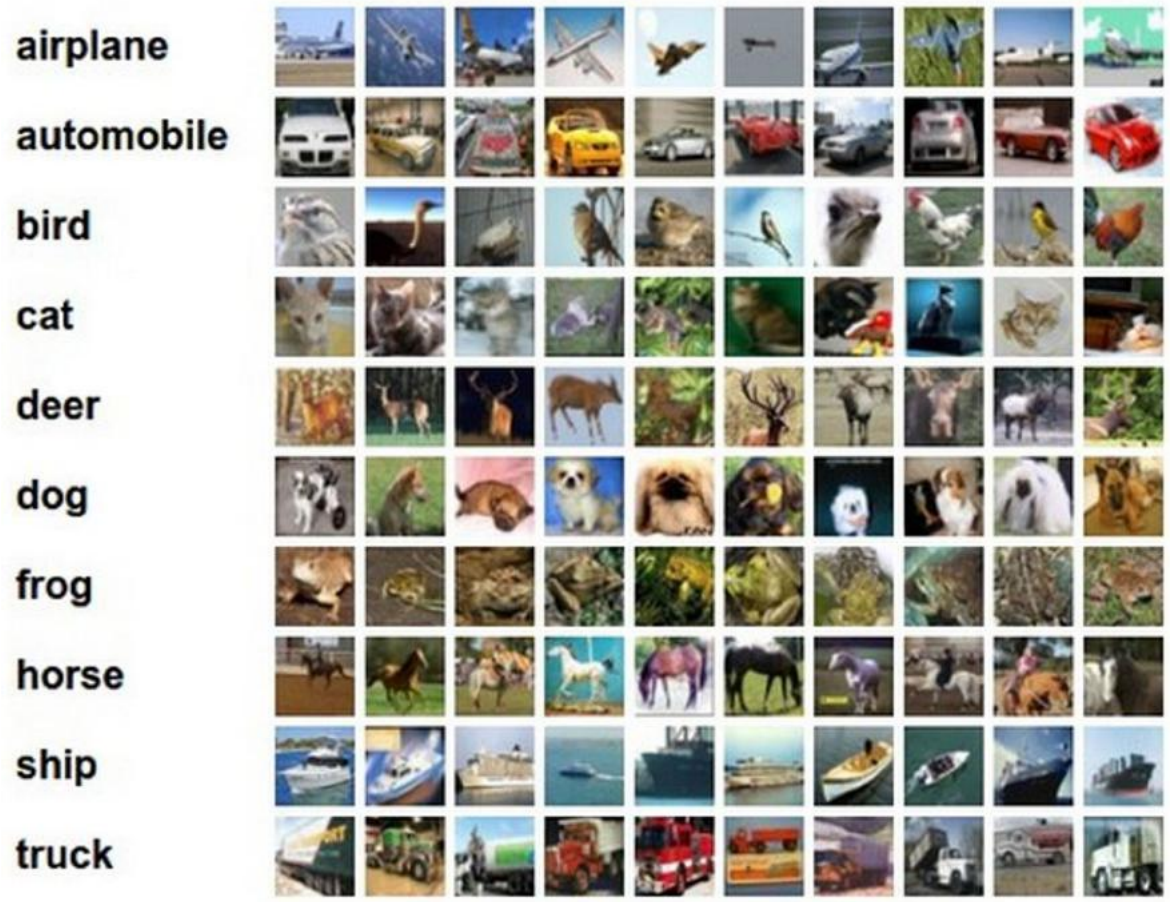
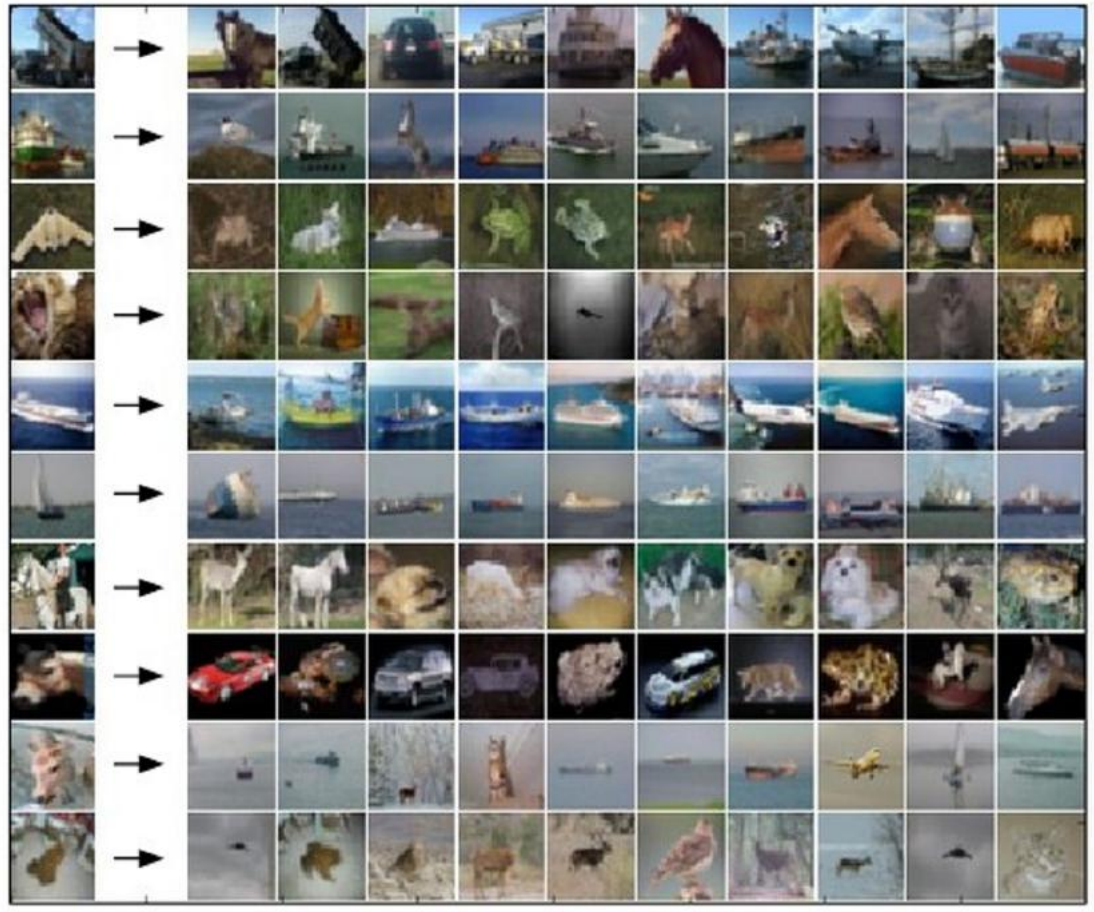
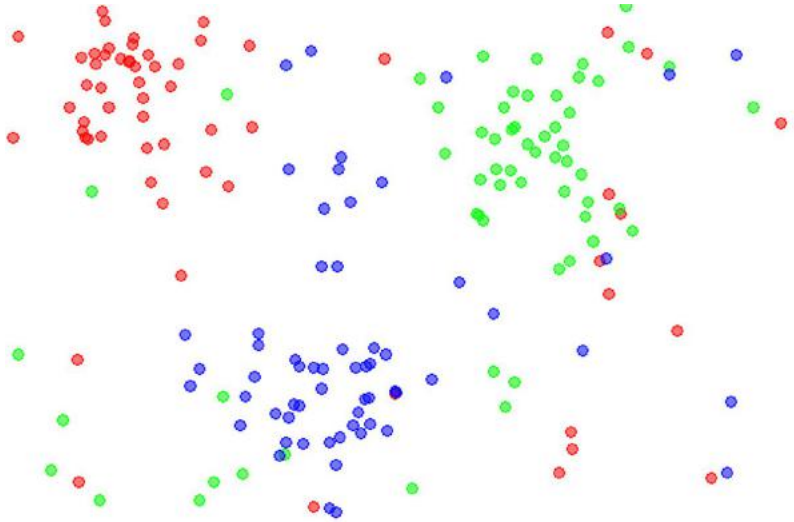


For every test image (first column), examples of nearest neighbors in rows



the data



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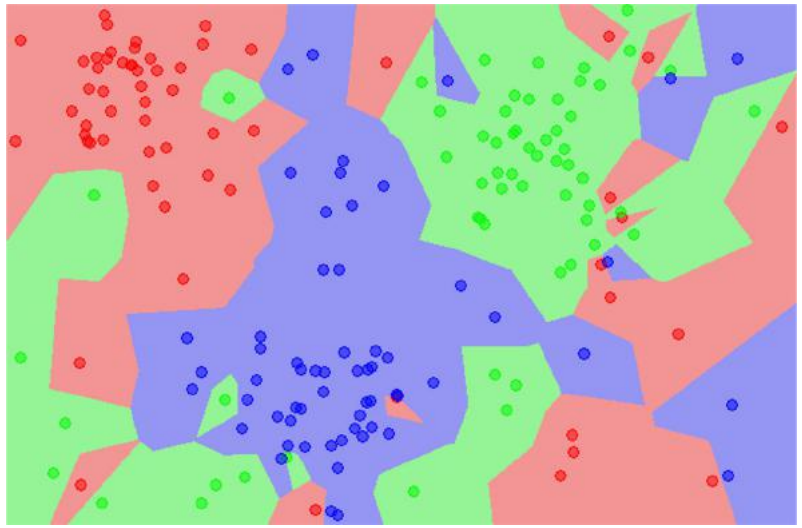

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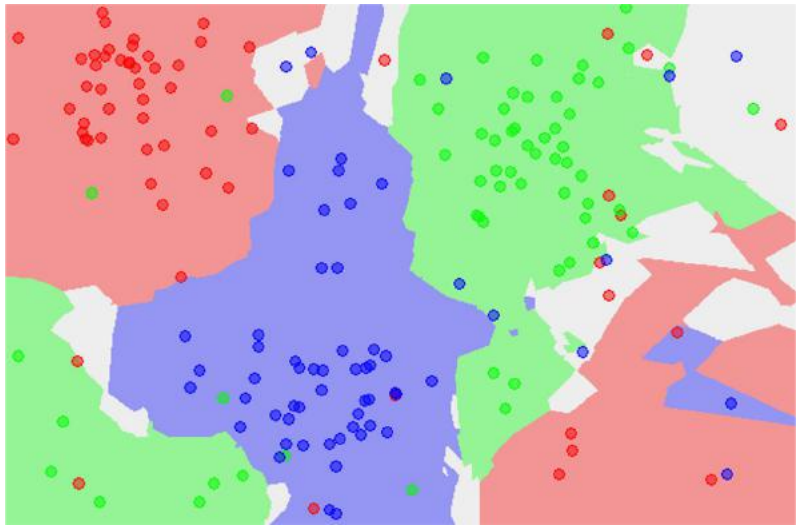
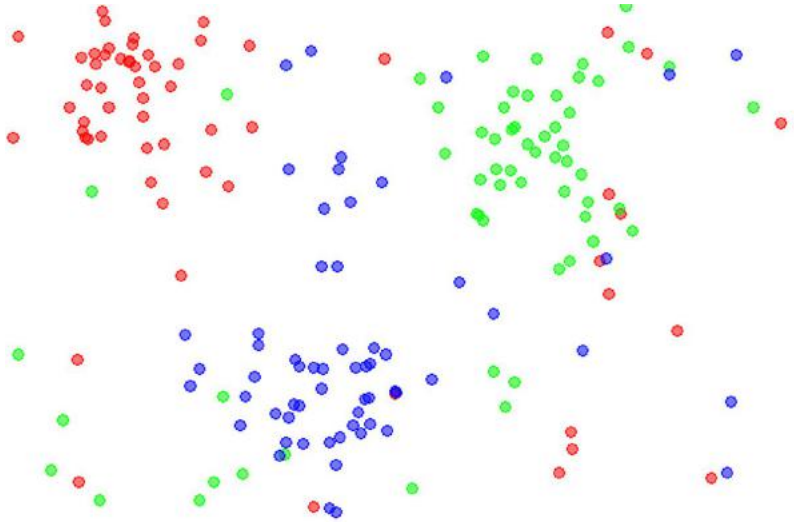
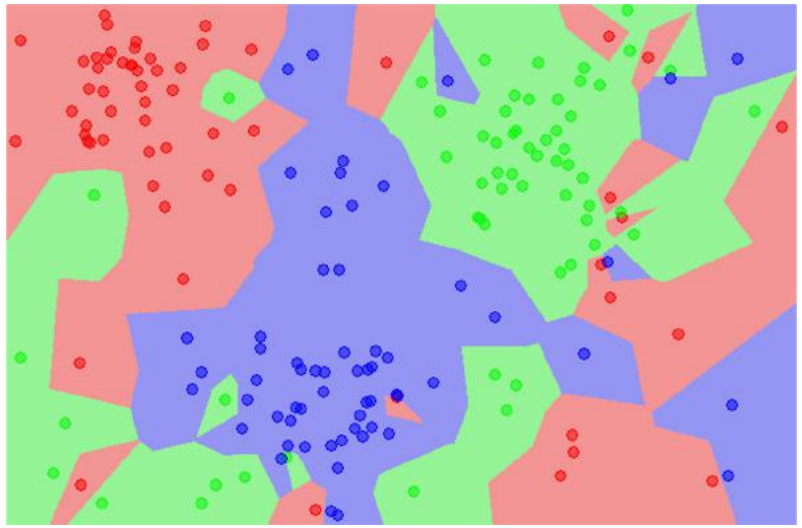


Q: what is the accuracy of the nearest neighbor classifier on the training data, when using the Euclidean distance?

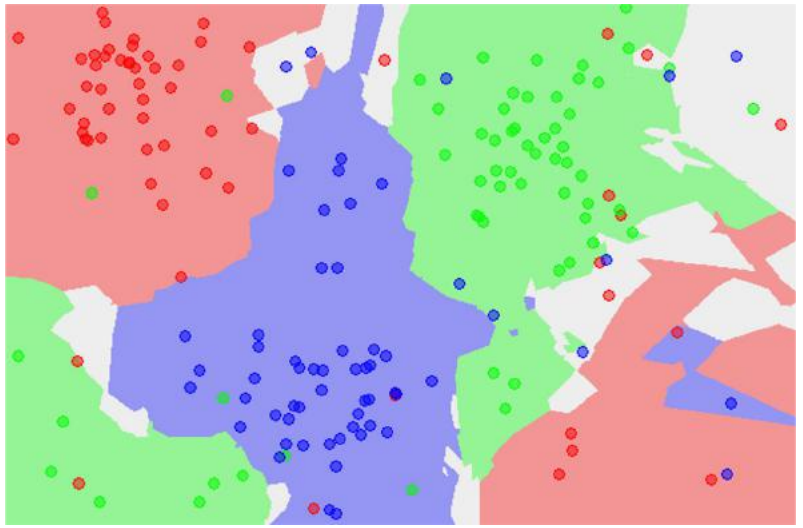
the data



NN classifier



5-NN classifier



Q2: what is the accuracy of the **k**-nearest neighbor classifier on the training data?

What is the best **distance** to use?
What is the best value of **k** to use?

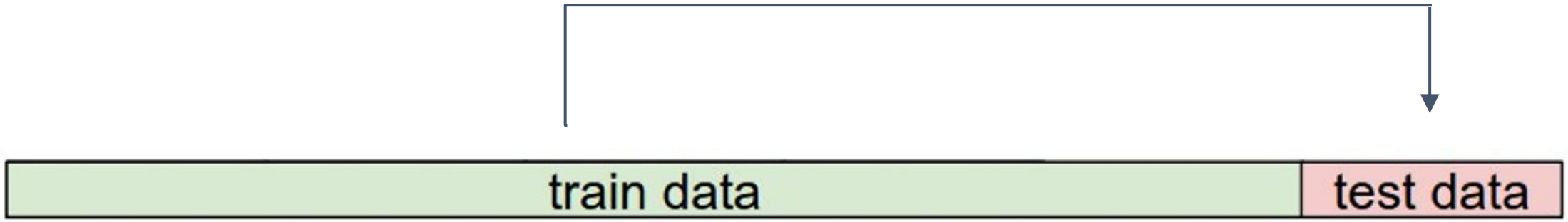
i.e. how do we set the **hyperparameters**?

What is the best **distance** to use?
What is the best value of **k** to use?

i.e. how do we set the **hyperparameters**?

Very problem-dependent.
Must try them all out and see what works best.

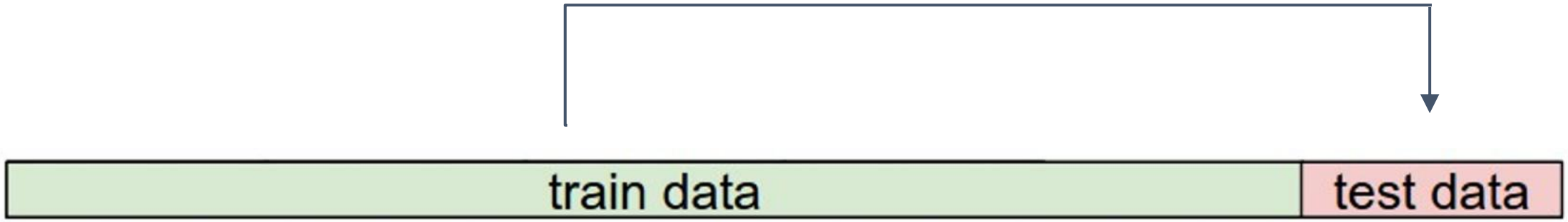
Try out what hyperparameters work best on test set.

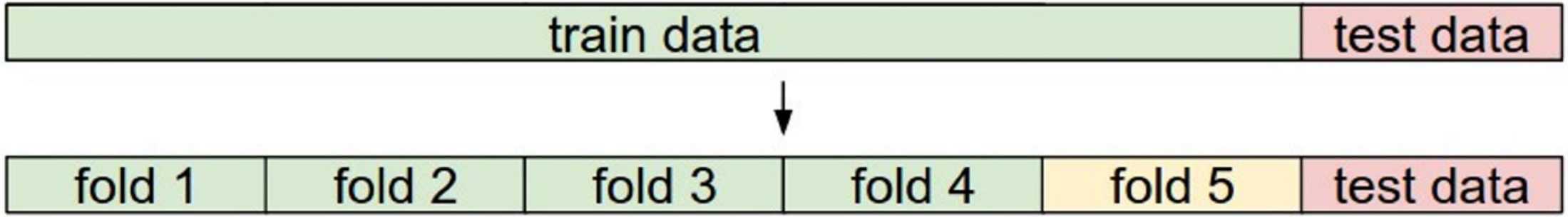


Trying out what hyperparameters work best on test set:

Very bad idea. The test set is a proxy for the generalization performance!

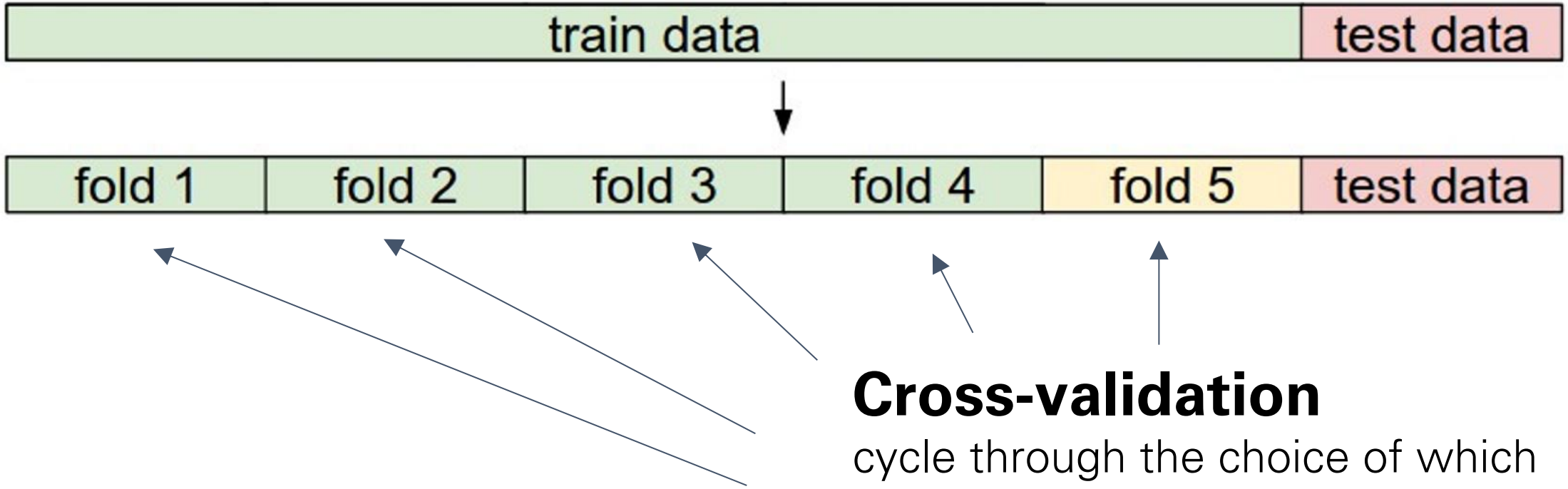
Use only **VERY SPARINGLY**, at the end.





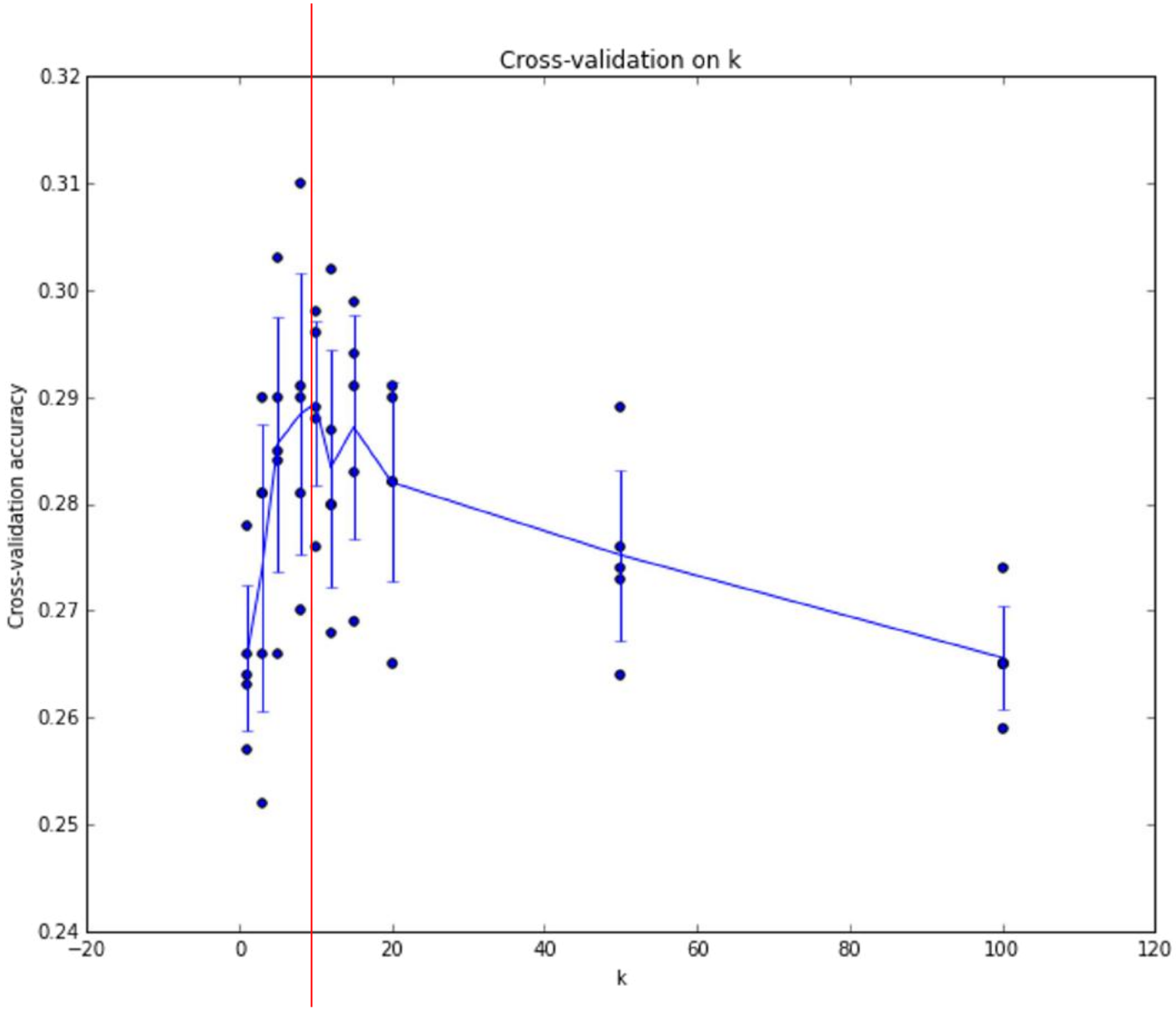
Validation data

use to tune hyperparameters



Cross-validation

cycle through the choice of which fold is the validation fold, average results.



Example of
5-fold cross-validation
for the value of **k**.

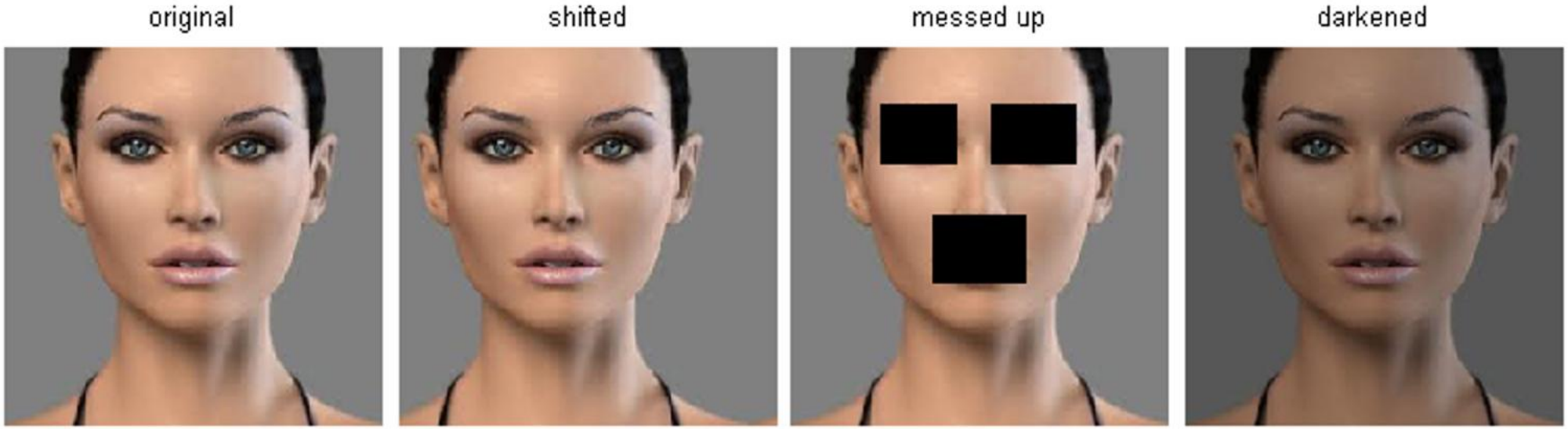
Each point: single outcome.

The line goes through the mean, bars indicated standard deviation

(Seems that k ~= 7 works the best for this data)

k-Nearest Neighbor on images **never used.**

- terrible performance at test time
- distance metrics on level of whole images can be very unintuitive



(all 3 images have same L2 distance to the one on the left)

The learning problem

— linear classification
— hypothesis class, estimation algorithm
— loss and estimation criterion
— sampling, empirical and expected losses

The Learning Problem

Digit Recognition

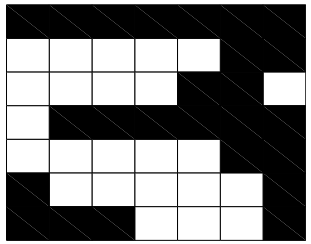


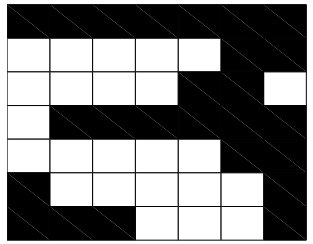
Image Classification

- Steps
  - —entertain a (biased) set of possibilities (hypothesis class)
  - —adjust predictions based on available examples (estimation)
  - —rethink the set of possibilities (model selection)
- Principles of learning are “universal”
  - —society (e.g., scientific community)
  - —animal (e.g., human)
  - —machine

Hypothesis class

- Representation: examples are binary vectors of length $d = 64$

$$\mathbf{x} = [111\ldots0001]^T =$$



and labels $y \in \{-1, 1\}$ ("no","yes")

- The mapping from examples to labels is a "**linear classifier**"

$$\hat{y} = \text{sign}\,(\,\theta \cdot \mathbf{x}\,) = \text{sign}\,(\,\theta_1 x_1 + \ldots + \theta_d x_d\,)$$

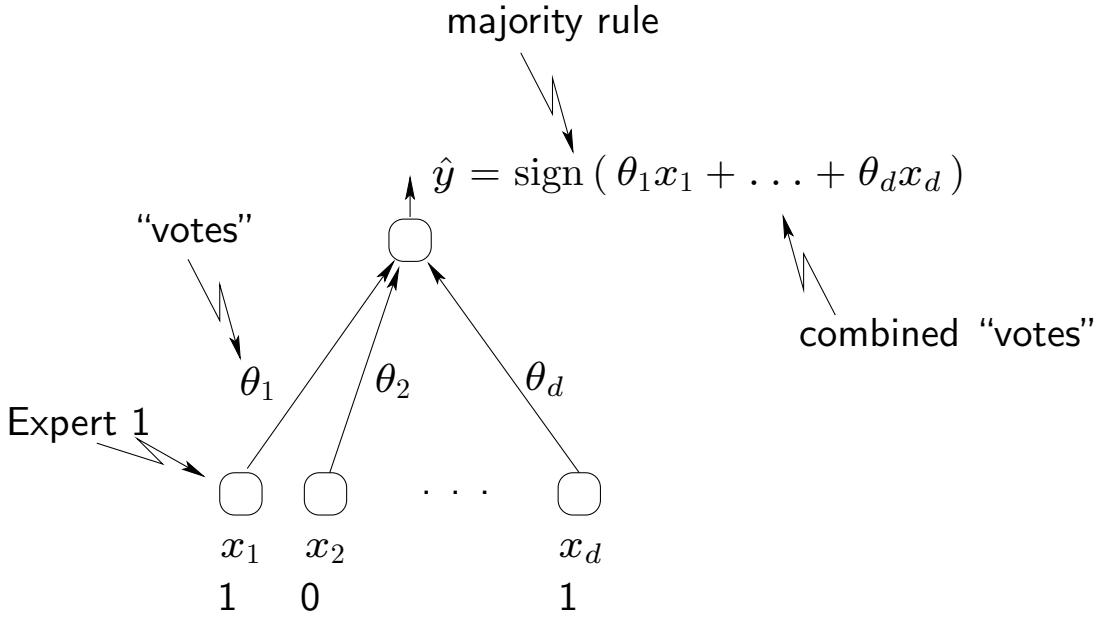
where θ is a vector of **parameters** we have to learn from examples.

Linear classifier/experts

- We can understand the simple linear classifier

$$\hat{y} = \text{sign}\,(\,\theta \cdot \mathbf{x}\,) = \text{sign}\,(\,\theta_1 x_1 + \ldots + \theta_d x_d\,)$$

as a way of combining expert opinion (in this case simple binary features)



Estimation

$\mathbf{x}$	y
0111111001110010000001000000010011111101110111110011101111110001	+1
0001111100000011000001110000011001111101111110011111111000000011	+1
1111111000000110000011000111111000000111100000111110001101111111	−1
...	...

- How do we adjust the parameters θ based on the labeled examples?

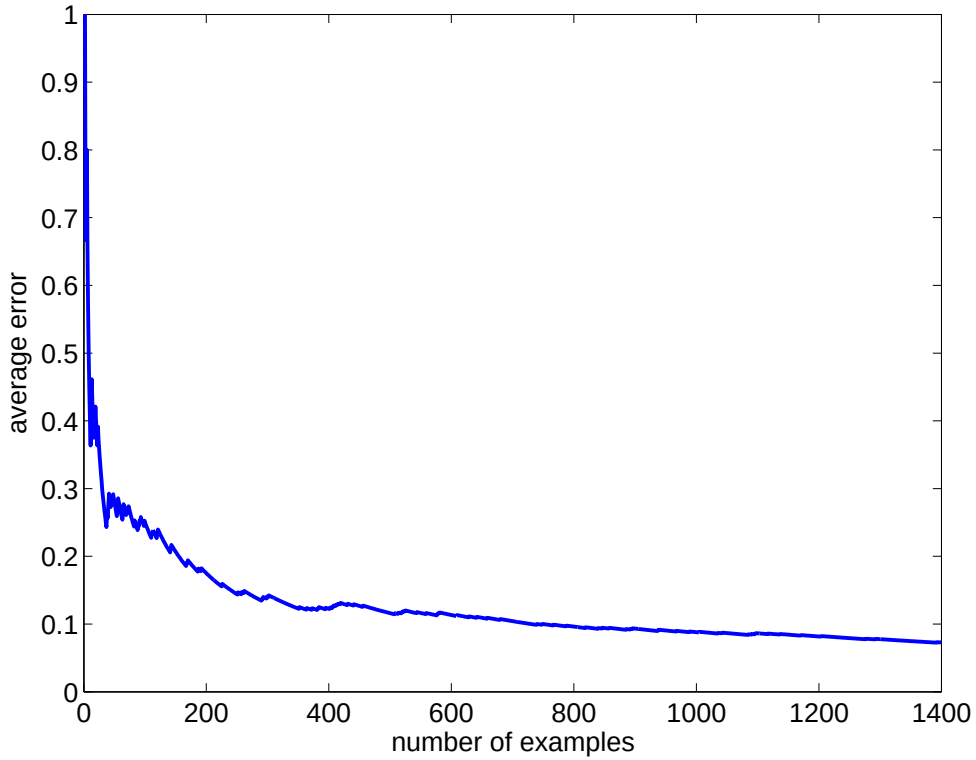
$$\hat{y} = \text{sign}\,(\,\theta \cdot \mathbf{x}\,)$$

For example, we can simply refine/update the parameters whenever we make a mistake (**perceptron algorithm**):

$$\theta_i \leftarrow \theta_i + y\,x_i,\ i = 1, \ldots, d \qquad \text{if prediction was wrong}$$

Evaluation

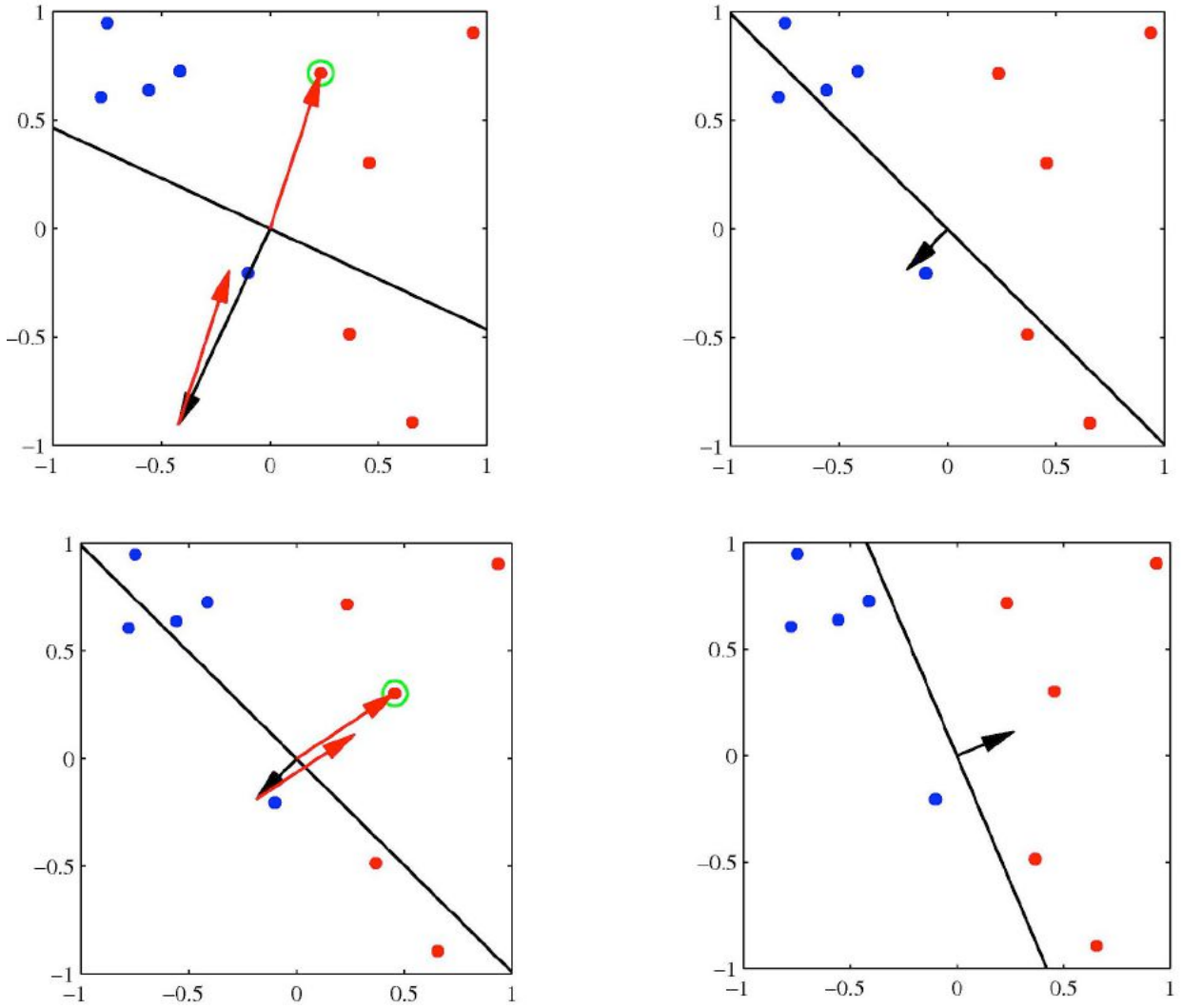
- Does the simple mistake driven algorithm work?



(average classification error as a function of the number of examples and labels seen so far)

Illustration of Convergence

- Convergence of the perceptron learning algorithm



Slide credit: Russ Salakhutdinov

Linear classifier: image classification

image parameters

$$f(x, W)$$

[32x32x3]
array of numbers 0...1
(3072 numbers total)

10 numbers, indicating class scores

Linear classifier: image classification

$$f(x, W) = Wx$$

[32x32x3]
array of numbers 0...1

10 numbers, indicating class scores

Linear classifier: image classification

$$f(x, W) = Wx$$

3072x1

10x1

10x3072

[32x32x3]
array of numbers 0...1

10 numbers, indicating class scores

parameters, or "weights"

Linear classifier: image classification

$$f(x, W) = Wx$$

3072x1

(+b) 10x1

10x1

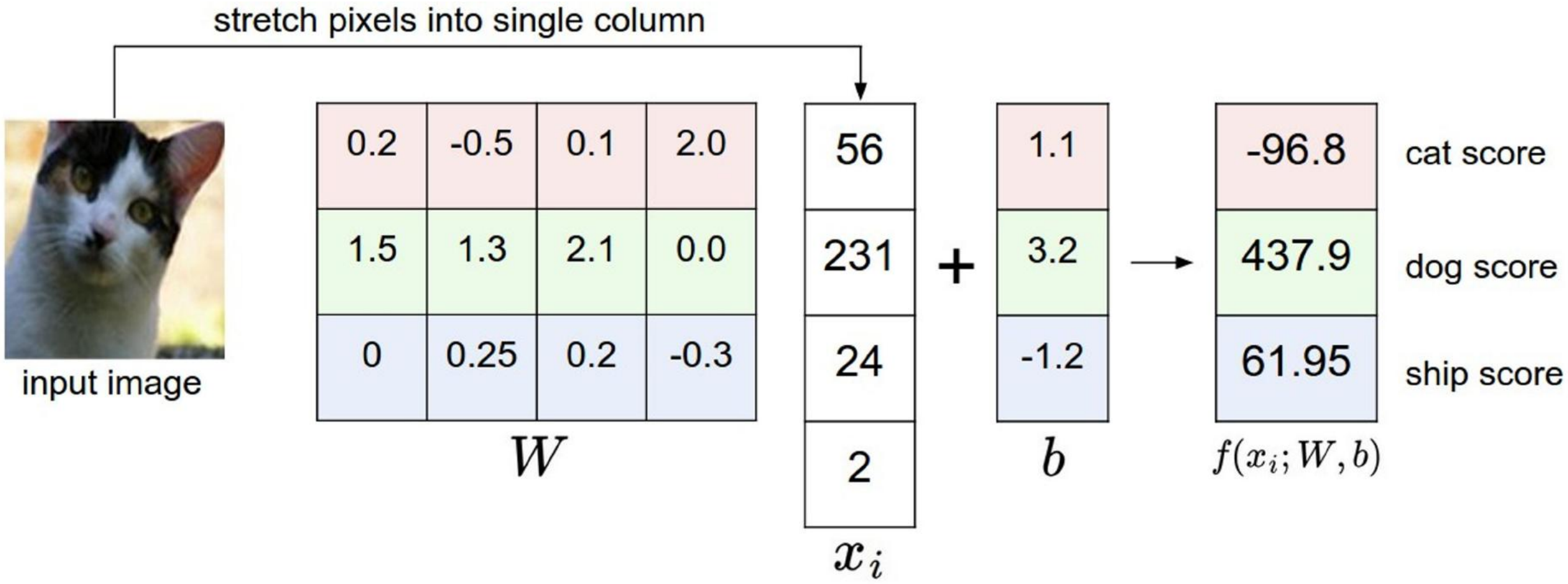
10x3072

[32x32x3]
array of numbers 0...1

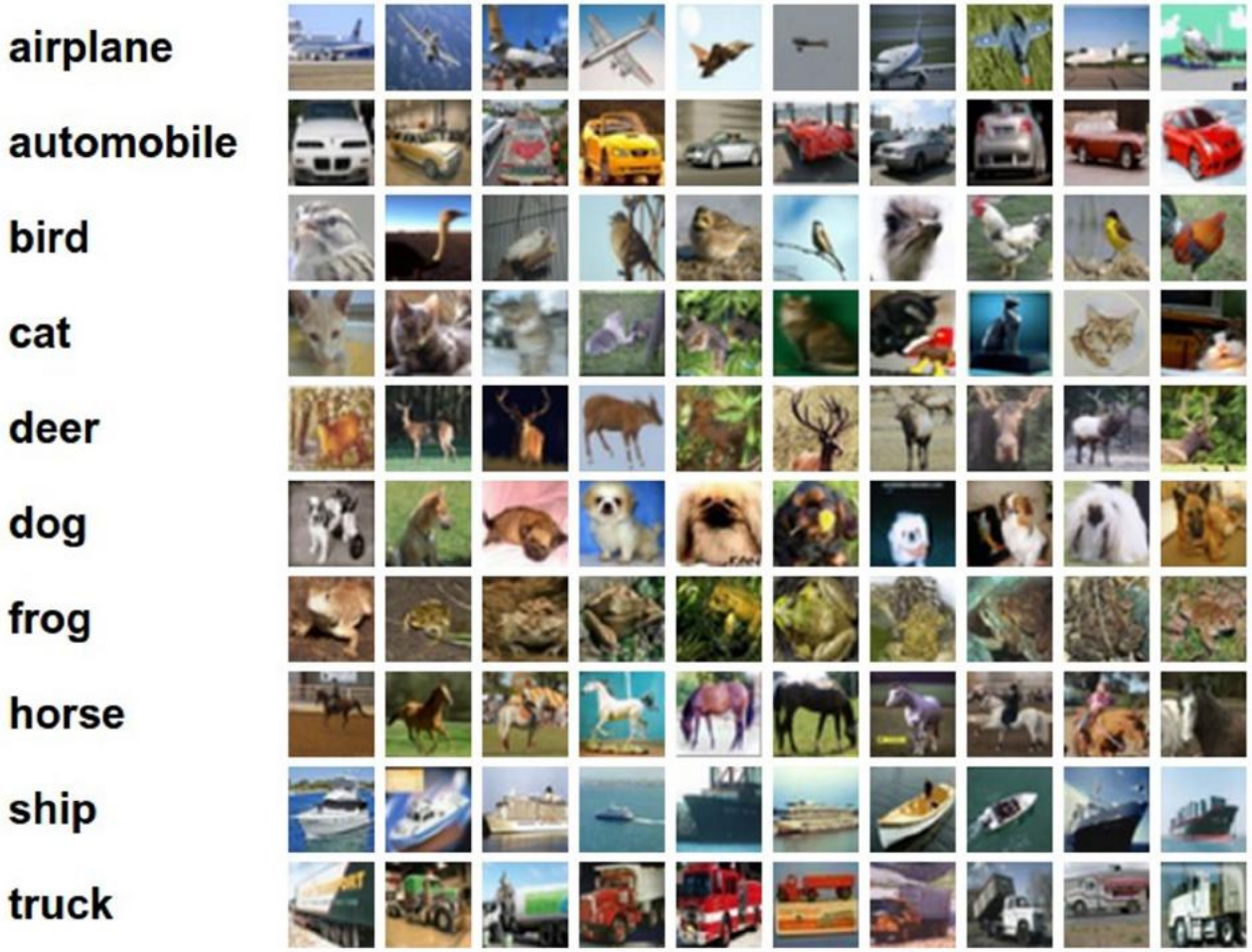
10 numbers, indicating class scores

parameters, or "weights"

Example with an image with 4 pixels, and 3 classes (cat/dog/ship)



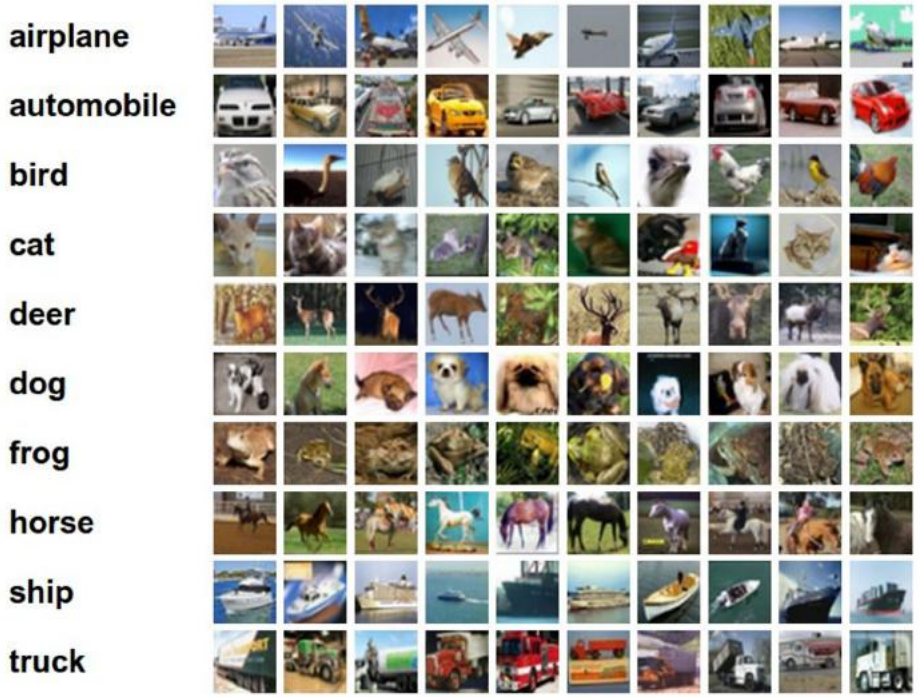
Interpreting a Linear Classifier



$$f(x_i, W, b) = Wx_i + b$$

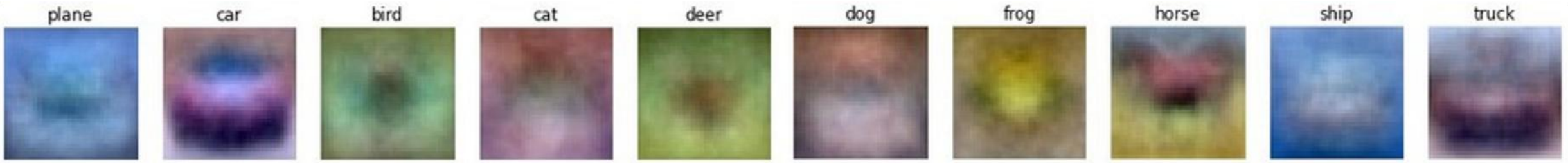
Q: what does the linear classifier do, in English?

Interpreting a Linear Classifier

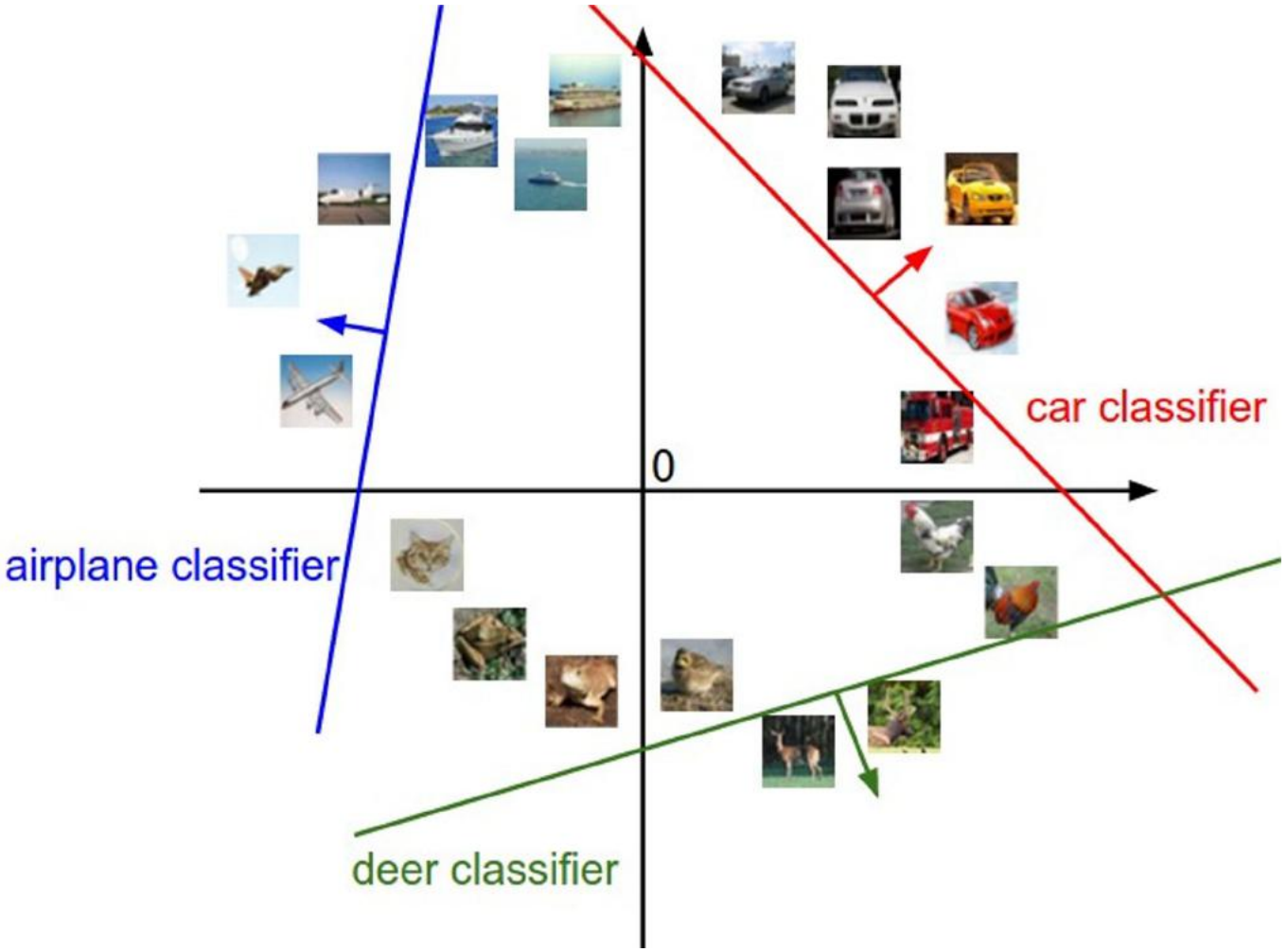


$$f(x_i, W, b) = Wx_i + b$$

Example trained weights of a linear classifier trained on CIFAR-10:



Interpreting a Linear Classifier

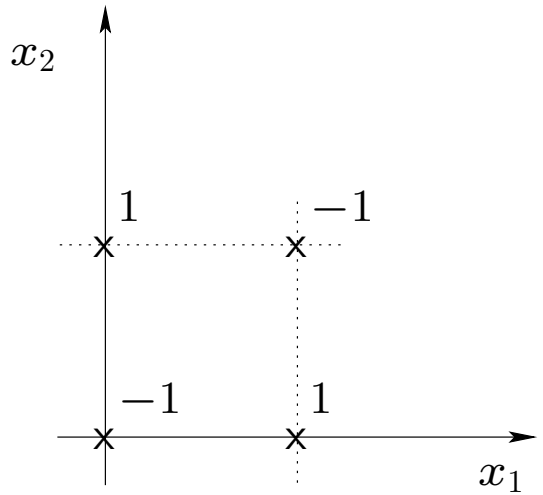


$$f(x_i, W, b) = Wx_i + b$$

[32x32x3]
array of numbers 0...1
(3072 numbers total)

Model selection

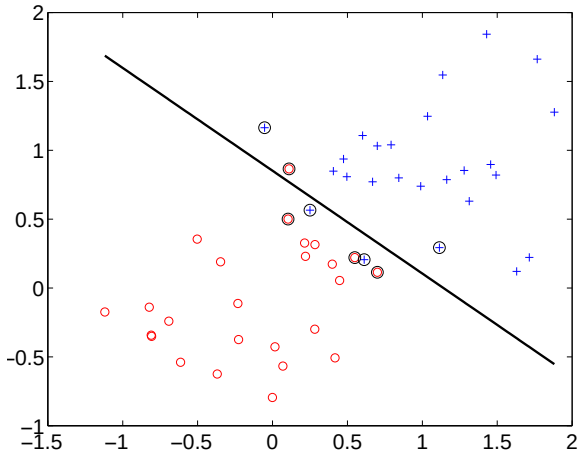
- The simple linear classifier cannot solve all the problems (e.g., XOR)



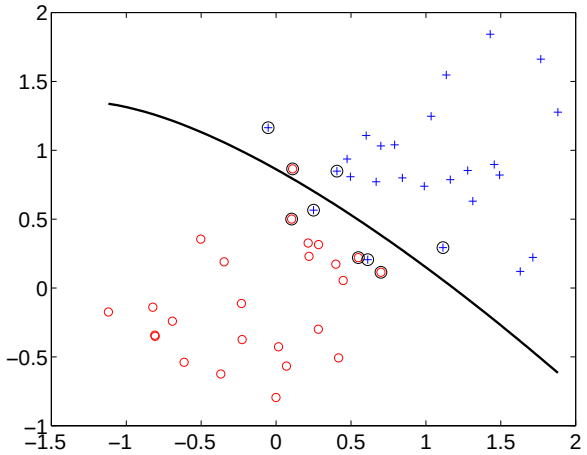
- Can we rethink the approach to do even better?
- We can, for example, add "polynomial experts"

$$\hat{y} = \text{sign}\left(\theta_1 x_1 + \ldots + \theta_d x_d + \theta_{12} x_1 x_2 + \ldots\right)$$

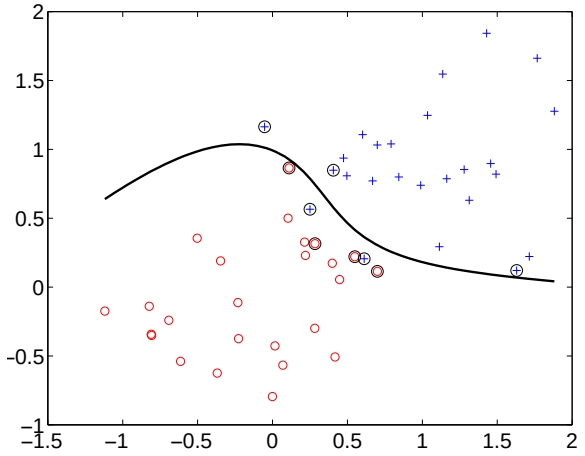
Model selection (cont'd)



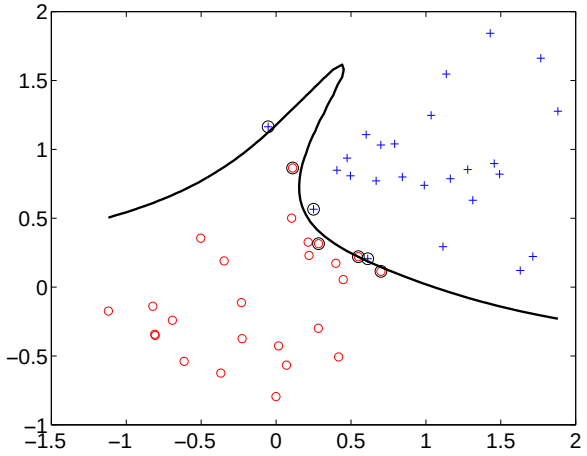
linear



2nd order polynomial



4th order polynomial



8th order polynomial

Review: The learning problem

Image Classification

- **Hypothesis class:** we consider some **restricted** set $\mathcal{F}$ of mappings $f : \mathcal{X} \rightarrow \mathcal{L}$ from images to labels
- **Estimation:** on the basis of a training set of examples and labels, $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$, we find an estimate $\hat{f} \in \mathcal{F}$
- **Evaluation:** we measure how well $\hat{f}$ **generalizes** to yet unseen examples, i.e., whether $\hat{f}(\mathbf{x}_{new})$ agrees with y_{new}

Hypothesis and estimation

- We used a simple linear classifier, a parameterized mapping $f(\mathbf{x}; \theta)$ from images $\mathcal{X}$ to labels $\mathcal{L}$, to solve a binary image classification problem (2's vs 3's):

$$\hat{y} \quad = \quad f(\mathbf{x}; \theta) = \text{sign}\Big(\theta \cdot \mathbf{x} \Big)$$

  where $\mathbf{x}$ is a pixel image and $\hat{y} \in \{-1, 1\}$.

- The parameters θ were adjusted on the basis of the training examples and labels according to a simple mistake driven update rule (written here in a vector form)

$$\theta \leftarrow \theta + y_i \mathbf{x}_i, \quad \text{whenever} \quad y_i \neq \text{sign}\Big(\theta \cdot \mathbf{x}_i \Big)$$

- The update rule attempts to minimize the number of errors that the classifier makes on the training examples

Estimation criterion

- We can formulate the binary classification problem more explicitly by defining a **zero-one loss:**

$$\text{Loss}\big(y, \hat{y}\big) = \begin{cases} 0, y = \hat{y} \\ 1, y \neq \hat{y} \end{cases}$$

  so that

$$\frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, \hat{y}_i\big) = \frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, f(\mathbf{x}_i; \theta)\big)$$

  gives the fraction of prediction errors on the training set.

- This is a function of the parameters θ and we can try to minimize it directly.

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**

Multiclass SVM loss:

Given an example (x_i, y_i)
where x_i is the image and
where y_i is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

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cat	**3.2**	1.3	2.2
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Losses:	2.9		

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and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 5.1 - 3.2 + 1)
+max(0, -1.7 - 3.2 + 1)
= max(0, 2.9) + max(0, -3.9)
= 2.9 + 0
= 2.9

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
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the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	10.9

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the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

= max(0, 2.2 - (-3.1) + 1)
+max(0, 2.5 - (-3.1) + 1)
= max(0, 5.3) + max(0, 5.6)
= 5.3 + 5.6
= 10.9

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
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where x_i is the image and
where y_i is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

and the full training loss is the mean over all examples in the training data:

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i$$

L = (2.9 + 0 + 10.9)/3
= 4.6

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	10.9

Multiclass SVM loss:

Given an example (x_i, y_i)
where x_i is the image and
where y_i is the (integer) label,

and using the shorthand for the scores vector: $s = f(x_i, W)$

the SVM loss has the form:

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Q: what is the min/max possible loss?

There is something missing in the loss:

$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

e.g. suppose that we found a W such that L = 0.
Is this W unique?

Suppose: 3 training examples, 3 classes.
With some W the scores $f(x, W) = Wx$ are:



cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

Before:

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

With W twice as large:

= max(0, 2.6 - 9.8 + 1)
+max(0, 4.0 - 9.8 + 1)
= max(0, -6.2) + max(0, -4.8)
= 0 + 0
= 0

Weight Regularization

λ = regularization strength (hyperparameter)

$$L = \frac{1}{N}\sum_{i=1}^{N}\sum_{j\neq y_i}\max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1) + \lambda R(W)$$

In common use:

L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Max norm regularization

Dropout (will see later)

Batch normalization (will see later)

L2 regularization: motivation

$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$

$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1^T x = w_2^T x = 1$$

Estimation criterion (revisited)

- We have reduced the estimation problem to a minimization problem

$$\text{find } \theta \text{ that minimizes } \overbrace{\frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, f(\mathbf{x}_i;\theta)\big)}^{\text{empirical loss}}$$

  —valid for any parameterized class of mappings from examples to predictions

  —valid when the predictions are discrete labels, real valued, or other provided that the loss is defined appropriately

  —may be ill-posed (under-constrained) as stated

- But why is it sensible to minimize the empirical loss in the first place since we are only interested in the performance on new examples?

Training and test performance: sampling

- We assume that each training **and** test example-label pair, $(\mathbf{x}, y)$ is drawn **independently at random** from the **same** but unknown population of examples and labels.
- We can represent this population as a joint probability distribution $P(\mathbf{x}, y)$ so that each training/test example is a **sample** from this distribution

$(\mathbf{x}_i, y_i) \sim P$

Training and test performance: sampling

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- We can represent this population as a joint probability distribution $P(\mathbf{x}, y)$ so that each training/test example is a **sample** from this distribution

$$(\mathbf{x}_i, y_i) \sim P$$

$$\text{Empirical (training) loss} = \frac{1}{n}\sum_{i=1}^{n} \text{Loss}\big(y_i, f(\mathbf{x}_i; \theta)\big)$$

$$\text{Expected (test) loss} = E_{(\mathbf{x},y)\sim P}\left\{\text{Loss}\big(y, f(\mathbf{x}; \theta)\big)\right\}$$

- The training loss based on a few sampled examples and labels serves as a proxy for the test performance measured over the whole population

Regression, example
Linear regression
— Estimation, errors, analysis

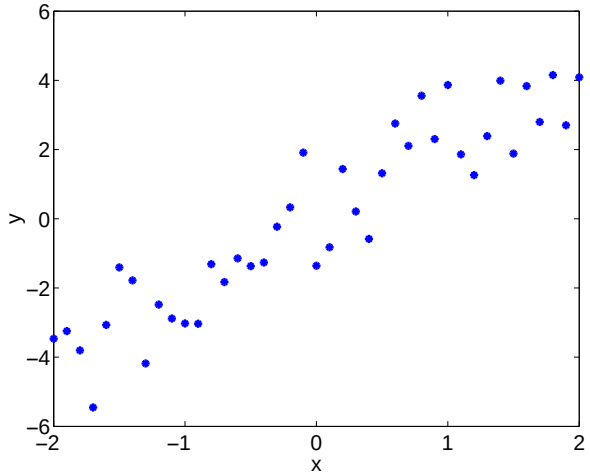
Regression

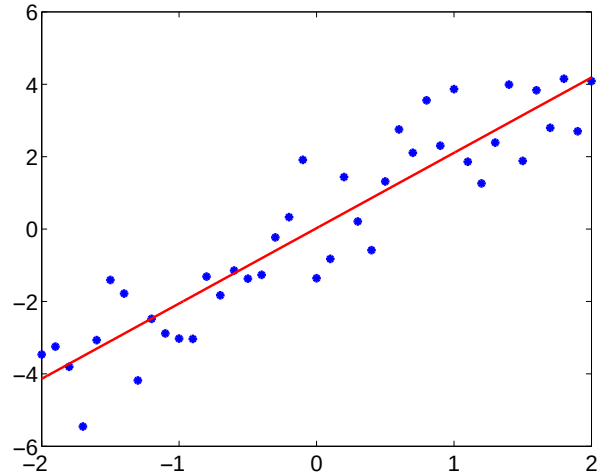
- The goal is to make quantitative (real valued) predictions on the basis of a (vector of) features or attributes
- Example: predicting vehicle fuel efficiency (mpg) from 8 attributes

y	$\mathbf{x}$				
	cyls	disp	hp	weight	. . .
18.0	8	307.0	130.00	3504	. . .
26.0	4	97.00	46.00	1835	. . .
33.5	4	98.00	83.00	2075	. . .
. . .					

- We need to
  - —specify the class of functions (e.g., linear)
  - —select how to measure prediction loss
  - —solve the resulting minimization problem

Linear regression





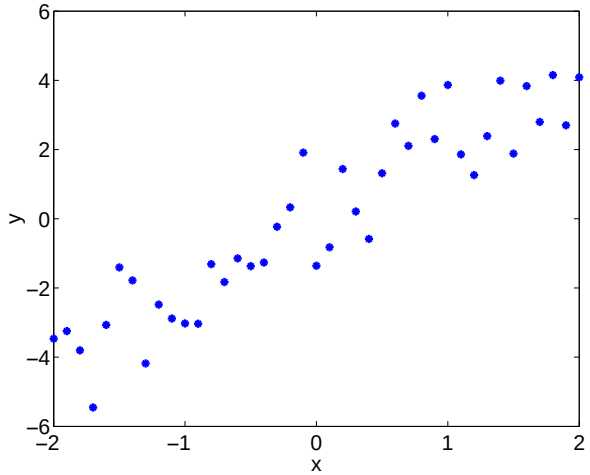
- We begin by considering linear regression (easy to extend to more complex predictions later on)

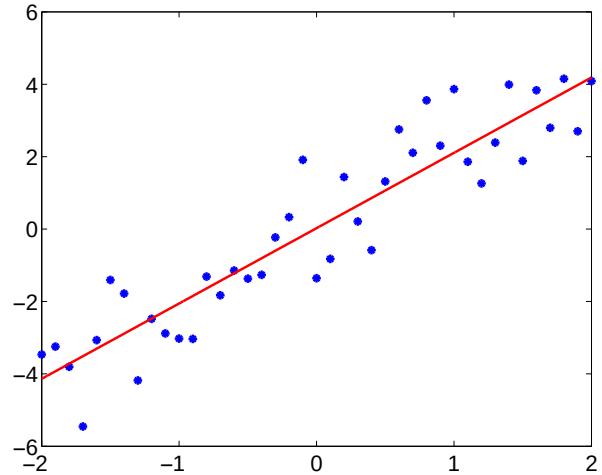
$$f : \mathcal{R} \rightarrow \mathcal{R} \qquad f(x; \mathbf{w}) = w_0 + w_1 x$$

$$f : \mathcal{R}^d \rightarrow \mathcal{R} \qquad f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

where $\mathbf{w}$ are **parameters** we need to set.

Linear regression: squared loss





$$f : \mathcal{R} \rightarrow \mathcal{R} \qquad f(x; \mathbf{w}) = w_0 + w_1 x$$

$$f : \mathcal{R}^d \rightarrow \mathcal{R} \qquad f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

- We can measure the prediction loss in terms of squared error, $\text{Loss}(y, \hat{y}) = (y - \hat{y})^2$, so that the empirical loss on n training samples becomes mean squared error

$$J_n(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f(\mathbf{x}_i; \mathbf{w}) \right)^2$$

Linear regression: estimation

- We have to minimize the **empirical** squared loss

$$
\begin{aligned}
J_n(\mathbf{w}) &= \frac{1}{n}\sum_{i=1}^{n}\big(y_i - f(\mathbf{x}_i;\mathbf{w})\big)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(y_i - w_0 - w_1 x_i)^2 \quad \text{(1-dim)}
\end{aligned}
$$

- By setting the derivatives with respect to w_1 and w_0 to zero, we get necessary conditions for the "optimal" parameter values

$$
\begin{aligned}
\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= 0 \\
\frac{\partial}{\partial w_0} J_n(\mathbf{w}) &= 0
\end{aligned}
$$

Optimality conditions: derivation

$$\frac{\partial}{\partial w_1} J_n(\mathbf{w}) \quad = \quad \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2$$

Optimality conditions: derivation

$$\begin{aligned}\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \\ &= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)^2\end{aligned}$$

Optimality conditions: derivation

$$
\begin{aligned}
\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i) \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)
\end{aligned}
$$

Optimality conditions: derivation

$$
\begin{aligned}
\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i) \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i) \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)(-x_i) = 0
\end{aligned}
$$

Optimality conditions: derivation

$$
\begin{aligned}
\frac{\partial}{\partial w_1} J_n(\mathbf{w}) &= \frac{\partial}{\partial w_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i)^2 \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i) \frac{\partial}{\partial w_1} (y_i - w_0 - w_1 x_i) \\
&= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)(-x_i) = 0 \\
\frac{\partial}{\partial w_0} J_n(\mathbf{w}) &= \frac{2}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)(-1) = 0
\end{aligned}
$$

Linear regression: matrix notation

- We can express the solution a bit more generally by resorting to a matrix notation

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \cdots \\ y_n \end{bmatrix}, \ \mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \cdots & \cdots \\ 1 & x_n \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

so that

$$\begin{aligned} \frac{1}{n}\sum_{t=1}^{n}(y_t - w_0 - w_1 x_t)^2 &= \frac{1}{n}\left\| \begin{bmatrix} y_1 \\ \cdots \\ y_n \end{bmatrix} - \begin{bmatrix} 1 & x_1 \\ \cdots & \cdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \right\|^2 \\ &= \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \end{aligned}$$

Linear regression: solution

- By setting the derivatives of $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2/n$ to zero, we get the same optimality conditions as before, now expressed in a matrix form

$$\frac{\partial}{\partial \mathbf{w}} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \quad = \quad \frac{\partial}{\partial \mathbf{w}} \frac{1}{n} (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

Linear regression: solution

- By setting the derivatives of $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2/n$ to zero, we get the same optimality conditions as before, now expressed in a matrix form

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 &= \frac{\partial}{\partial \mathbf{w}} \frac{1}{n}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \frac{2}{n}\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w})\end{aligned}$$

Linear regression: solution

- By setting the derivatives of $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2/n$ to zero, we get the same optimality conditions as before, now expressed in a matrix form

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \frac{1}{n}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 &= \frac{\partial}{\partial \mathbf{w}} \frac{1}{n}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \frac{2}{n}\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) \\ &= \frac{2}{n}(\mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\mathbf{w}) = \mathbf{0}\end{aligned}$$

  which gives

$$\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

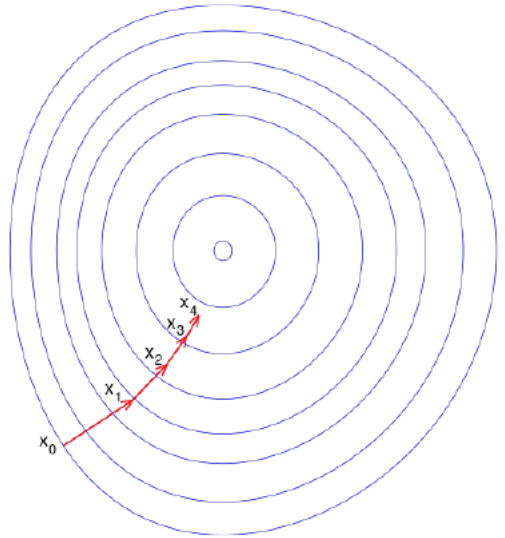
- The solution is a linear function of the outputs y

Alternative: Gradient Descent Algorithm

- One straightforward method: **gradient descent**
  - initialize $\boldsymbol{\theta}$ (e.g., randomly)
  - repeatedly update $\boldsymbol{\theta}$ based on the gradient

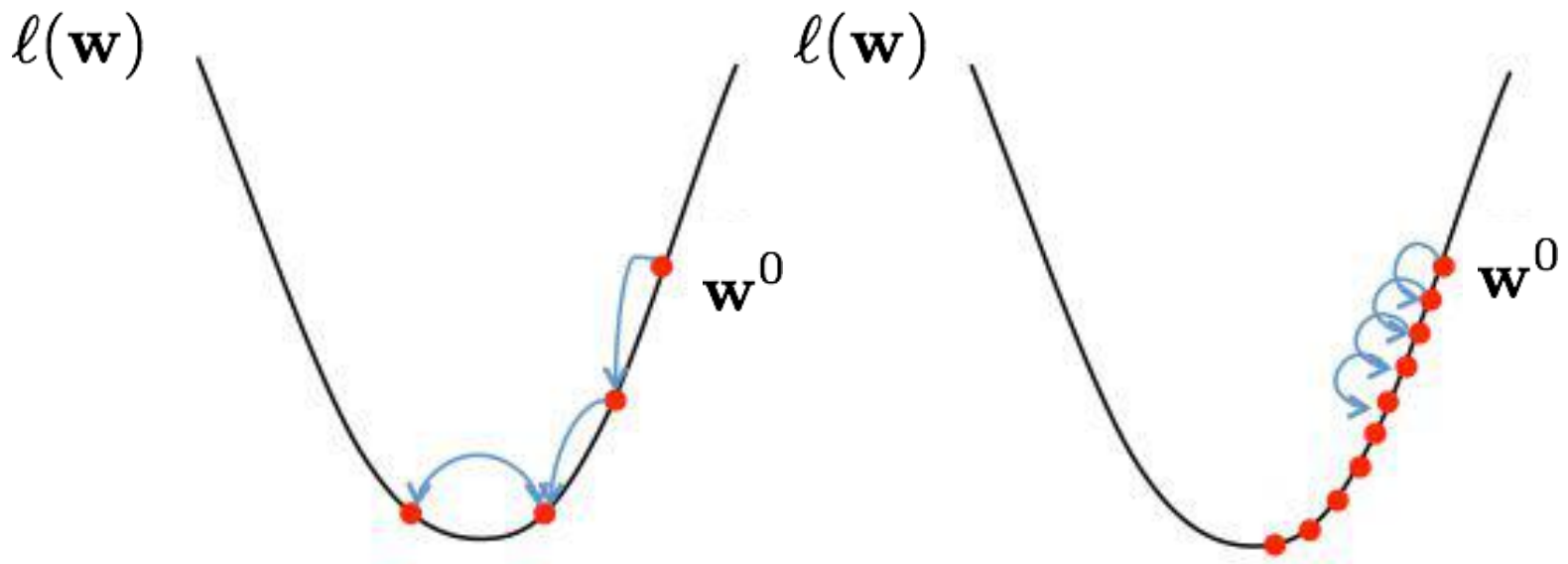
$$\Delta = -\frac{1}{T}\sum_t \nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)};\boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$$
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\, \Delta$$

- α is the **learning rate**



Slide adapted from Sanja Fidler

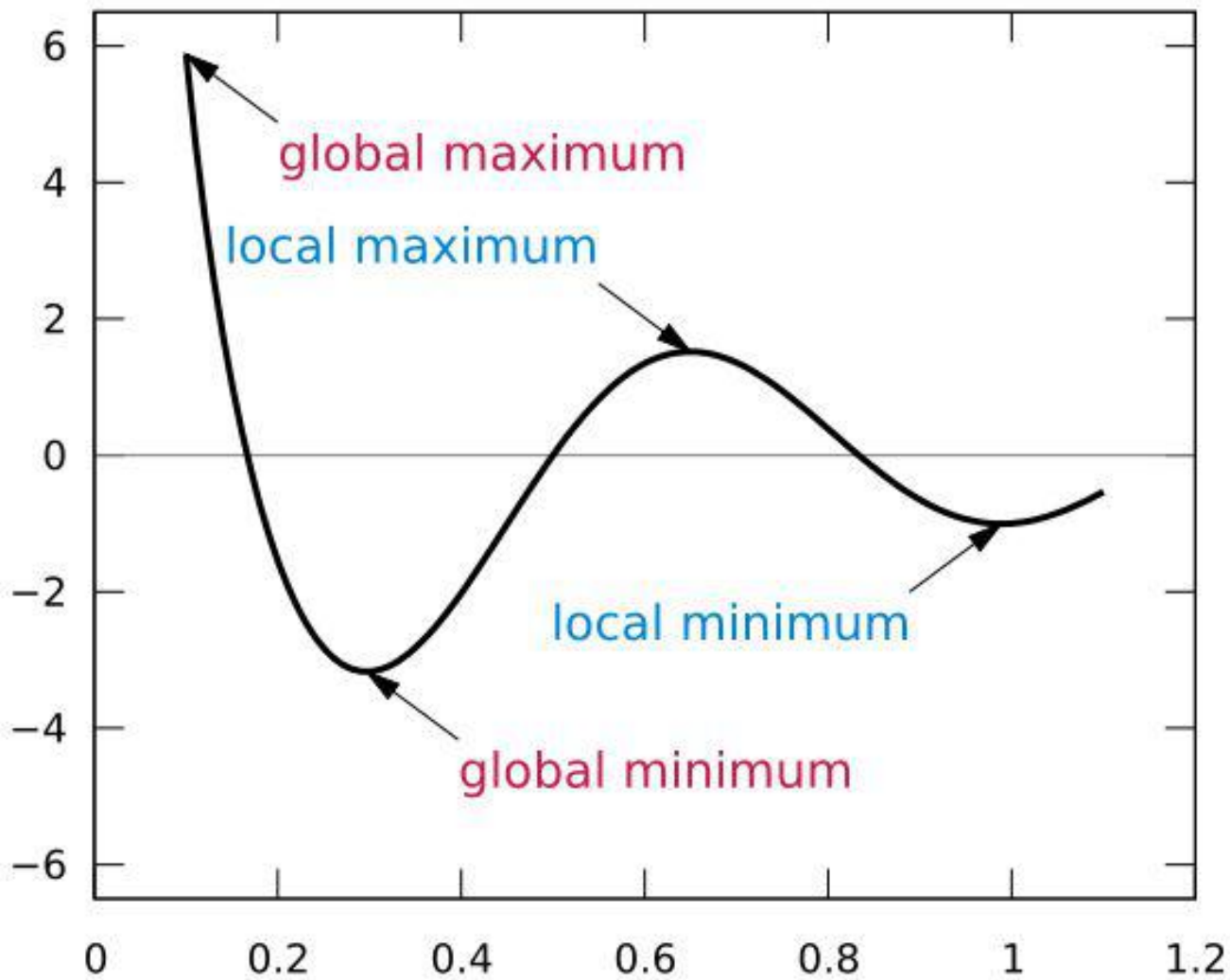
Effect of learning rate λ



- Large λ => Fast convergence but larger residual error
  Also possible oscillations
- Small λ => Slow convergence but small residual error

Slide credit: Erik Sudderth

Local and Global Optima



Stochastic Gradient Descent

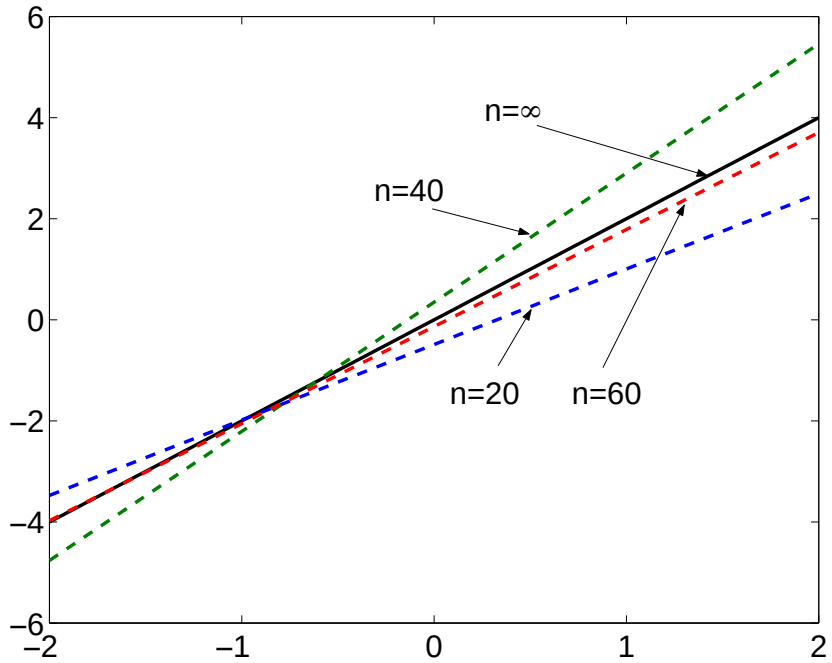
- Two ways to generalize this for all examples in training set:
  1. **Batch updates:** sum or average updates across every example n, then change the parameter values
  2. **Stochastic/online updates:** update the parameters for each training case in turn, according to its own gradients

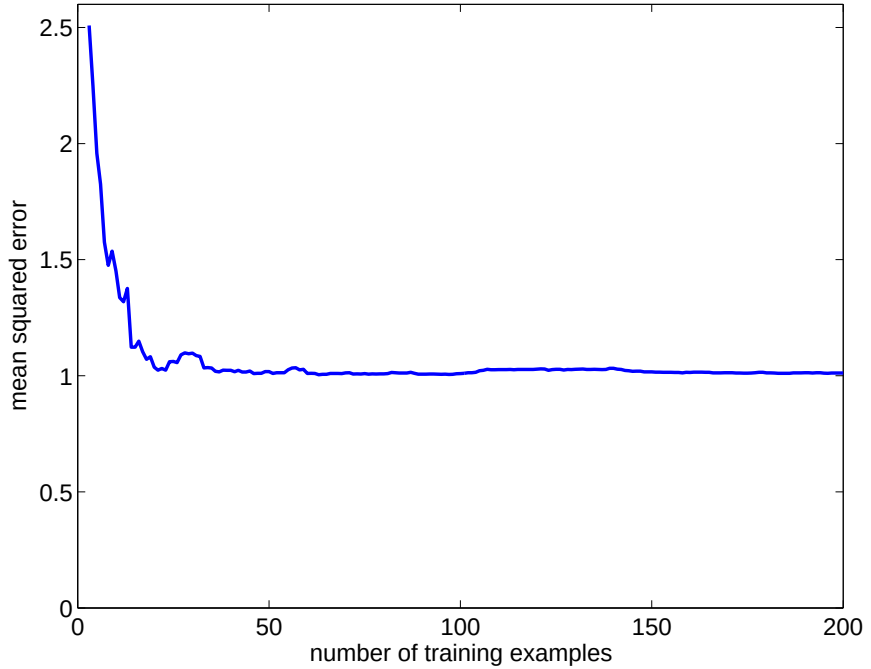
$$\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \, \Delta$$

Linear regression: generalization

- As the number of training examples increases our solution gets "better"





We'd like to understand the error a bit better

Linear regression: types of errors

related to the **capacity** of the model

- **Structural error** measures the error introduced by the limited function class (infinite training data):

$$\min_{w_1,w_0} E_{(x,y)\sim P}\left(y - w_0 - w_1 x\right)^2 = E_{(x,y)\sim P}\left(y - w_0^* - w_1^* x\right)^2$$

  where (w_0^*, w_1^*) are the optimal linear regression parameters.

- **Approximation error** measures how close we can get to the optimal linear predictions with limited training data:

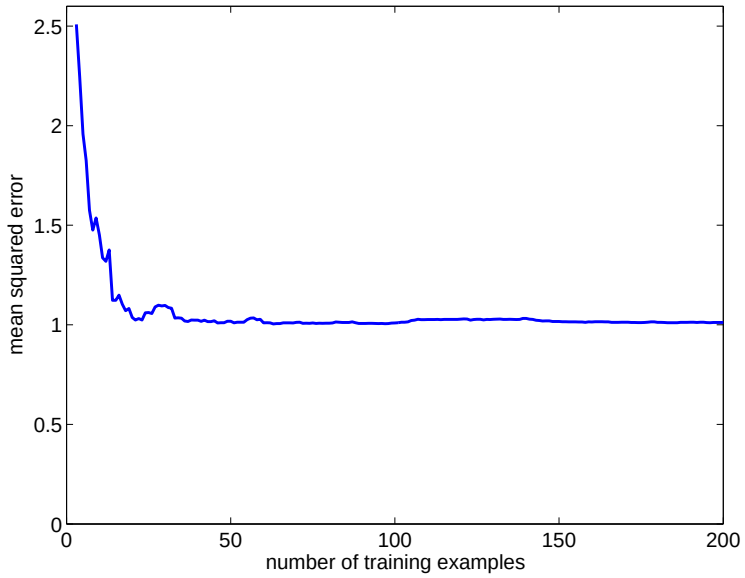
$$E_{(x,y)\sim P}\left(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x\right)^2$$

  where $(\hat{w}_0, \hat{w}_1)$ are the parameter estimates based on a small training set (therefore themselves random variables).

Linear regression: error decomposition

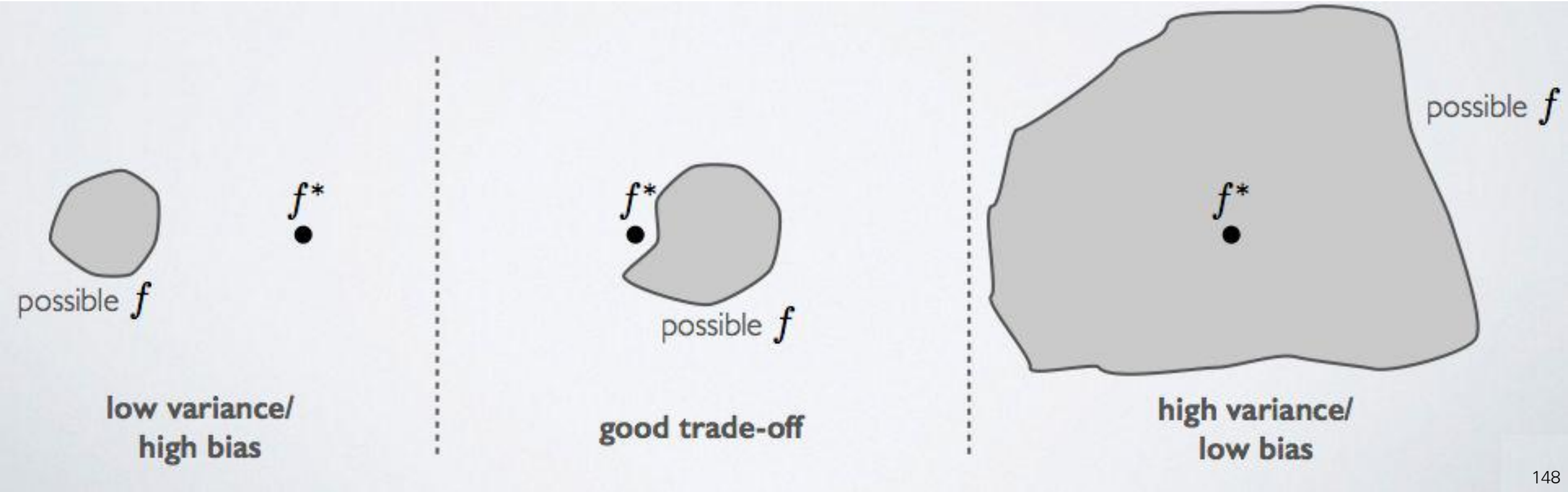
- The expected error of our linear regression function decomposes into the sum of structural and approximation errors

$$E_{(x,y)\sim P}\left(y - \hat{w}_0 - \hat{w}_1 x\right)^2 =$$
$$E_{(x,y)\sim P}\left(y - w_0^* - w_1^* x\right)^2 +$$
$$E_{(x,y)\sim P}\left(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x\right)^2$$



Bias-Variance Tradeoff

- **Variance** of trained model: does it vary a lot if the training set changes
- **Bias** of trained model: is the average model close to the true solution?
- Generalization error can be seen as the sum of bias and the variance



Parametric vs. non-parametric models

- **Parametric model:** its capacity is fixed and does not increase with the amount of training data
  - examples: linear classifier, neural network with fixed number of hidden units, etc.

- **Non-parametric model:** the capacity increases with the amount of training data
  - examples: k nearest neighbors classifier, neural network with adaptable hidden layer size, etc.

Beyond linear regression models

— additive regression models, examples
— generalization and cross-validation
— population minimizer

Linear regression

- Linear regression functions,

$$f : \mathcal{R} \rightarrow \mathcal{R} \qquad f(x; \mathbf{w}) = w_0 + w_1 x, \quad \text{or}$$
$$f : \mathcal{R}^d \rightarrow \mathcal{R} \qquad f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

  combined with the squared loss, are convenient because they are **linear in the parameters.**

—we get closed form estimates of the parameters

$$\hat{\mathbf{w}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

  where, for example, $\mathbf{y} = [y_1, \ldots, y_n]^T$.

—the resulting prediction errors $\epsilon_i = y_i - f(\mathbf{x}_i; \hat{\mathbf{w}})$ are uncorrelated with any linear function of the inputs $\mathbf{x}$.

—we can easily extend these to non-linear functions of the inputs while still keeping them linear in the parameters

Beyond linear regression

- Example extension: m^{th} order polynomial regression where $f : \mathcal{R} \rightarrow \mathcal{R}$ is given by

$$f(x; \mathbf{w}) = w_0 + w_1 x + \ldots + w_{m-1} x^{m-1} + w_m x^m$$

—linear in the parameters, non-linear in the inputs

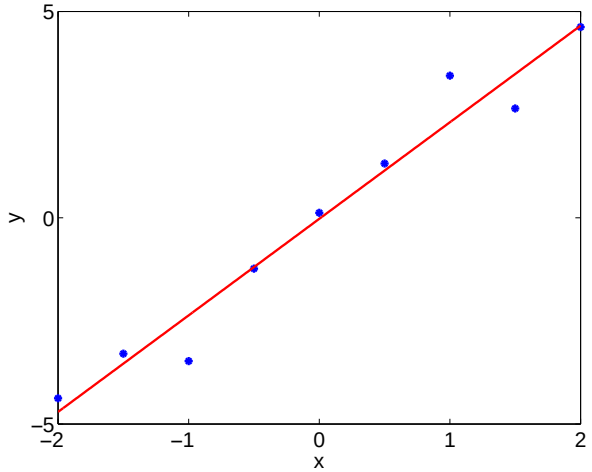
—solution as before

$$\hat{\mathbf{w}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

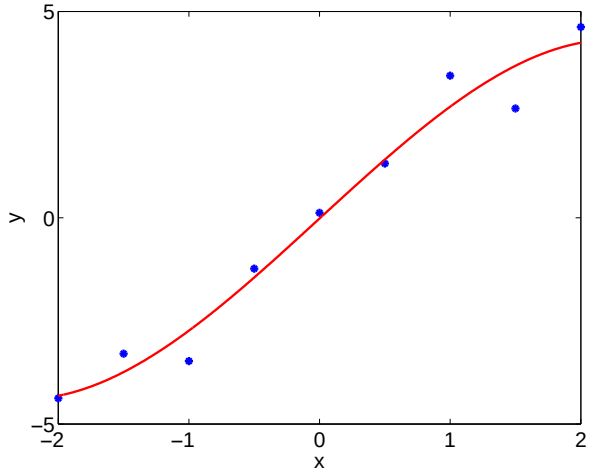
where

$$\hat{\mathbf{w}} = \begin{bmatrix} \hat{w}_0 \\ \hat{w}_1 \\ \ldots \\ \hat{w}_m \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^m \\ 1 & x_2 & x_2^2 & \ldots & x_2^m \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_n & x_n^2 & \ldots & x_n^m \end{bmatrix}$$

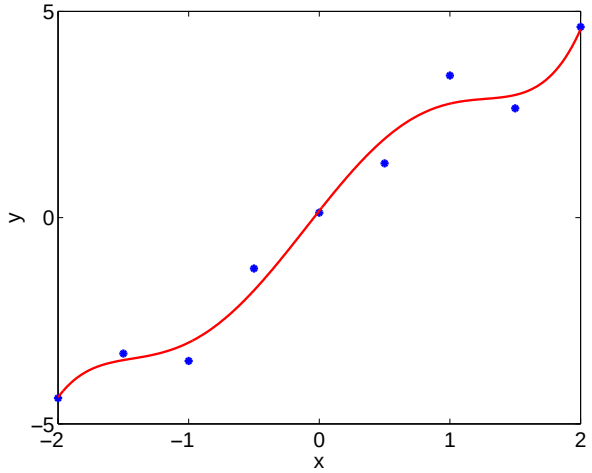
Polynomial regression



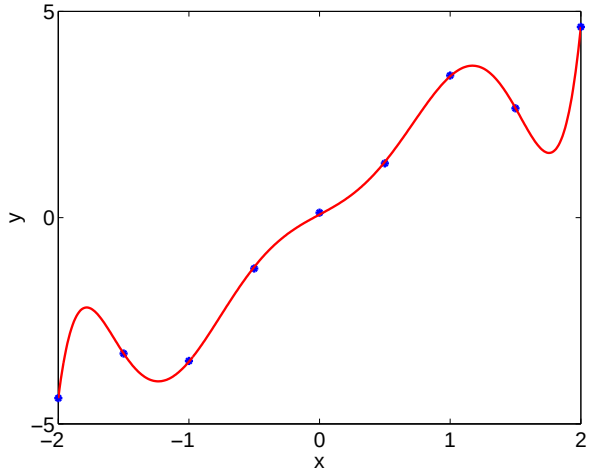
degree $= 1$



degree $= 3$



degree $= 5$



degree $= 7$

Underfitting and Overfitting

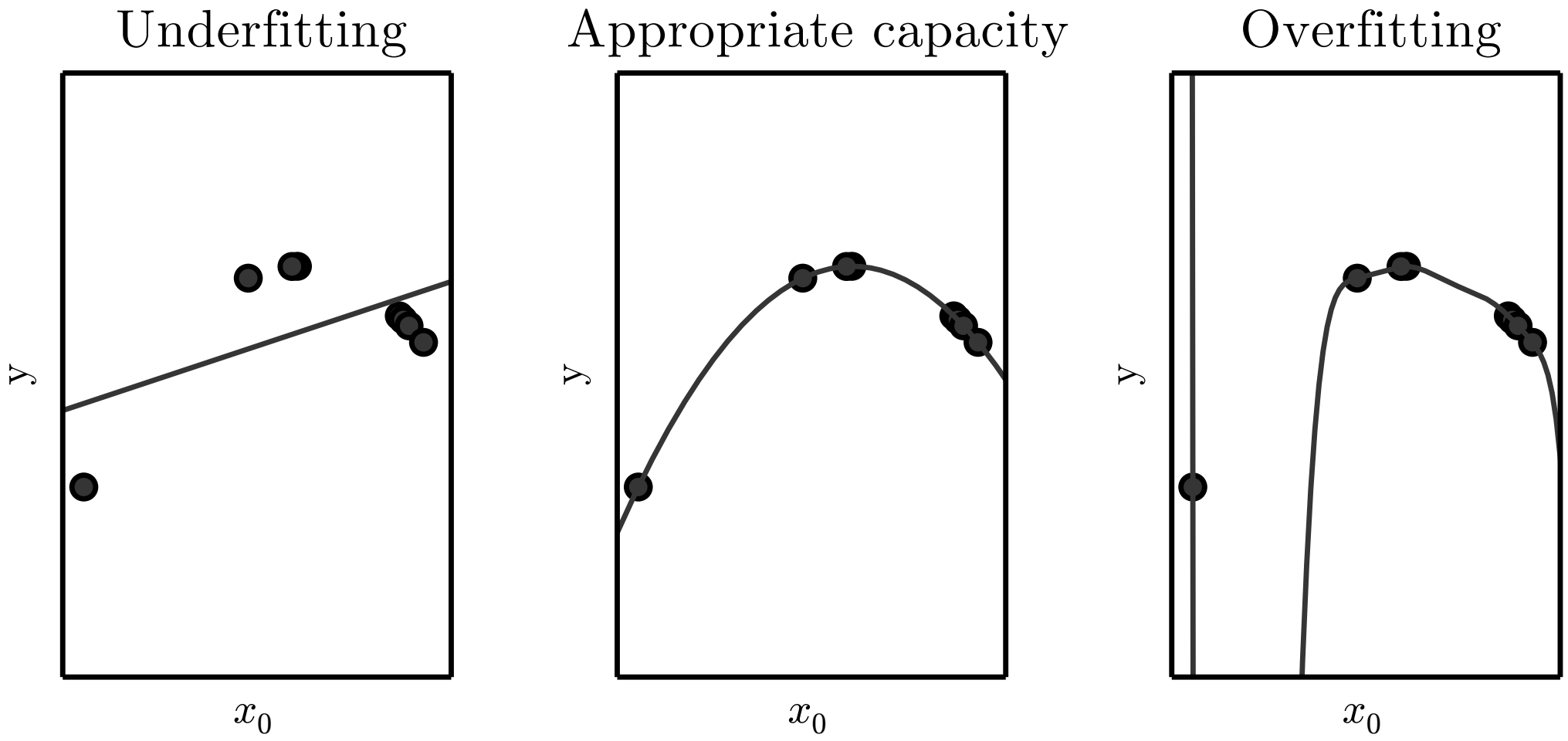


Image credit: Ian Goodfellow

Generalization and Capacity

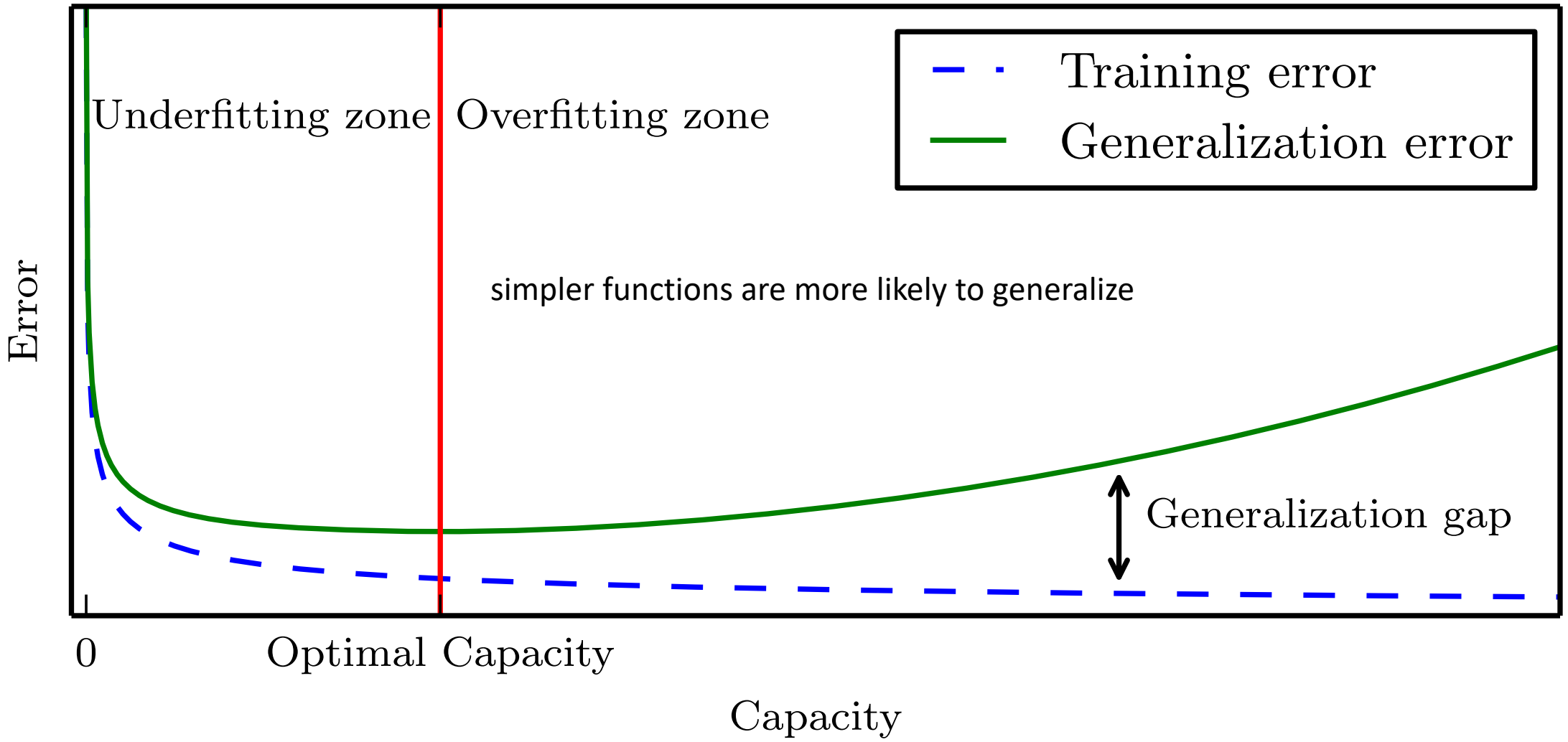


Image credit: Ian Goodfellow

Bias and Variance

sufficiently simpler models are more likely to generalize

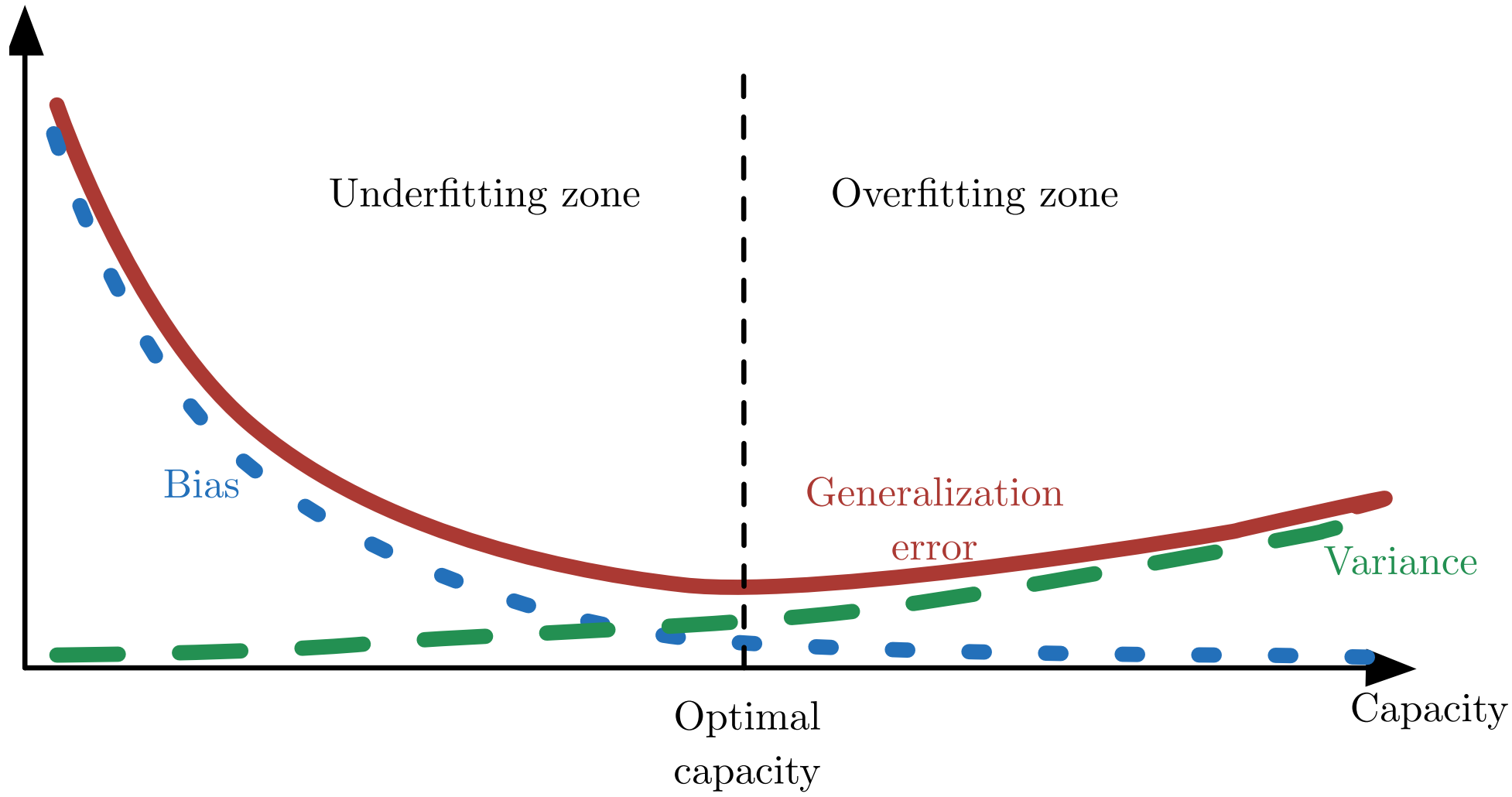


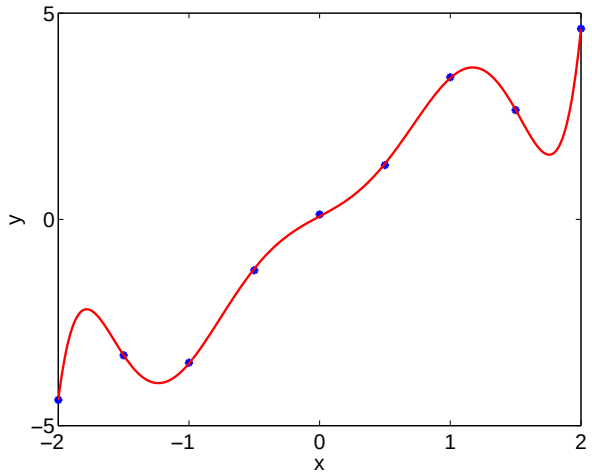
Image credit: Ian Goodfellow

Complexity and overfitting

- With limited training examples our polynomial regression model may achieve zero training error but nevertheless has a large test (generalization) error

$$\text{train} \quad \frac{1}{n}\sum_{t=1}^{n}(y_t - f(x_t; \hat{\mathbf{w}}))^2 \approx 0$$

$$\text{test} \quad E_{(x,y)\sim P}\,(y - f(x; \hat{\mathbf{w}}))^2 \gg 0$$



- We suffer from **overfitting** when the training error no longer bears any relation to the generalization error

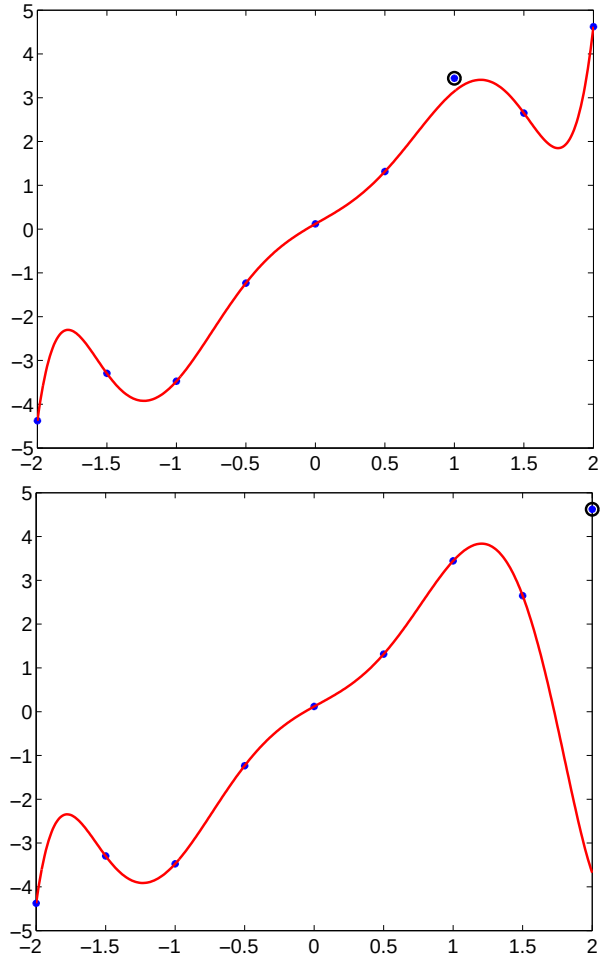
Avoiding overfitting: cross-validation

- **Cross-validation** allows us to estimate the generalization error based on training examples alone

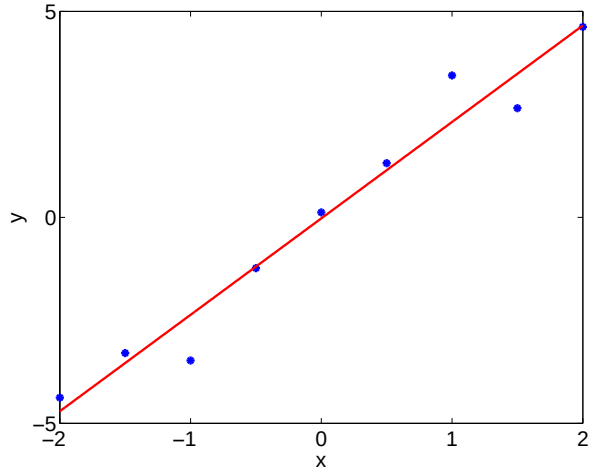
  Leave-one-out cross-validation treats each training example in turn as a test example:

$$\text{CV} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(x_i; \hat{\mathbf{w}}^{-i})\right)^2$$

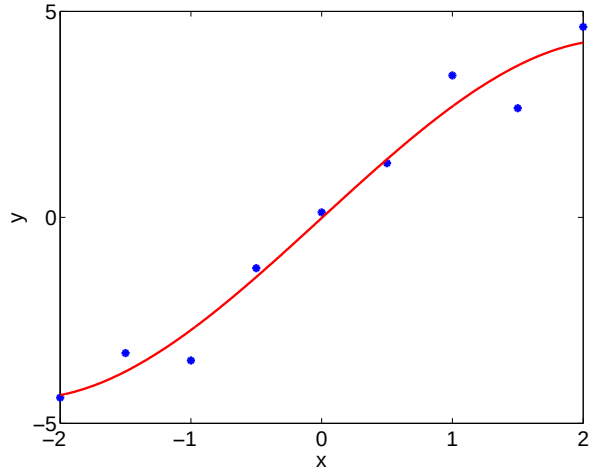
  where $\hat{\mathbf{w}}^{-i}$ are the least squares estimates of the parameters without the i^{th} training example.



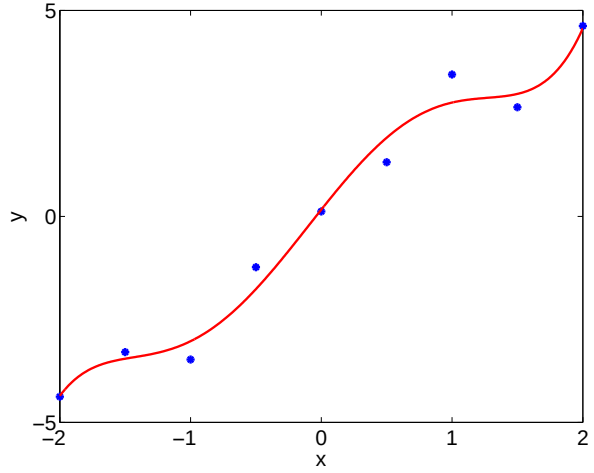
Polynomial regression: example (cont'd)



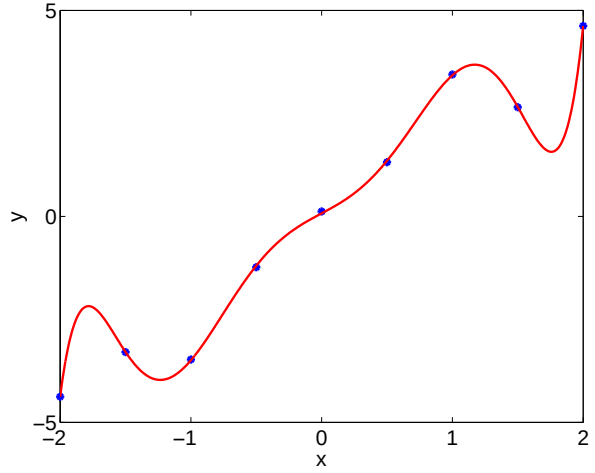
degree $= 1$, CV $= 0.6$



degree $= 3$, CV $= 1.5$



degree $= 5$, CV $= 6.0$



degree $= 7$, CV $= 15.6$

Additive models

- More generally, predictions can be based on a linear combination of a set of basis functions (or features) $\{\phi_1(\mathbf{x}), \ldots, \phi_m(\mathbf{x})\}$, where each $\phi_i(\mathbf{x}) \ : \ \mathcal{R}^d \ \rightarrow \ \mathcal{R}$, and

$$f(\mathbf{x}; \mathbf{w}) = w_0 + w_1\phi_1(\mathbf{x}) + \ldots + w_m\phi_m(\mathbf{x})$$

- Examples

If $\phi_i(x) = x^i$, $i = 1, \ldots, m$, then

$$f(x; \mathbf{w}) = w_0 + w_1 x + \ldots + w_{m-1}x^{m-1} + w_m x^m$$

Additive models

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- Examples

If $\phi_i(x) = x^i$, $i = 1, \ldots, m$, then

$$f(x; \mathbf{w}) = w_0 + w_1 x + \ldots + w_{m-1}x^{m-1} + w_m x^m$$

If $m = d$, $\phi_i(\mathbf{x}) = x_i$, $i = 1, \ldots, d$, then

$$f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

Additive models (cont'd)

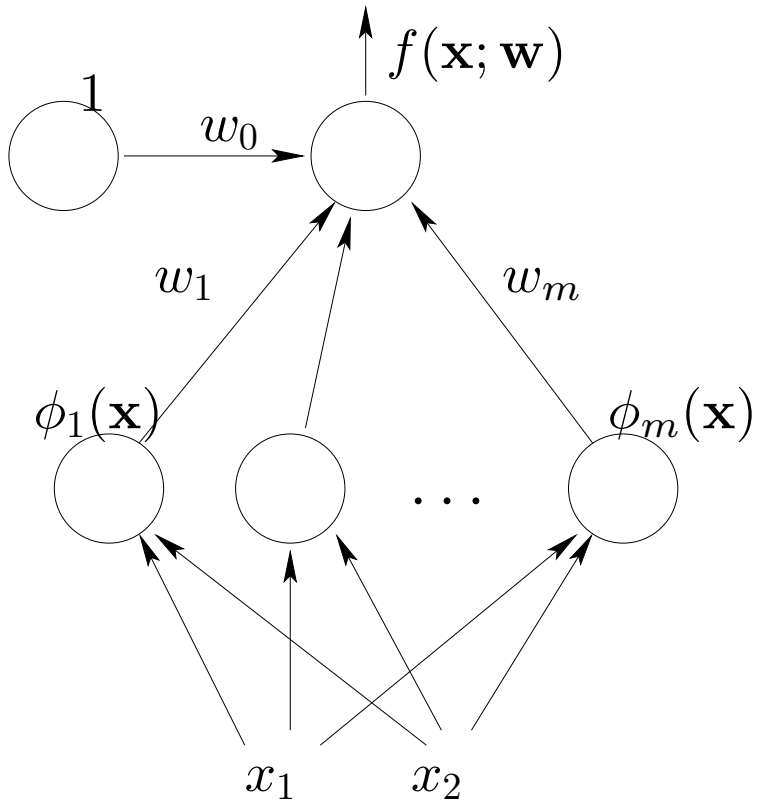
- The basis functions can capture various (e.g., qualitative) properties of the inputs.

- For example: we can try to rate companies based on text descriptions

$$
\begin{aligned}
\mathbf{x} &= \text{text document (collection of words)} \\
\phi_i(\mathbf{x}) &= \begin{cases} 1 \text{ if word } i \text{ appears in the document} \\ 0 \text{ otherwise} \end{cases} \\
f(\mathbf{x}; \mathbf{w}) &= w_0 + \sum_{i \in \text{words}} w_i \phi_i(\mathbf{x})
\end{aligned}
$$

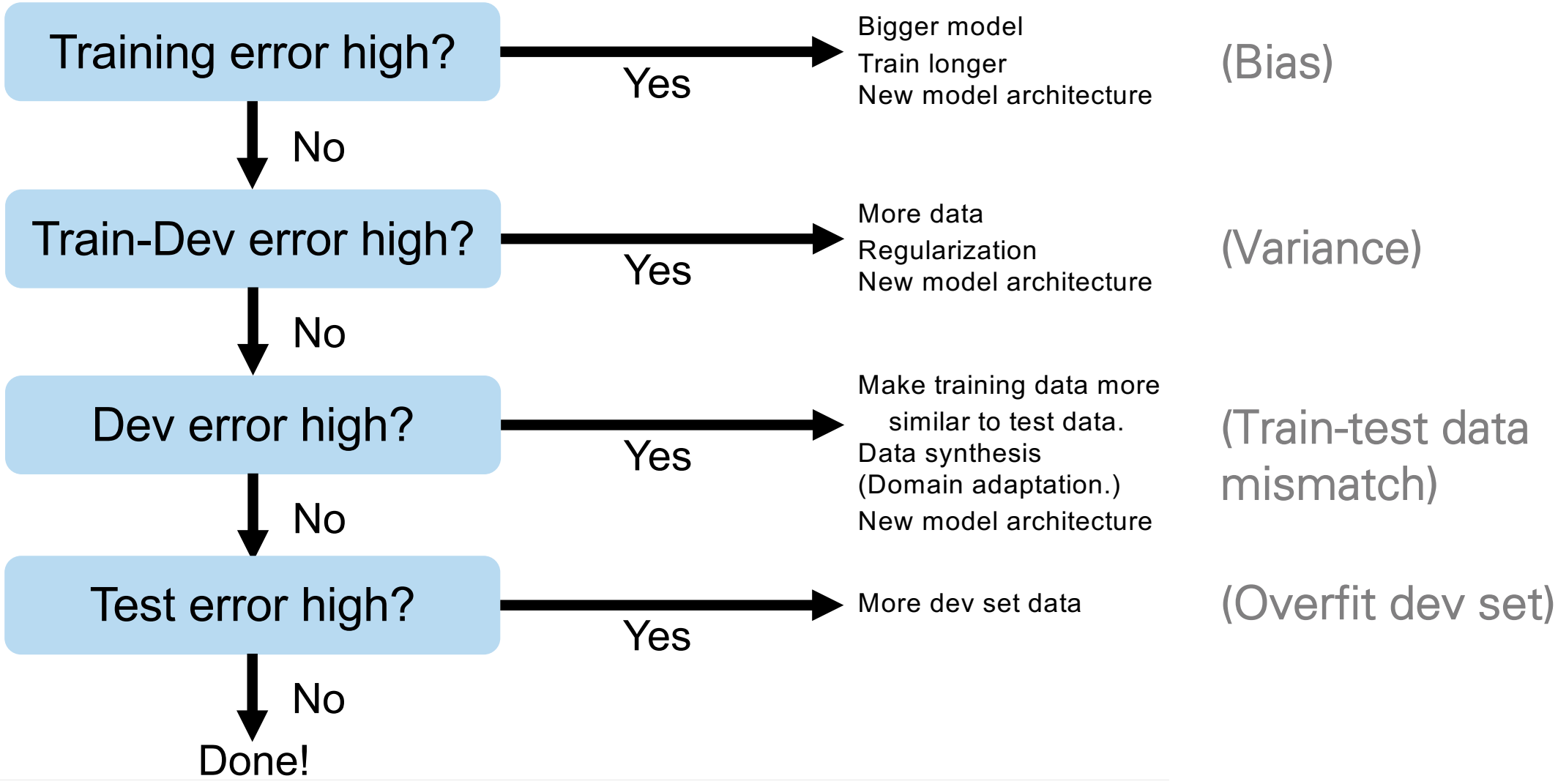
Additive models (cont'd)

- We can view the additive models graphically in terms of simple "units" and "weights"



- In **neural networks**, the basis functions themselves have adjustable parameters (cf. prototypes)

Take-home messages



Statistical regression models

— model formulation, motivation

— maximum likelihood estimation

Statistical view of linear regression

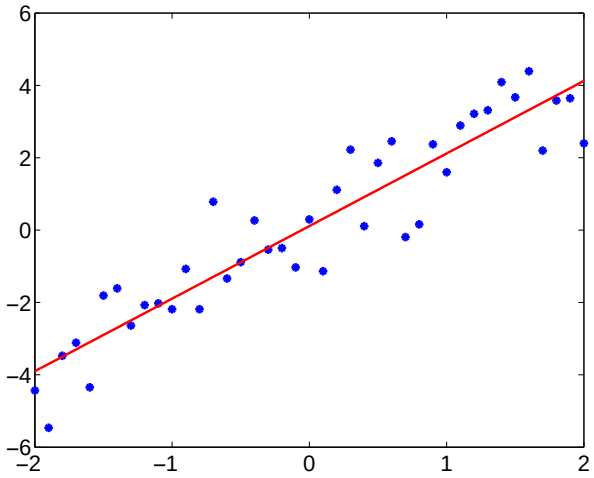
- In a statistical regression model we model both the function and noise

$$\textbf{Observed output} = \textbf{function} + \textbf{noise}$$

$$y = f(\mathbf{x}; \mathbf{w}) + \epsilon$$

where, e.g., $\epsilon \sim N(0, \sigma^2)$.

- Whatever we cannot capture with our chosen family of functions will be *interpreted* as noise

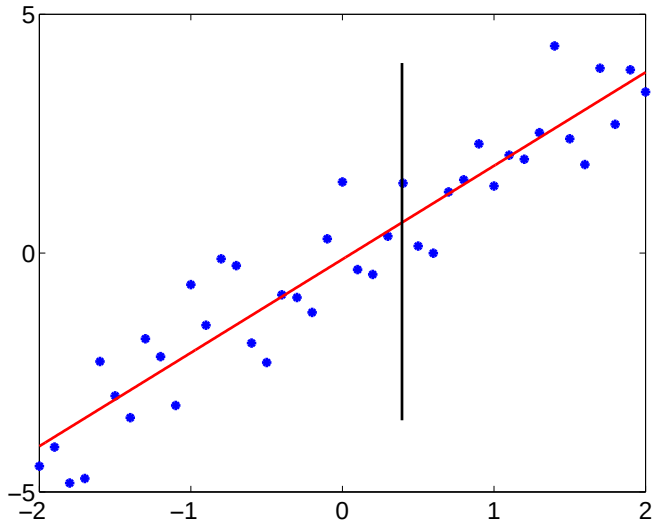


Statistical view of linear regression

- $f(\mathbf{x}; \mathbf{w})$ is trying to capture the mean of the observations y given the input $\mathbf{x}$:

$$\begin{aligned} E\{\, y \,|\, \mathbf{x} \,\} &= E\{\, f(\mathbf{x}; \mathbf{w}) + \epsilon \,|\, \mathbf{x} \,\} \\ &= f(\mathbf{x}; \mathbf{w}) \end{aligned}$$

where $E\{\, y \,|\, \mathbf{x} \,\}$ is the conditional expectation of y given $\mathbf{x}$, evaluated according to the model (not according to the underlying distribution P)



Statistical view of linear regression

- According to our statistical model

$$y = f(\mathbf{x}; \mathbf{w}) + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

the outputs y given $\mathbf{x}$ are normally distributed with mean $f(\mathbf{x}; \mathbf{w})$ and variance σ^2:

$$p(y|\mathbf{x}, \mathbf{w}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{ -\frac{1}{2\sigma^2}(y - f(\mathbf{x}; \mathbf{w}))^2 \}$$

(we model the uncertainty in the predictions, not just the mean)

- Loss function? Estimation?

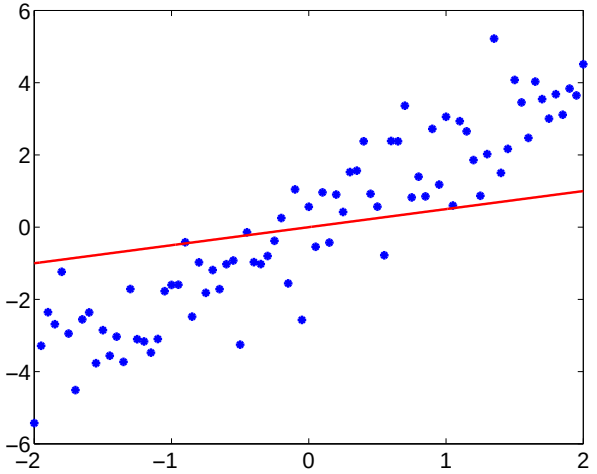
Maximum likelihood estimation

- Given observations $D_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ we find the parameters $\mathbf{w}$ that maximize the (conditional) likelihood of the outputs

$$L(D_n; \mathbf{w}, \sigma^2) = \prod_{i=1}^{n} p(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2)$$

- Example: linear function

$$p(y|\mathbf{x}, \mathbf{w}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{ -\frac{1}{2\sigma^2}(y - w_0 - w_1 x)^2 \}$$



(why is this a bad fit according to the likelihood criterion?)

Maximum likelihood estimation (cont'd)

Likelihood of the observed outputs:

$$L(D; \mathbf{w}, \sigma^2) = \prod_{i=1}^{n} P(y_i | \mathbf{x}_i, \mathbf{w}, \sigma^2)$$

- It is often easier (but equivalent) to try to maximize the log-likelihood:

$$\begin{aligned} l(D; \mathbf{w}, \sigma^2) &= \log L(D; \mathbf{w}, \sigma^2) = \sum_{i=1}^{n} \log P(y_i | \mathbf{x}_i, \mathbf{w}, \sigma^2) \\ &= \sum_{i=1}^{n} \left(-\frac{1}{2\sigma^2} (y_i - f(\mathbf{x}_i; \mathbf{w}))^2 - \log \sqrt{2\pi\sigma^2} \right) \\ &= \left(-\frac{1}{2\sigma^2} \right) \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i; \mathbf{w}))^2 + \dots \end{aligned}$$

Maximum likelihood estimation (cont'd)

- Maximizing log-likelihood is equivalent to minimizing empirical loss when the loss is defined according to

$$\text{Loss}(y_i, f(\mathbf{x}_i; \mathbf{w})) = -\log P(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2)$$

Loss defined as the negative log-probability is known as the log-loss.

Maximum likelihood estimation (cont'd)

- The log-likelihood of observations

$$\log L(D; \mathbf{w}, \sigma^2) = \sum_{i=1}^{n} \log P(y_i | \mathbf{x}_i, \mathbf{w}, \sigma^2)$$

  is a generic fitting criterion and can be used to estimate the noise variance σ^2 as well.

- Let $\hat{\mathbf{w}}$ be the maximum likelihood (here least squares) setting of the parameters. What is the maximum likelihood estimate of σ^2, obtained by solving

$$\frac{\partial}{\partial \sigma^2} \log L(D; \mathbf{w}, \sigma^2) = 0 \quad ?$$

Maximum likelihood estimation (cont'd)

- The log-likelihood of observations

$$\log L(D; \mathbf{w}, \sigma^2) = \sum_{i=1}^{n} \log P(y_i | \mathbf{x}_i, \mathbf{w}, \sigma^2)$$

  is a generic fitting criterion and can be used to estimate the noise variance σ^2 as well.

- Let $\hat{\mathbf{w}}$ be the maximum likelihood (here least squares) setting of the parameters. The maximum likelihood estimate of the noise variance σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i; \hat{\mathbf{w}}))^2$$

  i.e., the mean squared prediction error.

Polynomial regression

- Consider again a simple m^{th} degree polynomial regression model

$$y = w_0 + w_1 x + \ldots + w_m x^m + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

where σ^2 is assumed fixed (known).

- In this model the outputs $\{y_1,\ldots,y_n\}$ corresponding to any inputs $\{x_1,\ldots,x_n\}$ are generated according to

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \quad \text{where}$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \ldots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_1 & \ldots & x_1^m \\ \ldots & \ldots & \ldots & \\ 1 & x_n & \ldots & x_n^m \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} \epsilon_1 \\ \ldots \\ \epsilon_n \end{bmatrix}$$

and $\epsilon_i \sim N(0, \sigma^2)$, $i = 1, \ldots, n$.

ML estimator, uncertainty

- We are interested in studying how the choice of inputs $\{x_1,\ldots,x_n\}$ or, equivalently, $\mathbf{X}$, affects the accuracy of our regression model

- Our model for the outputs $\{y_1,\ldots,y_n\}$ given $\mathbf{X}$ is

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \quad \mathbf{e} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

- We assume also that the training outputs are actually generated by a model in this class with some fixed but unknown parameters $\mathbf{w^*}$ (same σ^2)

$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \mathbf{e}, \quad \mathbf{e} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

- We can now ask, for a given $\mathbf{X}$, how accurately we are able to recover the ''true'' parameters $\mathbf{w^*}$

ML estimator, uncertainty

- The ML estimator $\hat{\mathbf{w}}$ viewed here as a function of the outputs $\mathbf{y}$ for a fixed $\mathbf{X}$, is given by

$$\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- We need to understand how $\hat{\mathbf{w}}$ varies in relation to $\mathbf{w^*}$ when the outputs are generated according to

$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \mathbf{e}, \quad \mathbf{e} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

- In the absence of noise $\mathbf{e}$, the ML estimator would recover $\mathbf{w^*}$ exactly (with only minor constraints on $\mathbf{X}$)

$$\begin{aligned}\hat{\mathbf{w}} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}\mathbf{w}^*) \\ &= (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})\mathbf{w}^* \\ &= \mathbf{w}^*\end{aligned}$$

ML estimator, uncertainty

- In the presence of noise we can still use the fact that $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \mathbf{e}$ to simplify the parameter estimates

$$\begin{aligned}
\hat{\mathbf{w}} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\
&= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}\mathbf{w}^* + \mathbf{e}) \\
&= (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})\mathbf{w}^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{e} \\
&= \mathbf{w}^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{e}
\end{aligned}$$

- So the ML estimate is the correct parameter vector plus an estimate based purely on noise

Next Lecture:

Multi-layer Perceptrons