Illustration: Puppy or bagel? // Karen Zack

COMP541
DEEP LEARNING

Lecture #2 – Machine Learning Overview

KOÇ UNIVERSITY

Aykut Erdem // Koç University // Fall 2023

Previously on COMP541

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

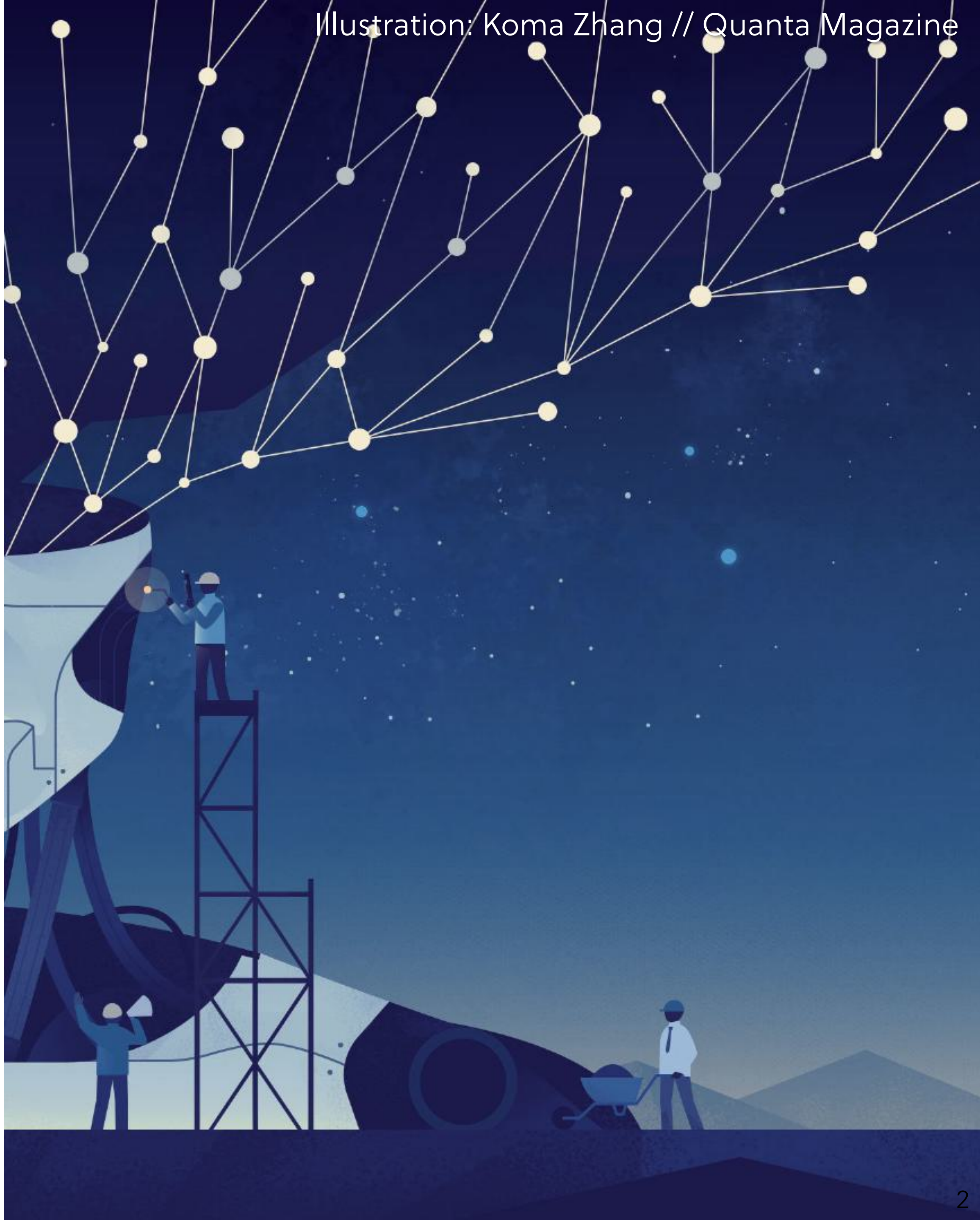


Illustration: Koma Zhang // Quanta Magazine

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 and Andrej Karpathy's CS231n class

—Justin Johnson's EECS598 class

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

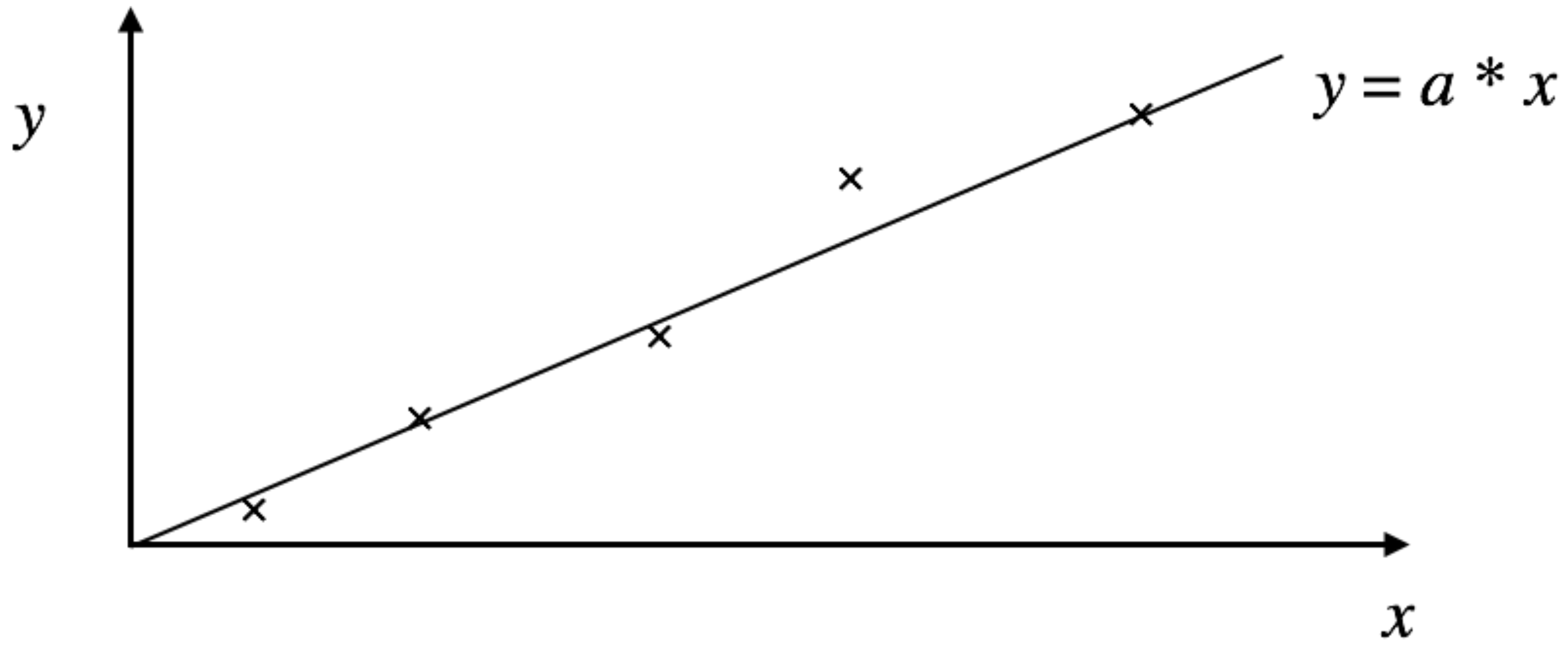
- Drawing conclusions from empirical data (observations, measurements)

- 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

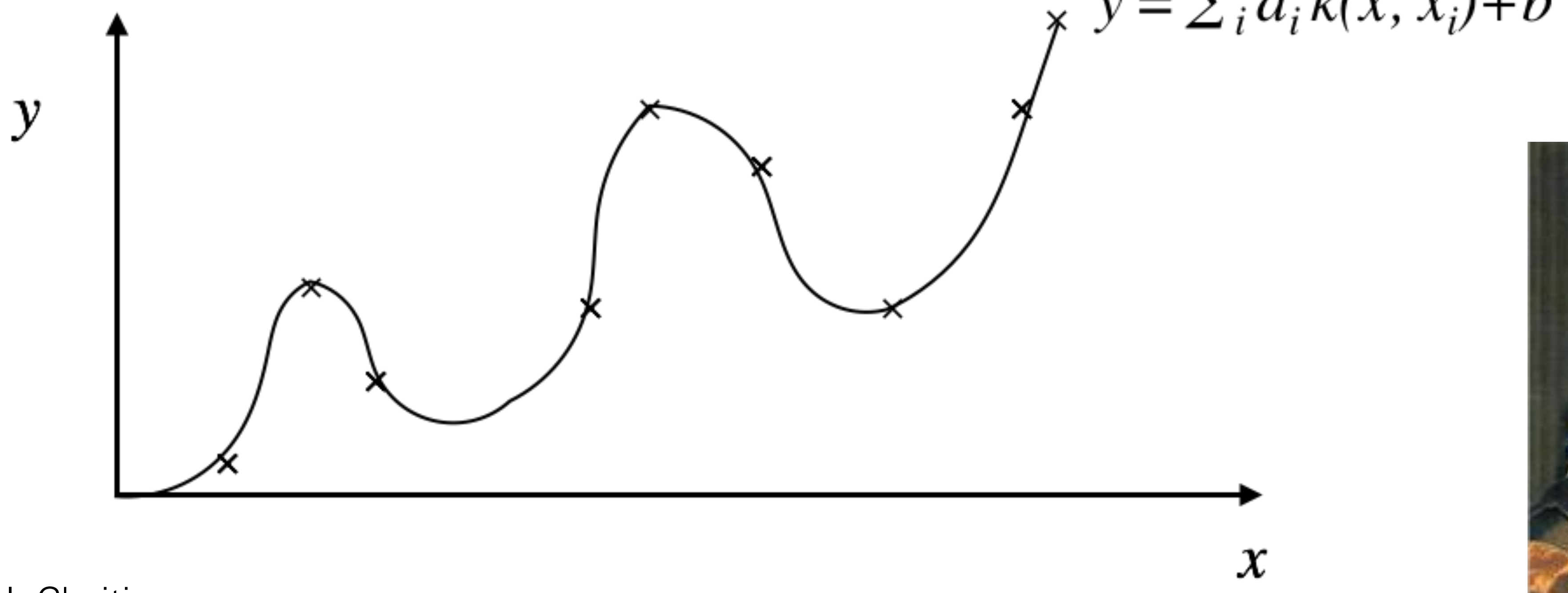
$$y = \sum_i a_i k(x, x_i) + b$$

Leibniz, Weyl, Chaitin

Empirical Inference

- Drawing conclusions from empirical data (observations, measurements)

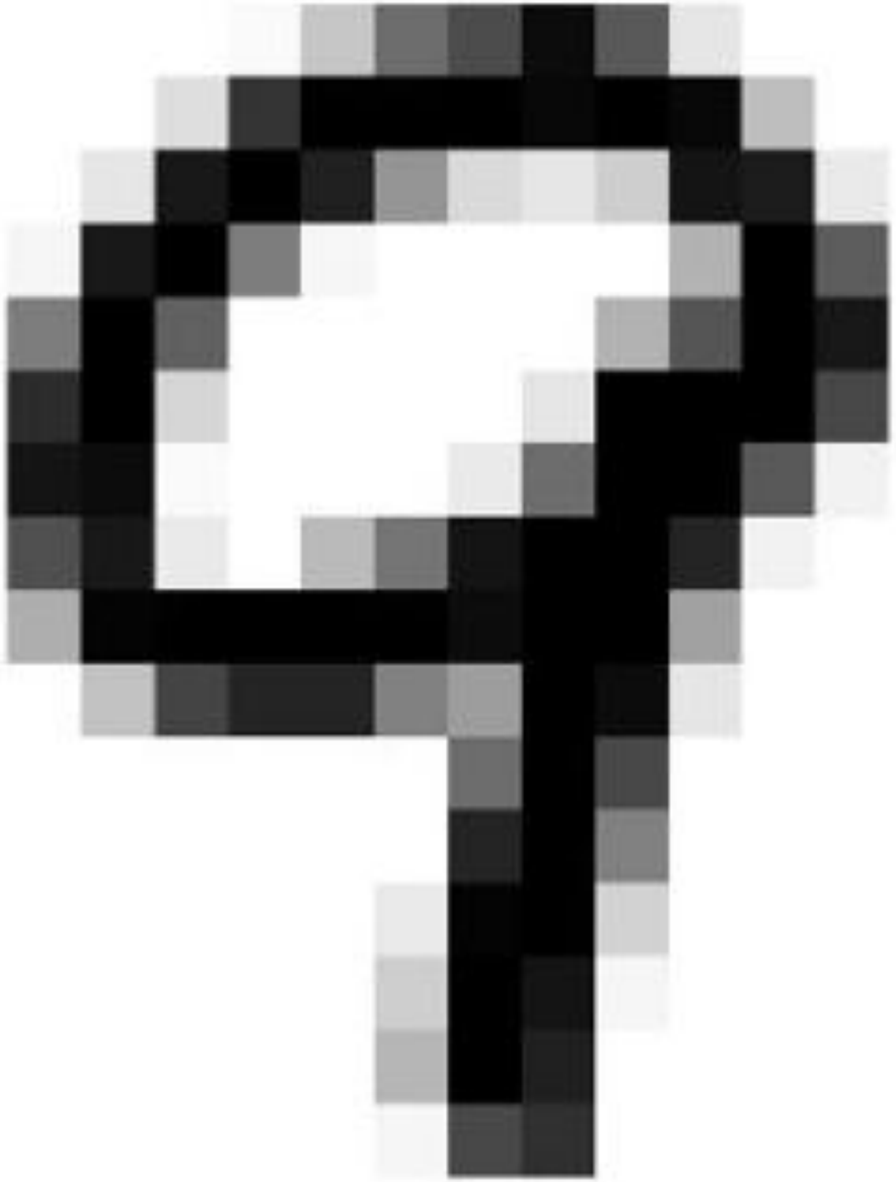
- Example 1: scientific inference



Leibniz, Weyl, Chaitin

Empirical Inference

- Example 2: perception



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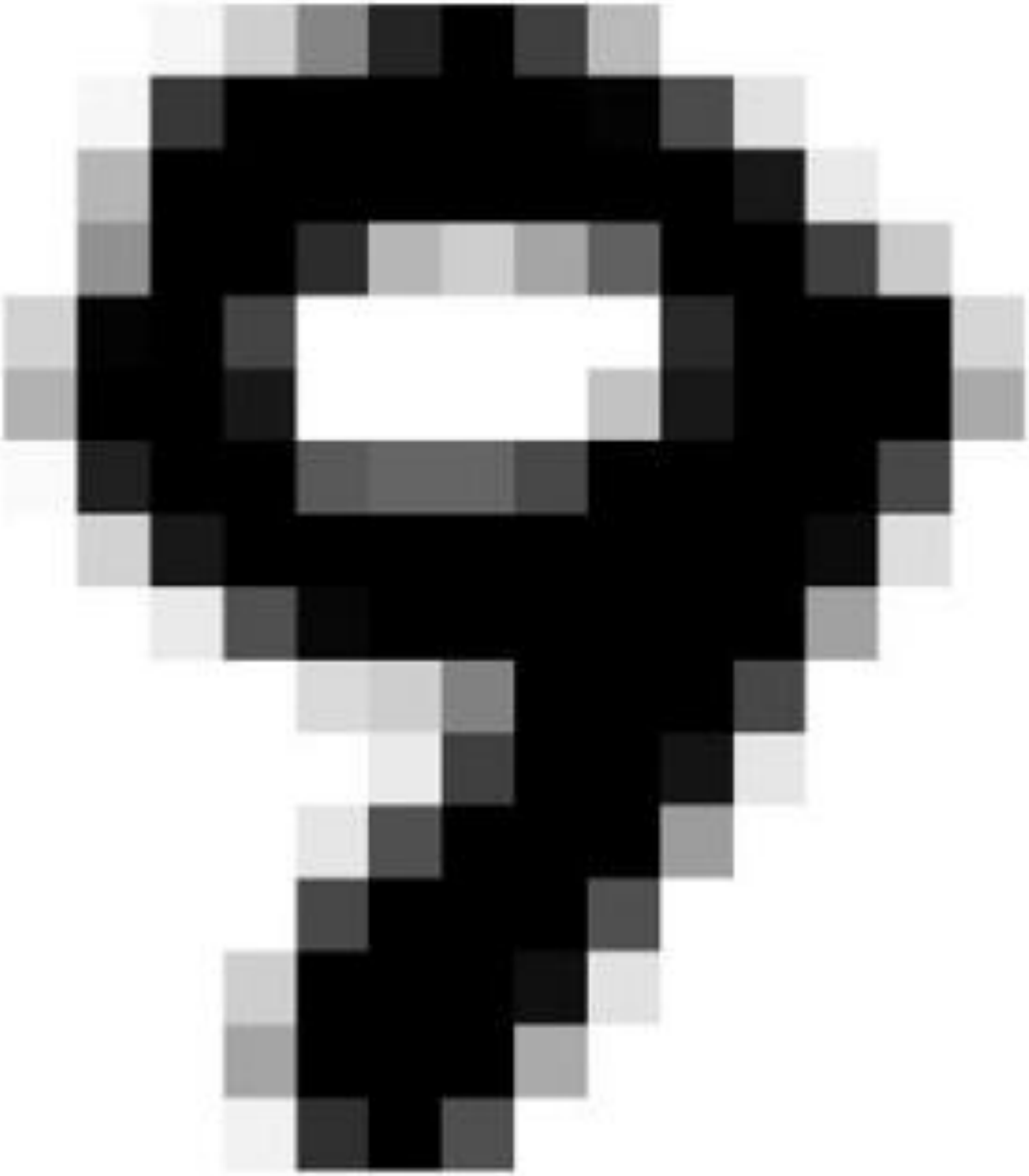

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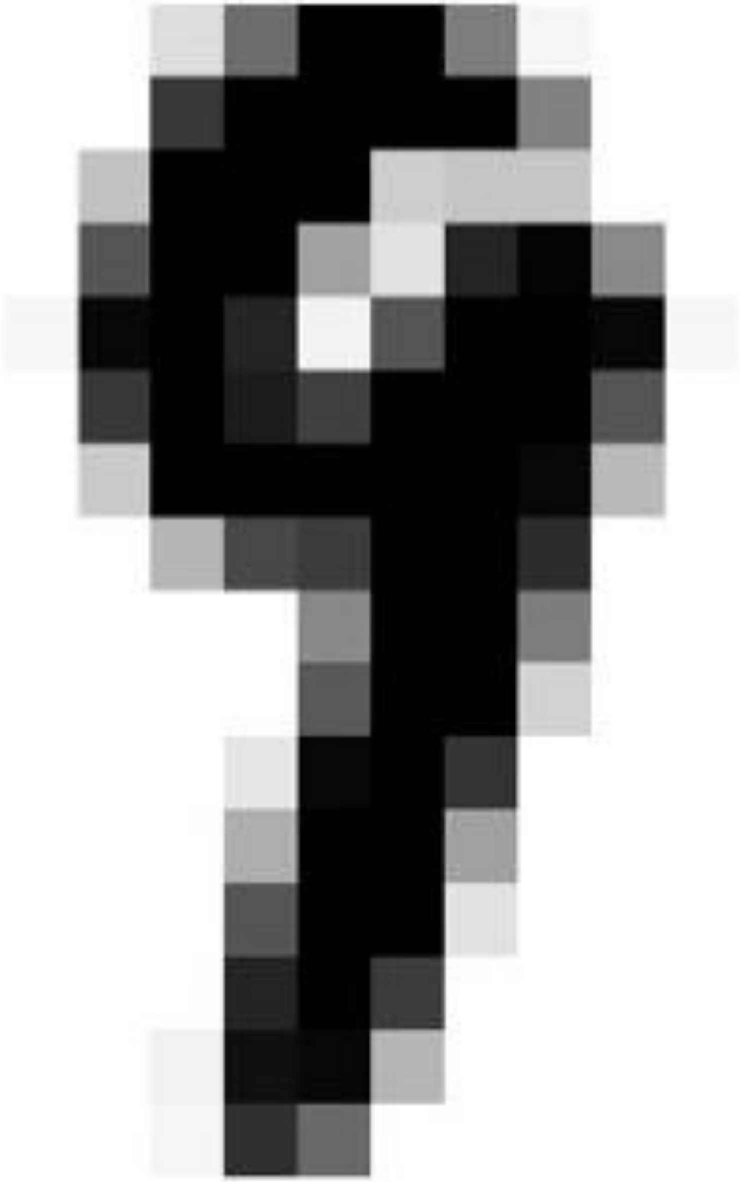

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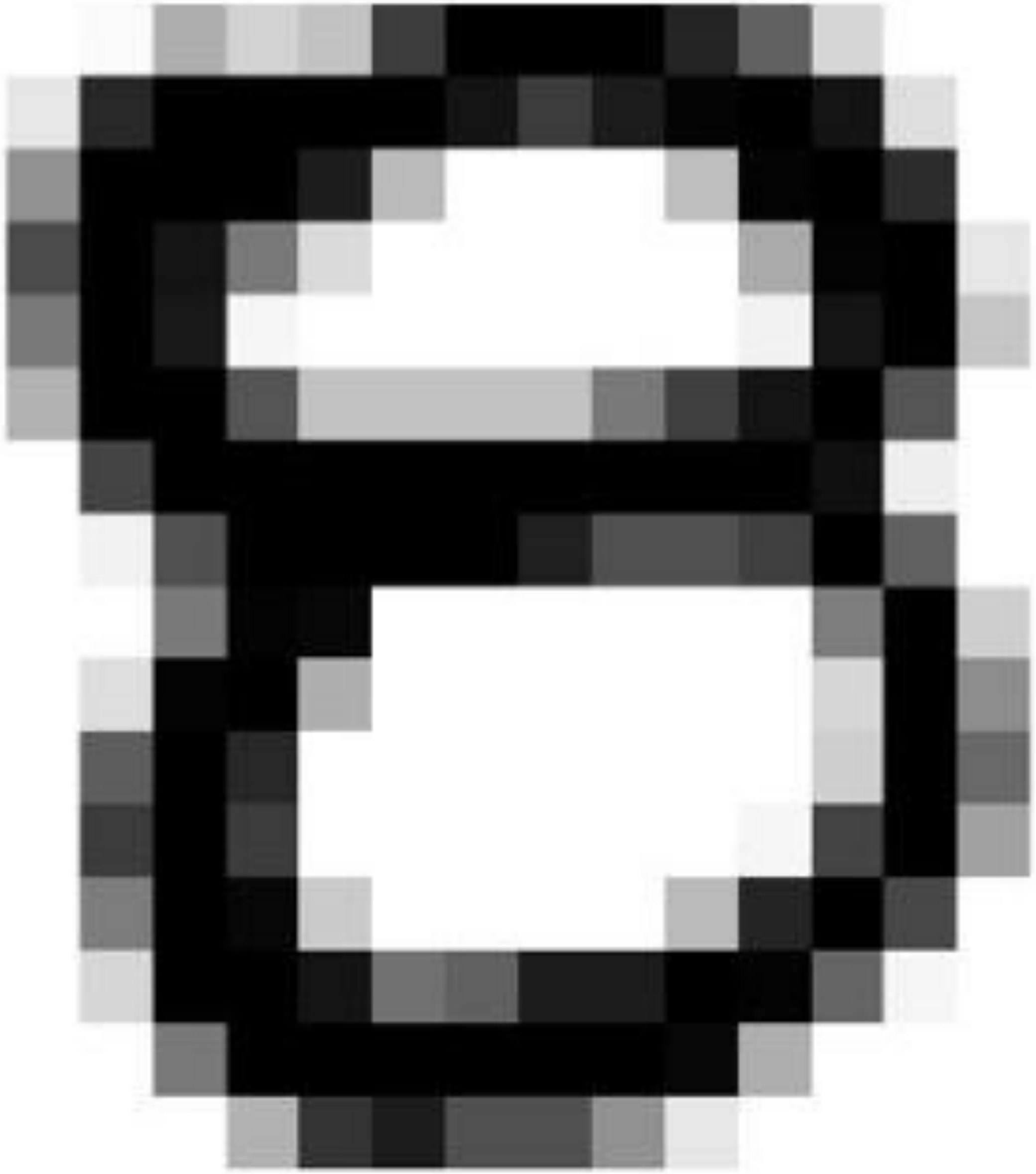

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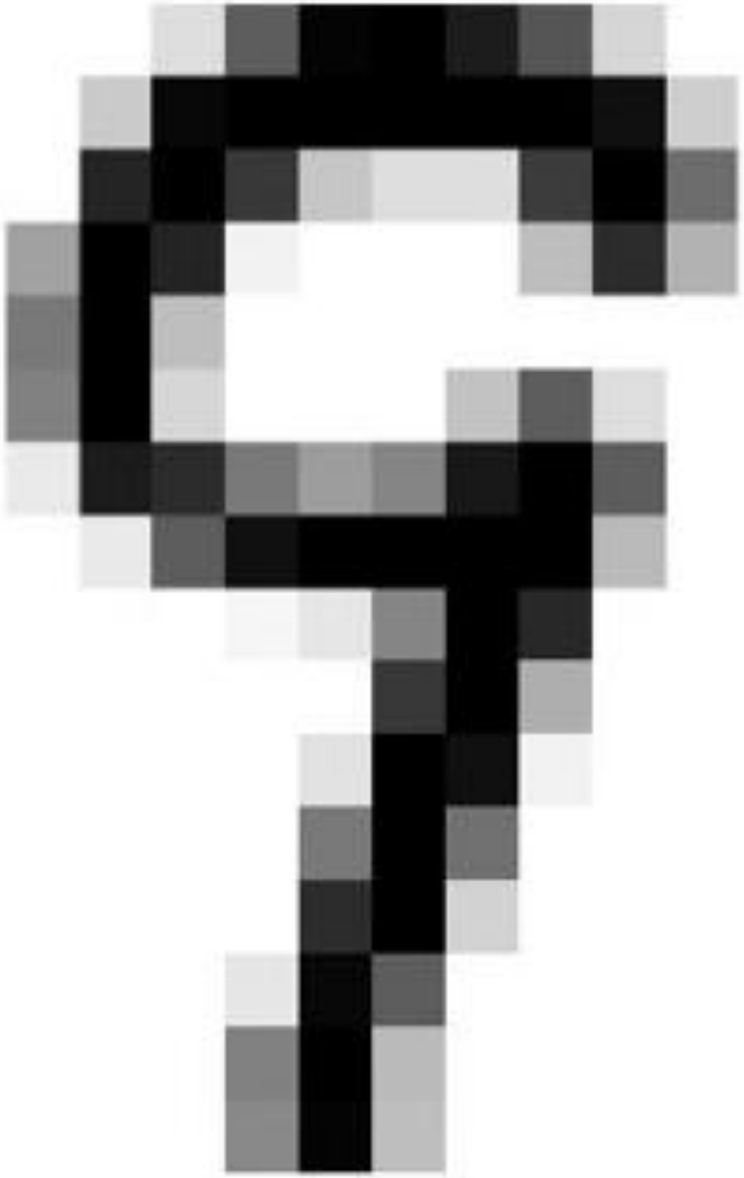

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The choice of representation may determine whether the learning task is very easy or very difficult!

Generalization

- *observe* 1, 2, 4, 7, …
- What’s next? +1 +2 +3

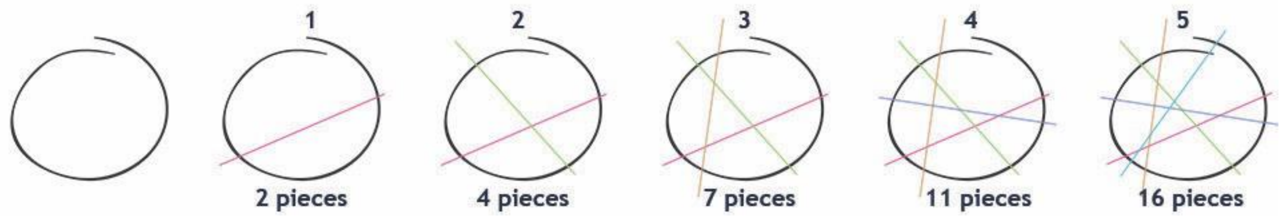


Image credit: mathspice.com

- 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: > 1300 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

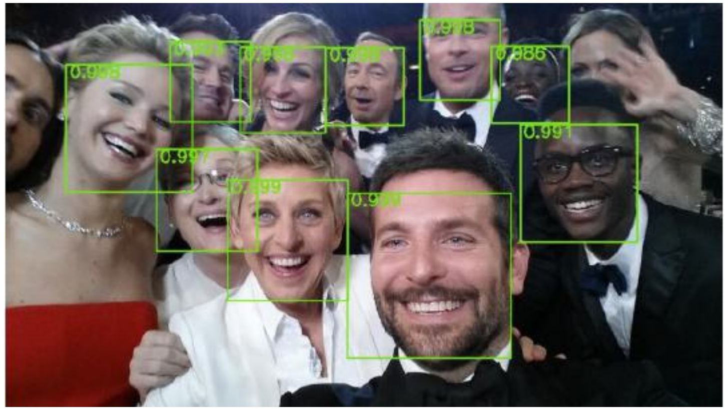
Supervised learning

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

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

cat

Image classification

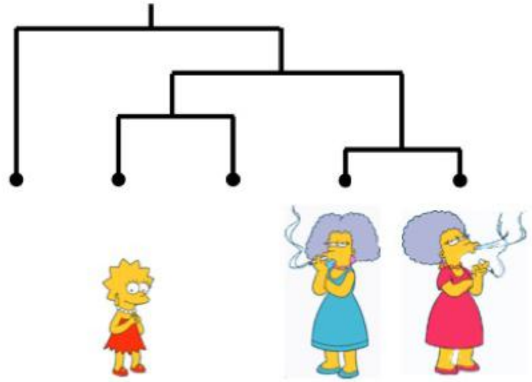


Face detection

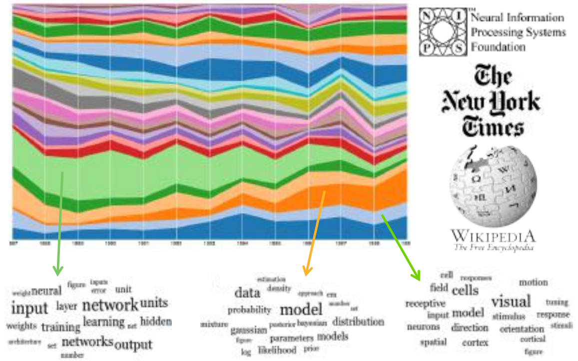
Unsupervised learning

- **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

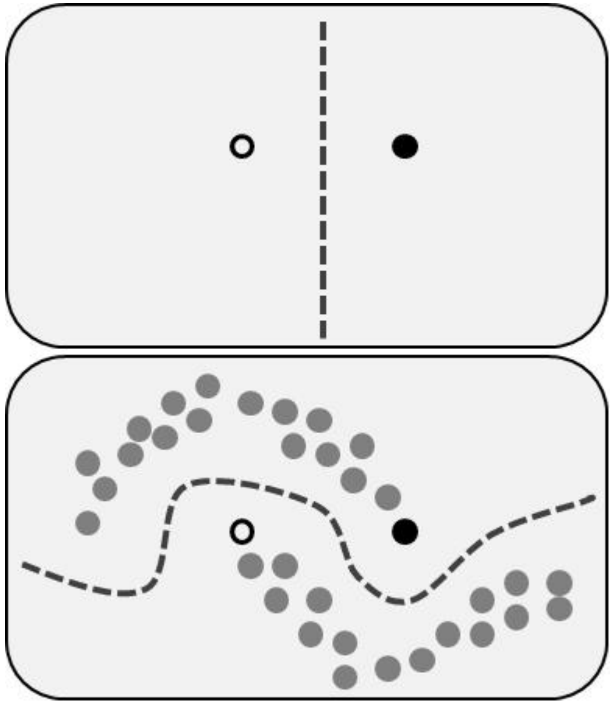
Semi-supervised learning

- **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

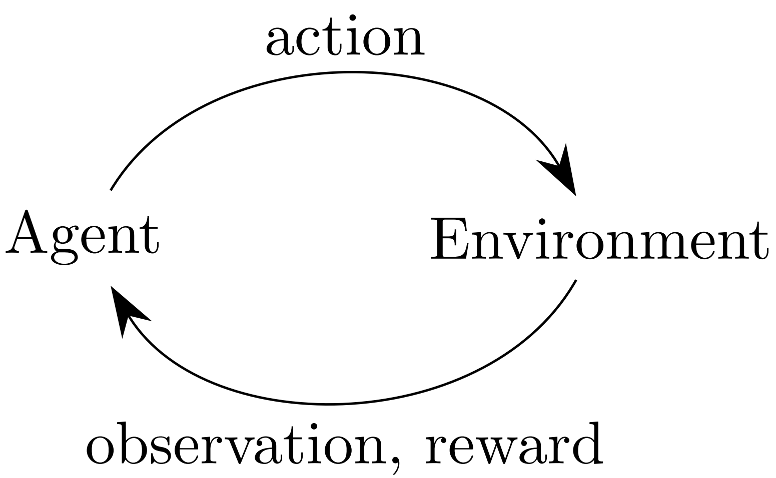
Try to improve predictions based on examples by making use of the additional "unlabeled" examples

Image credit: Wikipedia

Reinforcement learning

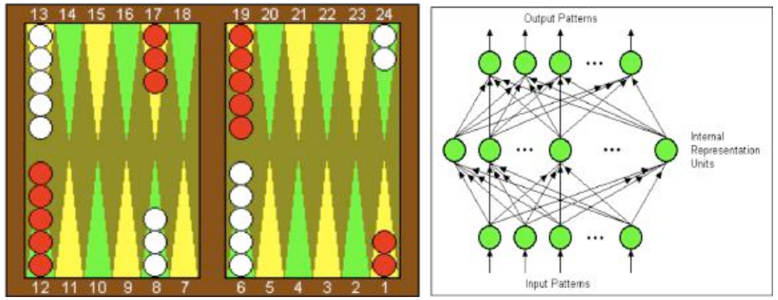
- **Input:**

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



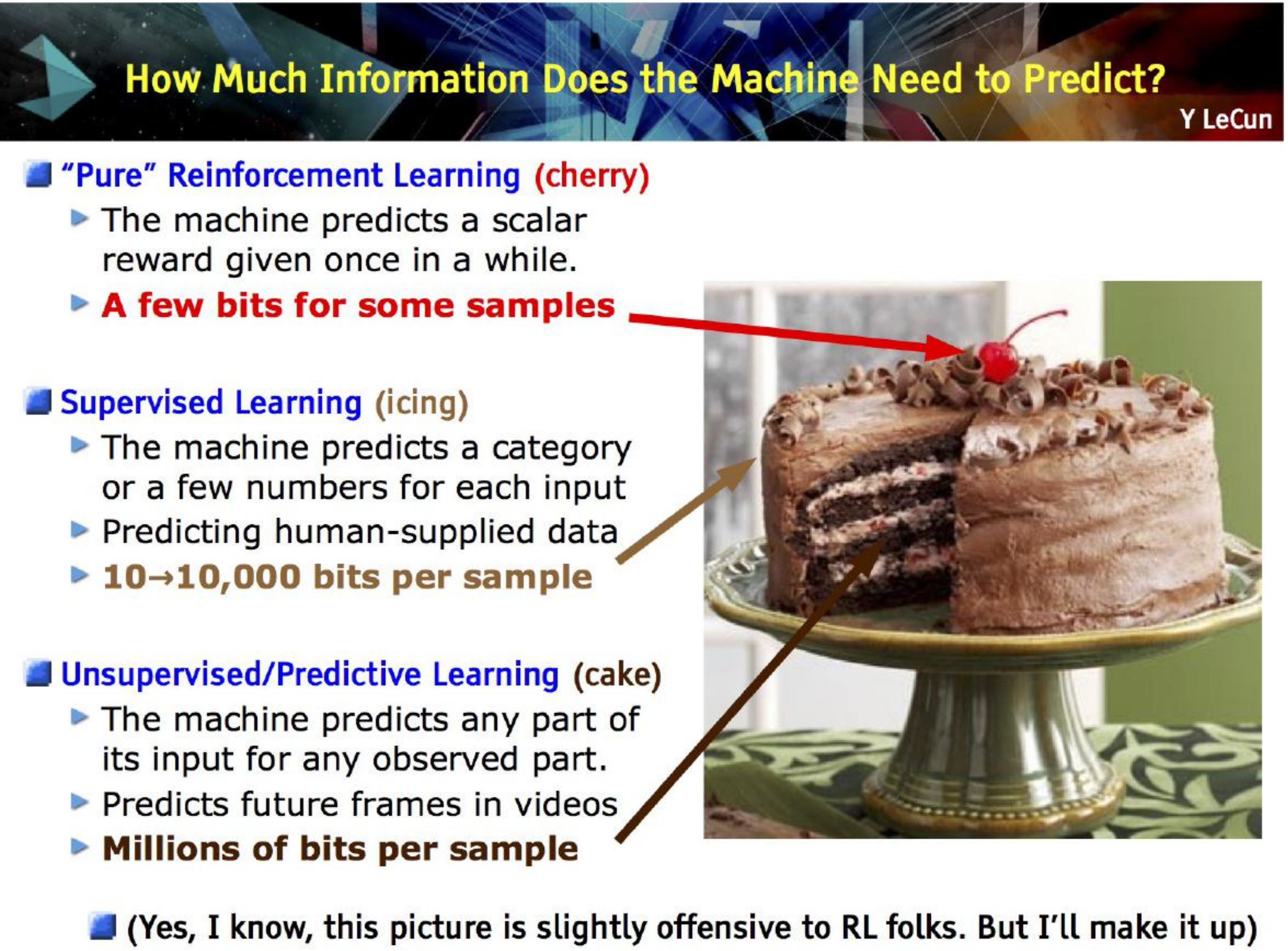
- **Task:** A way of behaving that is very rewarding in the long run

- 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

Input: image

Output: Assign image to one of a fixed set of categories

cat
bird
deer
dog
truck

The problem: **Semantic Gap**


```
[[105 112 108 111 104  99 106  99  96 103 112 119 104  97  93  87]
 [ 91  98 102 106 104  79  98 103  99 105 123 136 110 105  94  85]
 [ 76  85  90 105 128 105  87  96  95  99 115 112 106 103  99  85]
 [ 99  81  81  93 120 131 127 100  95  98 102  99  96  93 101  94]
 [106  91  61  64  69  91  88  85 101 107 109  98  75  84  96  95]
 [114 108  85  55  55  69  64  54  64  87 112 129  98  74  84  91]
 [133 137 147 103  65  81  80  65  52  54  74  84 102  93  85  82]
 [128 137 144 140 109  95  86  70  62  65  63  63  60  73  86 101]
 [125 133 148 137 119 121 117  94  65  79  80  65  54  64  72  98]
 [127 125 131 147 133 127 126 131 111  96  89  75  61  64  72  84]
 [115 114 109 123 150 148 131 118 113 109 100  92  74  65  72  78]
 [ 89  93  90  97 108 147 131 118 113 114 113 109 106  95  77  80]
 [ 63  77  86  81  77  79 102 123 117 115 117 125 125 130 115  87]
 [ 62  65  82  89  78  71  80 101 124 126 119 101 107 114 131 119]
 [ 63  65  75  88  89  71  62  81 120 138 135 105  81  98 110 118]
 [ 87  65  71  87 106  95  69  45  76 130 126 107  92  94 105 112]
 [118  97  82  86 117 123 116  66  41  51  95  93  89  95 102 107]
 [164 146 112  80  82 120 124 104  76  48  45  66  88 101 102 109]
 [157 170 157 120  93  86 114 132 112  97  69  55  70  82  99  94]
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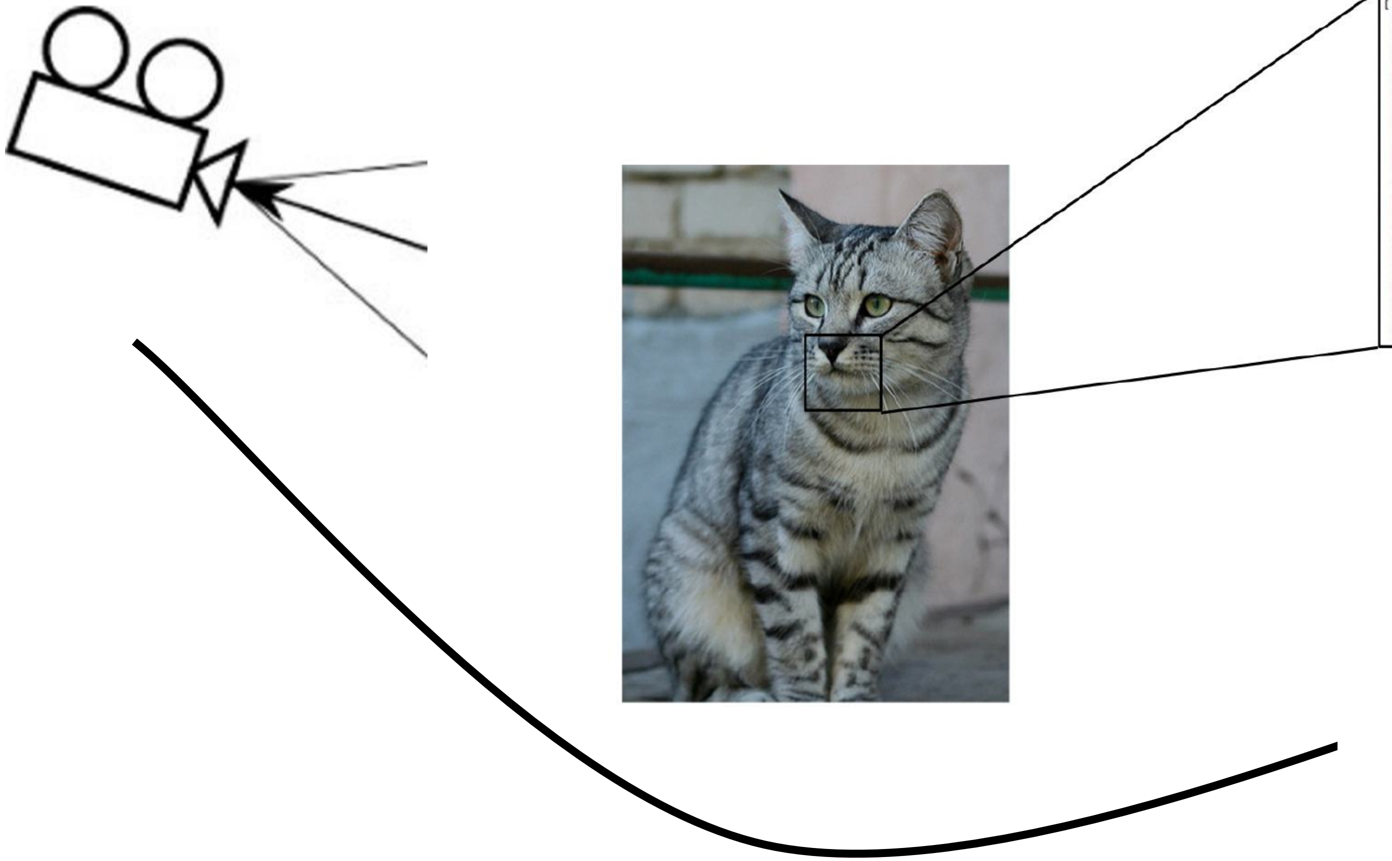
 [128 112  96 117 150 144 120 115 104 107 102  93  87  81  72  79]
 [123 107  96  86  83 112 153 149 122 109 104  75  80 107 112  99]
 [122 121 102  80  82  86  94 117 145 148 153 102  58  78  92 107]
 [122 164 148 103  71  56  78  83  93 103 119 139 102  61  69  84]]
```

What the computer sees

An image is just a big grid of numbers between [0, 255].

e.g. 800 x 600 x 3
(3 channels RGB)

Challenges: Viewpoint Variation



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[[105 112 108 111 104  99 106  99  96 103 112 119 104  97  93  87]
 [ 91  98 102 106 104  79  98 103  99 105 123 136 110 105  94  85]
 [ 76  85  90 105 128 105  87  96  95  99 115 112 106 103  99  85]
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 [122 164 148 103  71  56  78  83  93 103 119 139 102  61  69  84]]
```

All pixels change when
the camera moves!

Challenges: Intraclass Variation

Challenges: Fine-Grained Categories

Main Coon

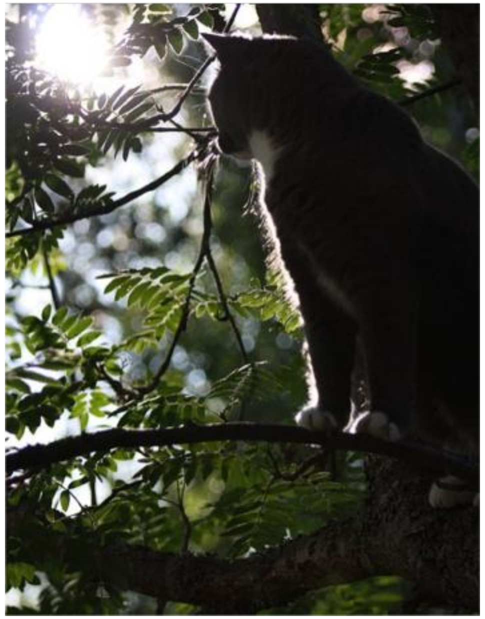
Ragdoll

American Shorthhair

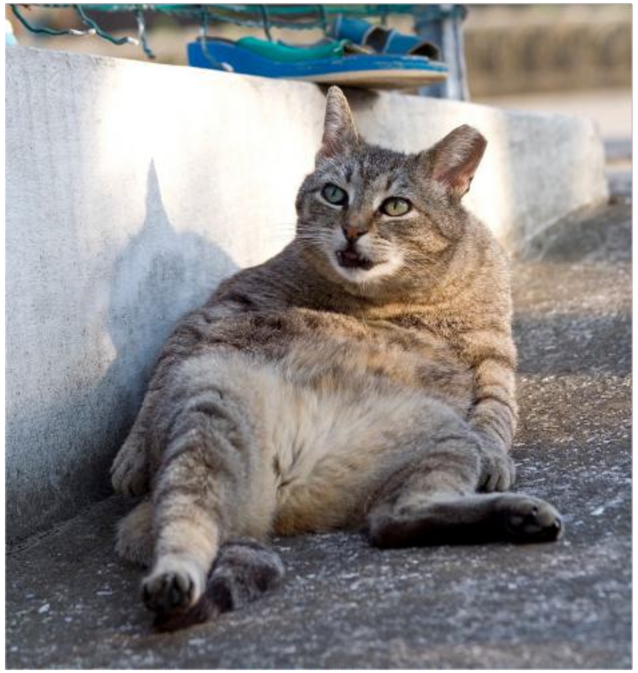
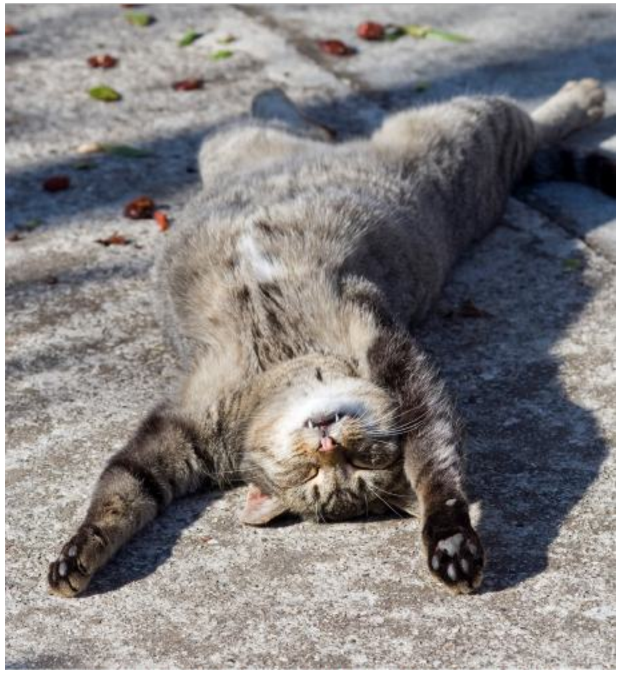
Challenges: Background clutter

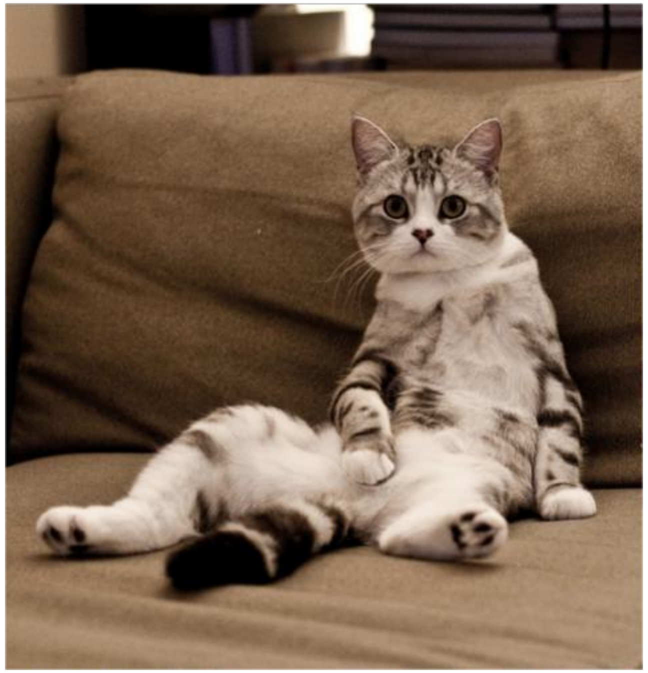
Challenges: Illumination Changes



Challenges: Deformation

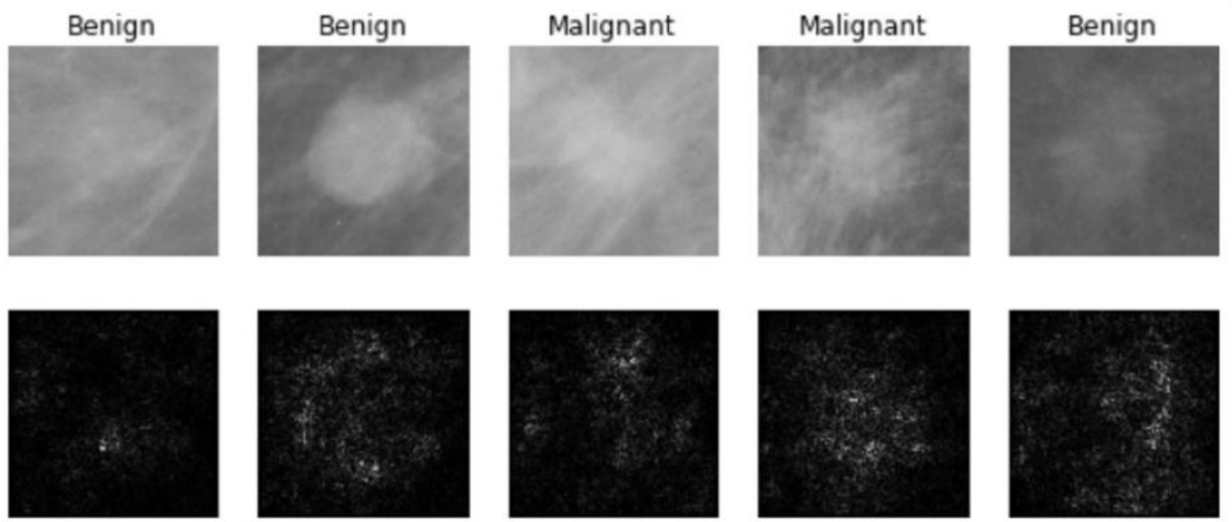





Challenges: Occlusion

Image Classification: Very Useful!

Medical Imaging



Galaxy Classification

Whale recognition

[Kaggle Challenge]

An image classifier

```
def classify_image(image):
  # Some magic here?
  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.

You could try …

Find edges

Find corners

?

Machine Learning: Data-Driven Approach

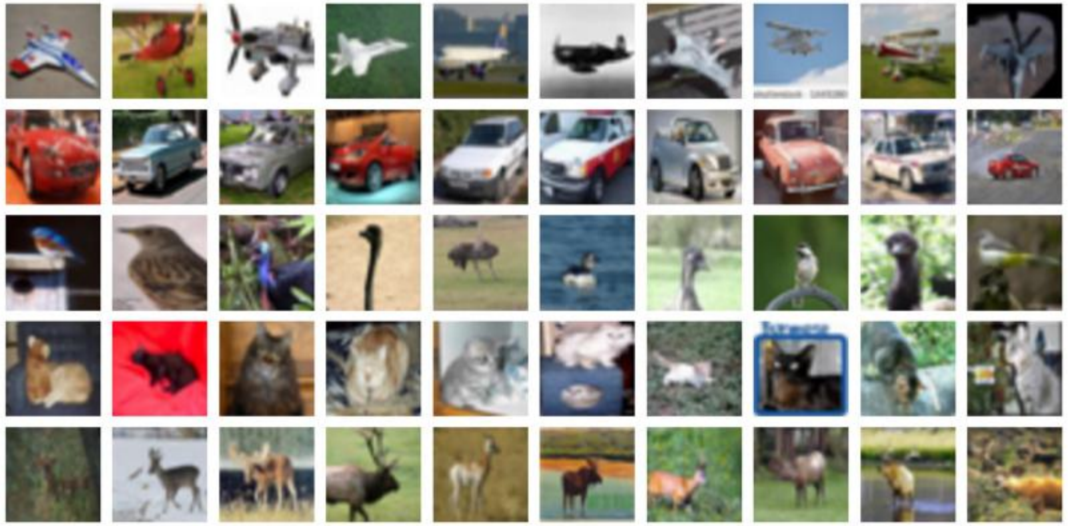
1. Collect a dataset of images and labels
2. Use Machine Learning to train an image classifier
3. Evaluate the classifier on a withheld set of test images

```python
def train(images, labels):
  # Machine learning!
  return model
```

```python
def predict(model, test_images):
  # Use model to predict labels
  return test_labels
```

Example training set

airplane
automobile
bird
cat
deer



First classifier: Nearest Neighbor Classifier

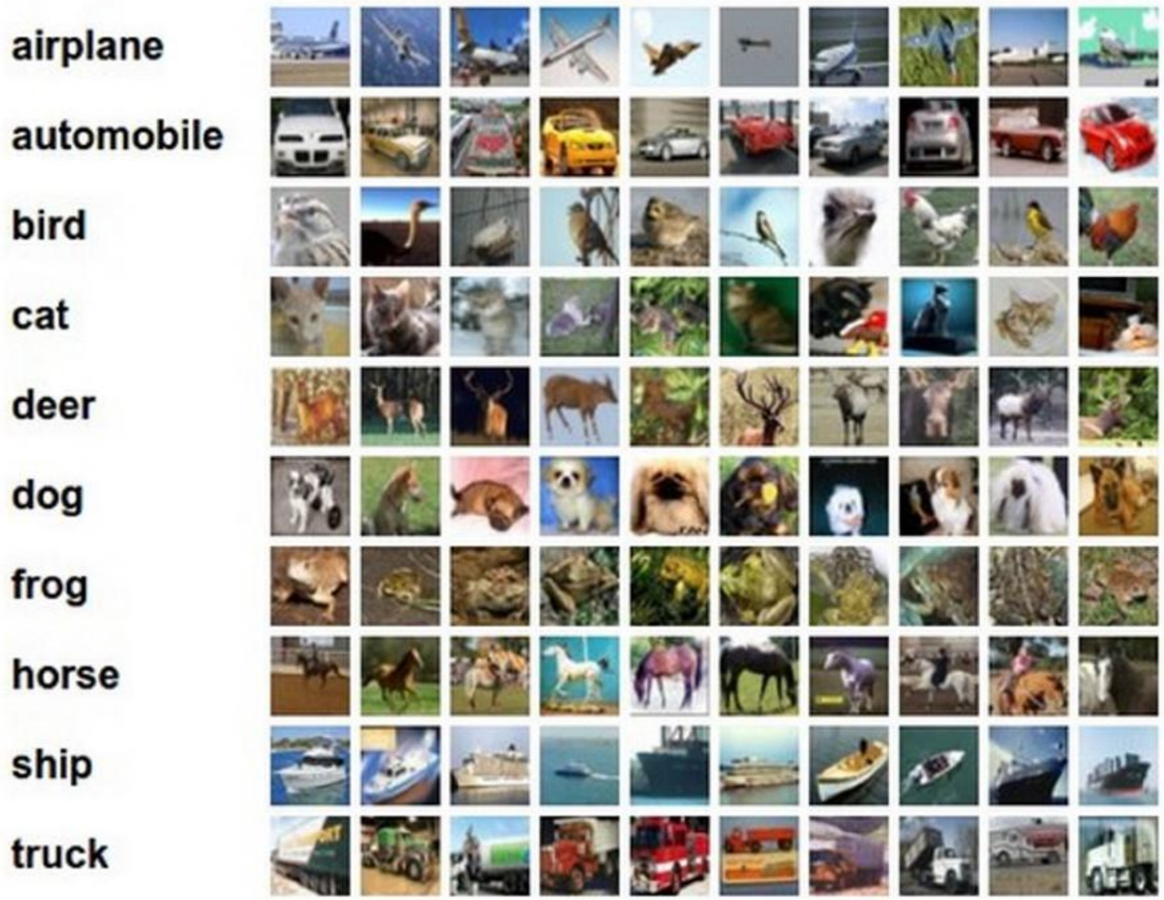
```
def train(images, labels):
  # Machine learning!
  return model
```

→ Memorize all data and labels

```
def predict(model, test_images):
  # Use model to predict labels
  return test_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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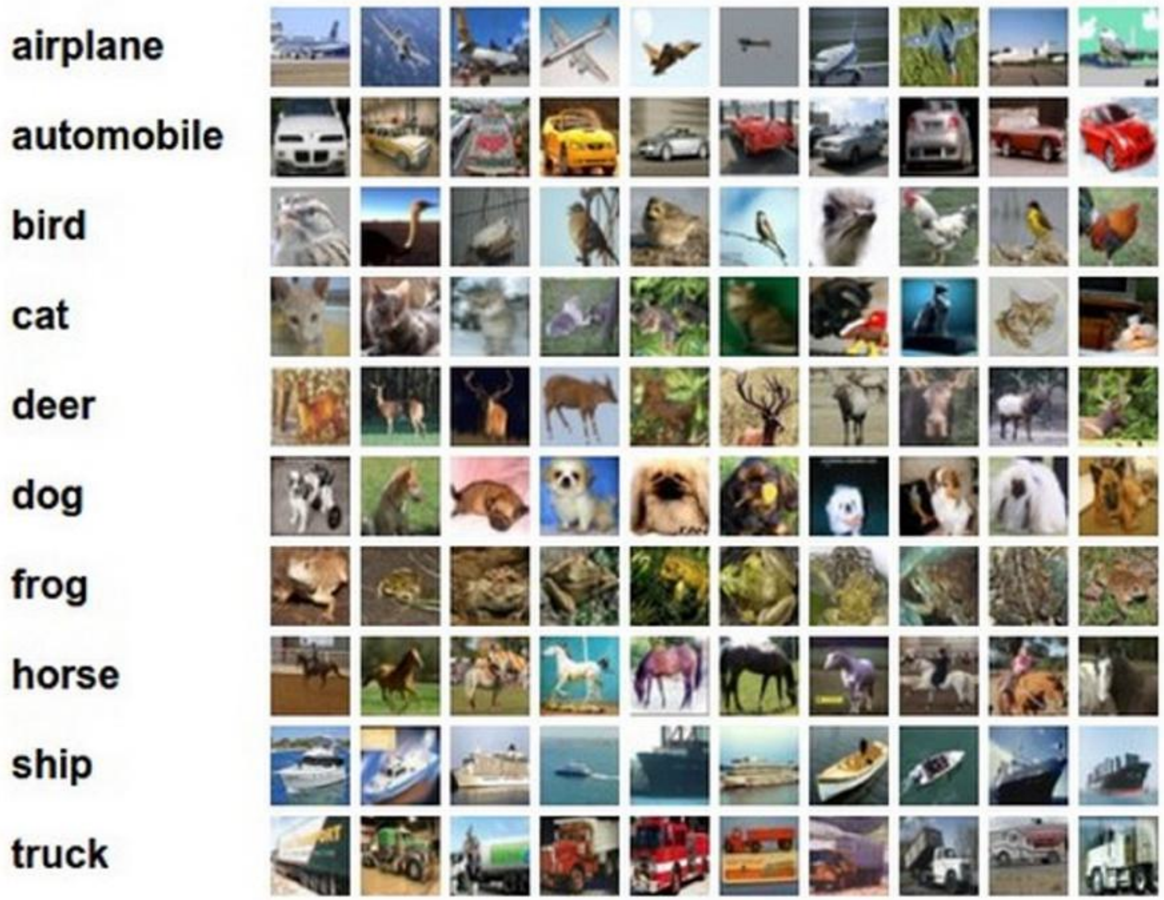
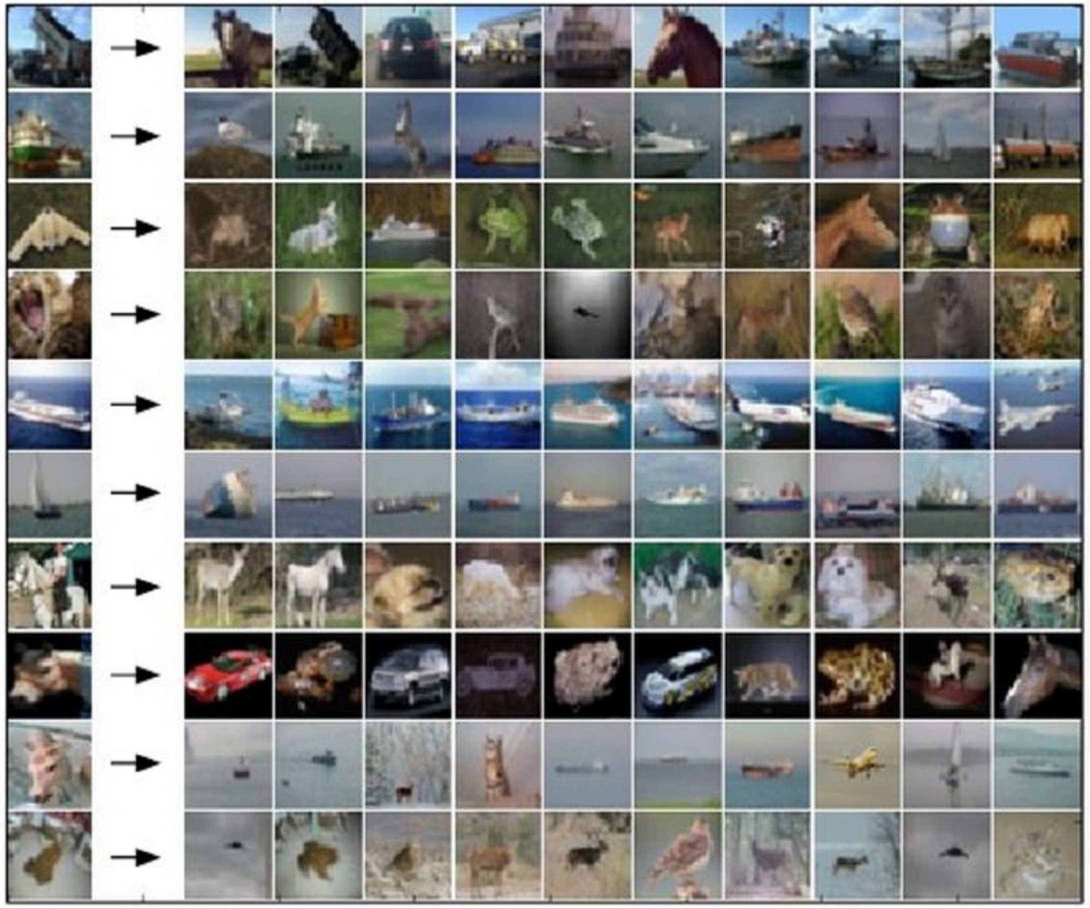


For every test image (first column), examples of nearest neighbors in rows



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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Memorize training data

Nearest Neighbor classifier

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```

For every test image:

- Find the nearest train image
- Return 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 :(**

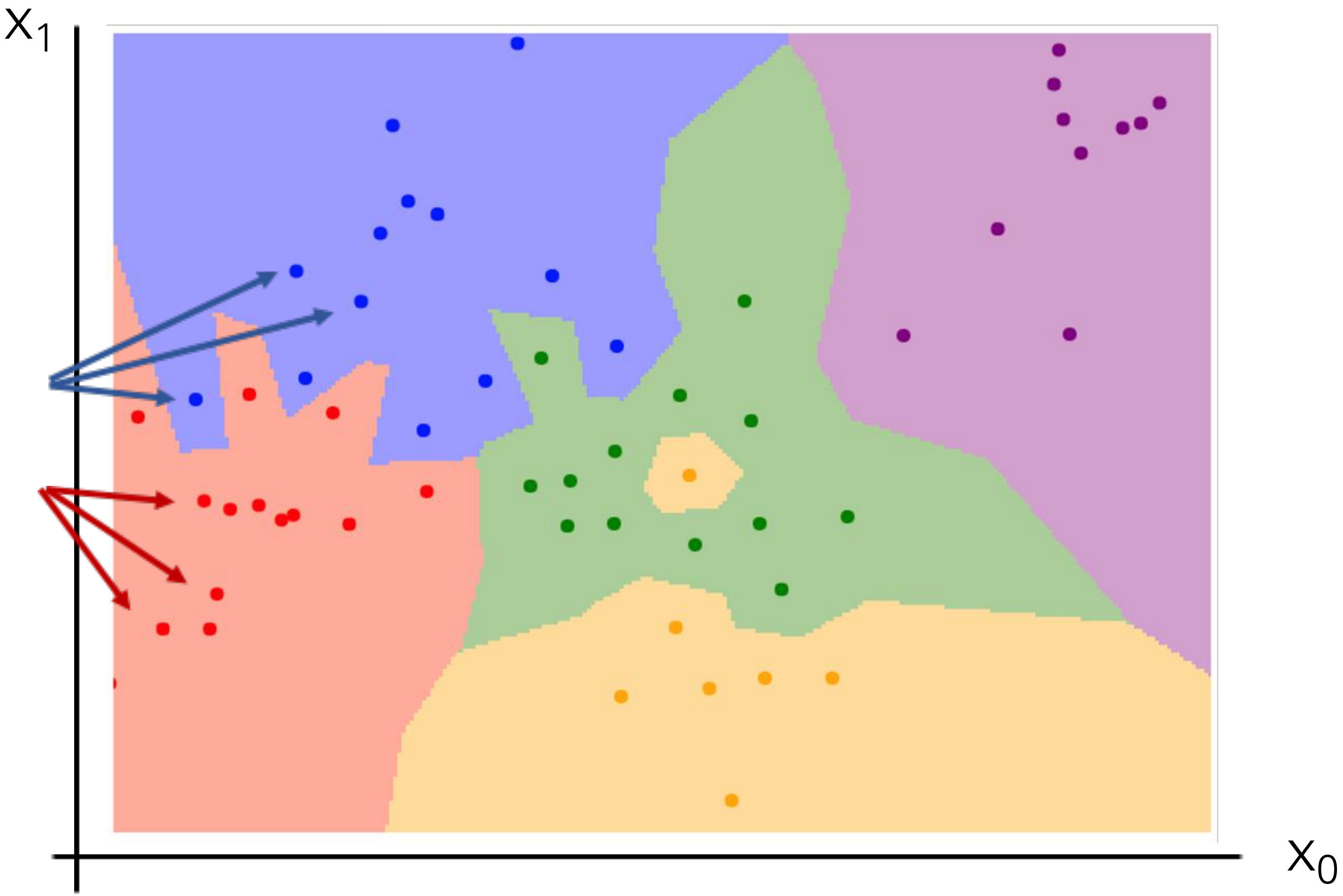
This is **backwards**:

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

Nearest Neighbor Decision Boundaries

Nearest neighbors in two dimensions

Points are training examples; colors give training labels

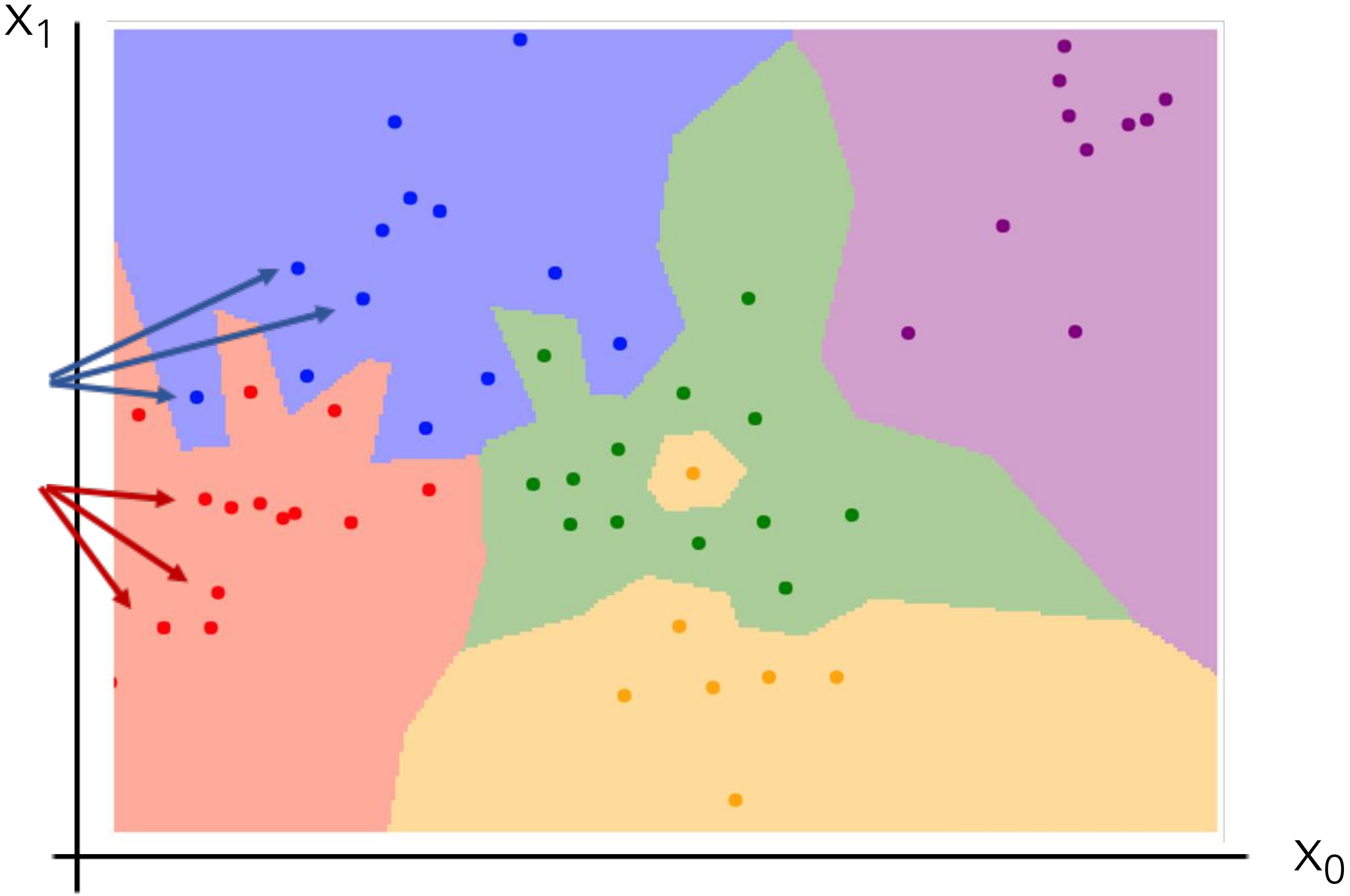


Nearest Neighbor Decision Boundaries

Nearest neighbors in two dimensions

Points are training examples; colors give training labels

Background colors give the category a test point would be assigned



Nearest Neighbor Decision Boundaries

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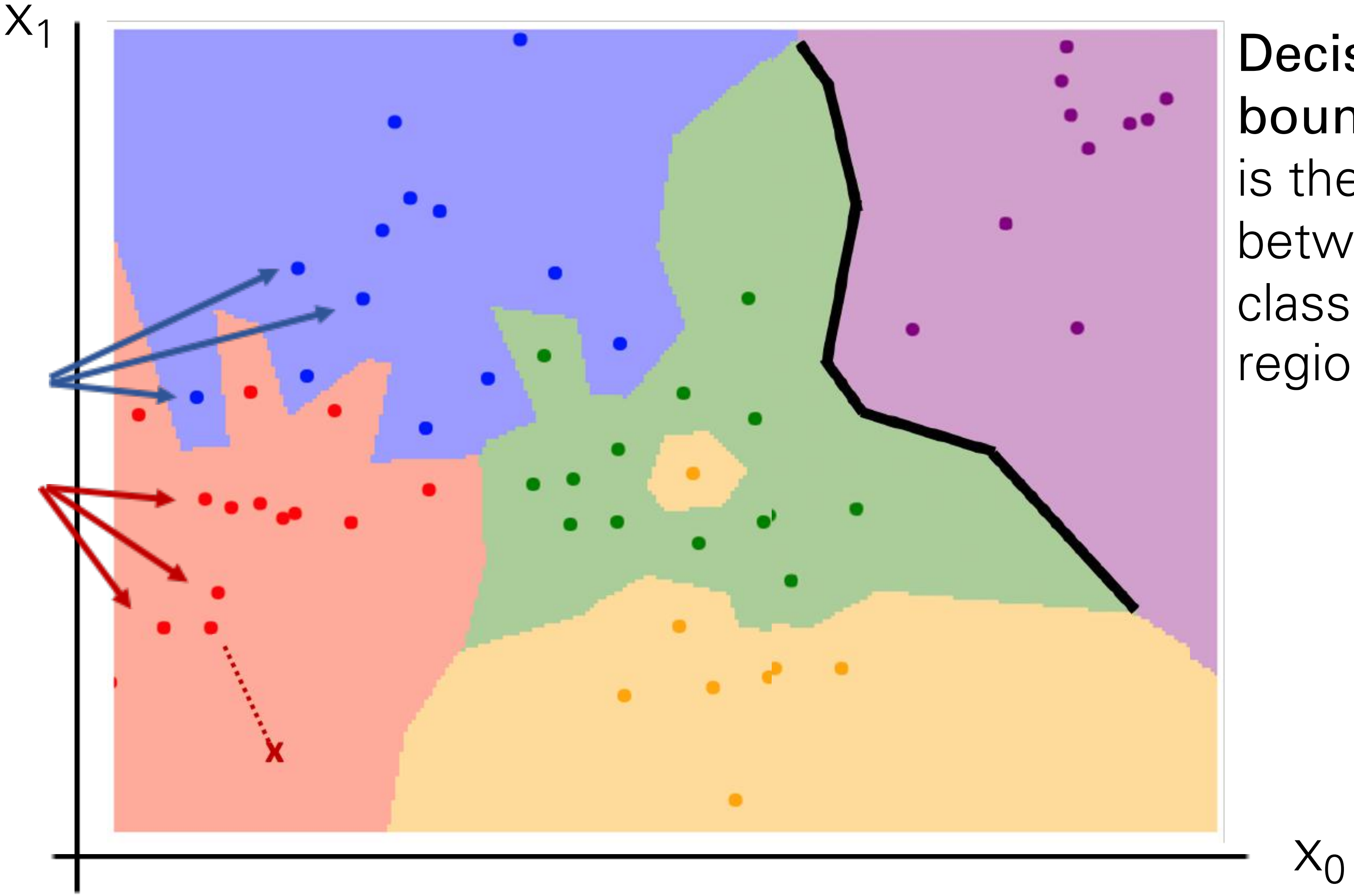
Points are training examples; colors give training labels

Background colors give the category a test point would be assigned



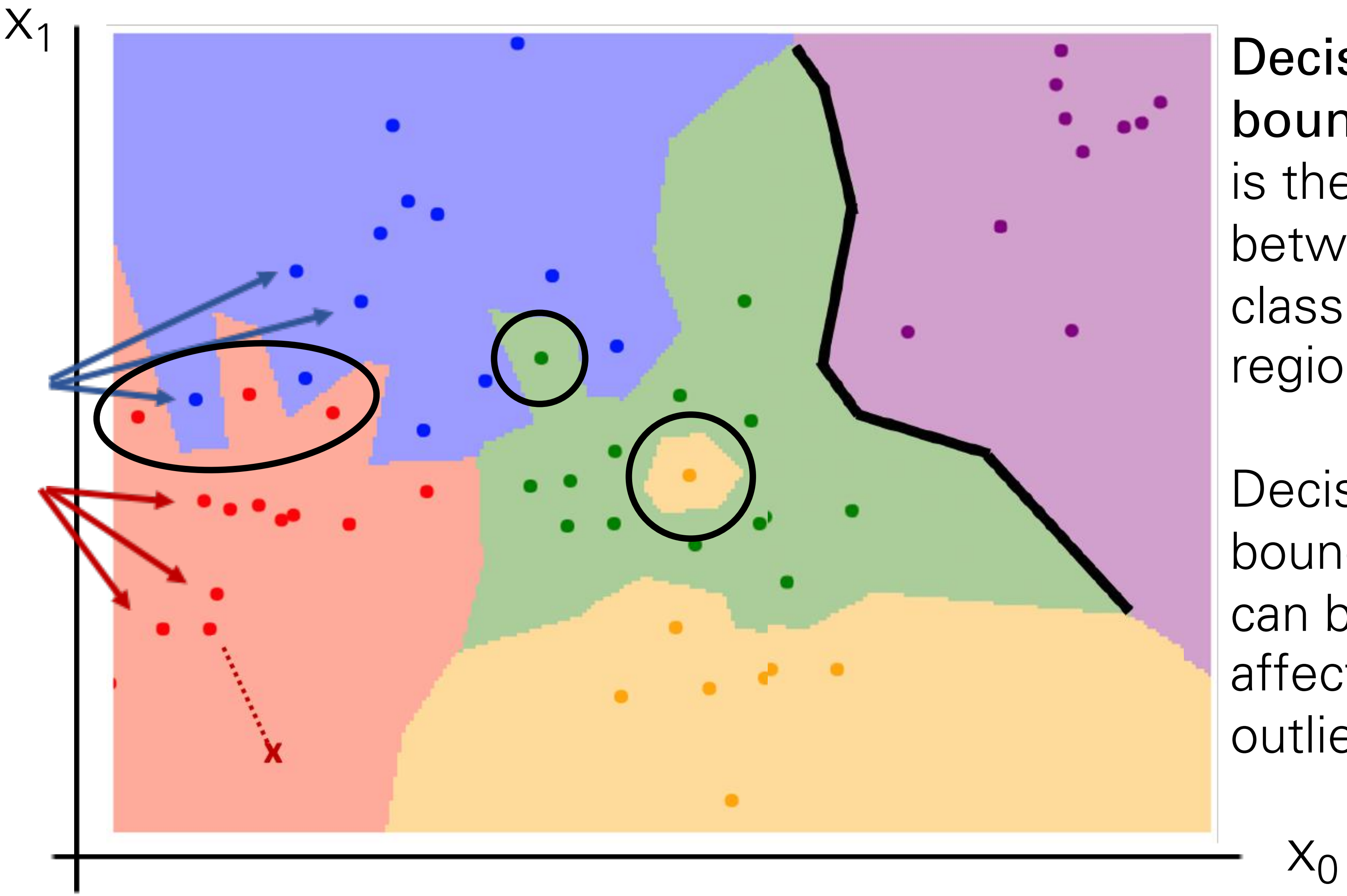
Decision boundary is the boundary between two classification regions

Nearest Neighbor Decision Boundaries

Nearest neighbors in two dimensions

Points are training examples; colors give training labels

Background colors give the category a test point would be assigned



Decision boundary is the boundary between two classification regions

Decision boundaries can be noisy; affected by outliers

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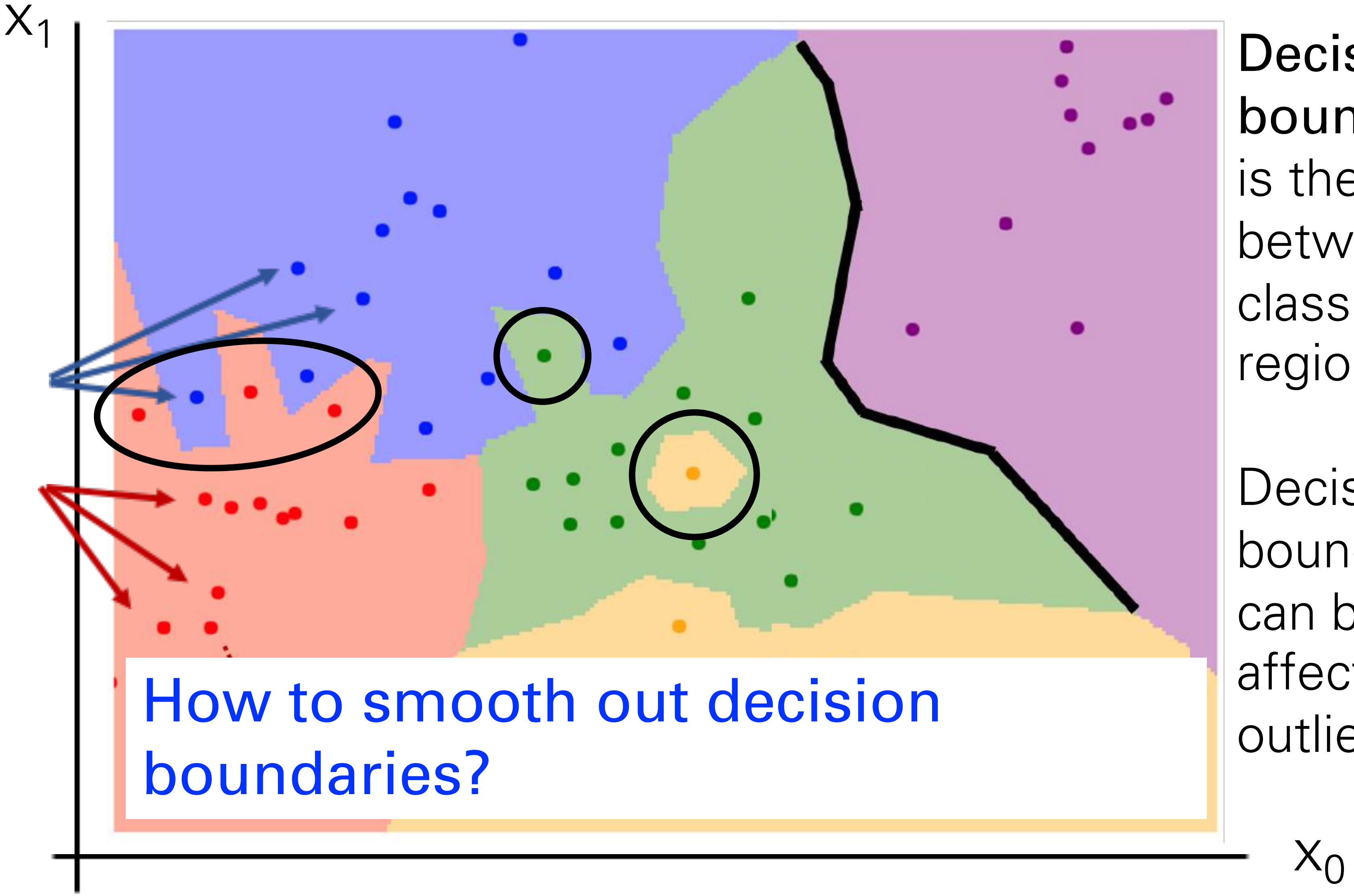

Decision boundary is the boundary between two classification regions

Decision boundaries can be noisy; affected by outliers

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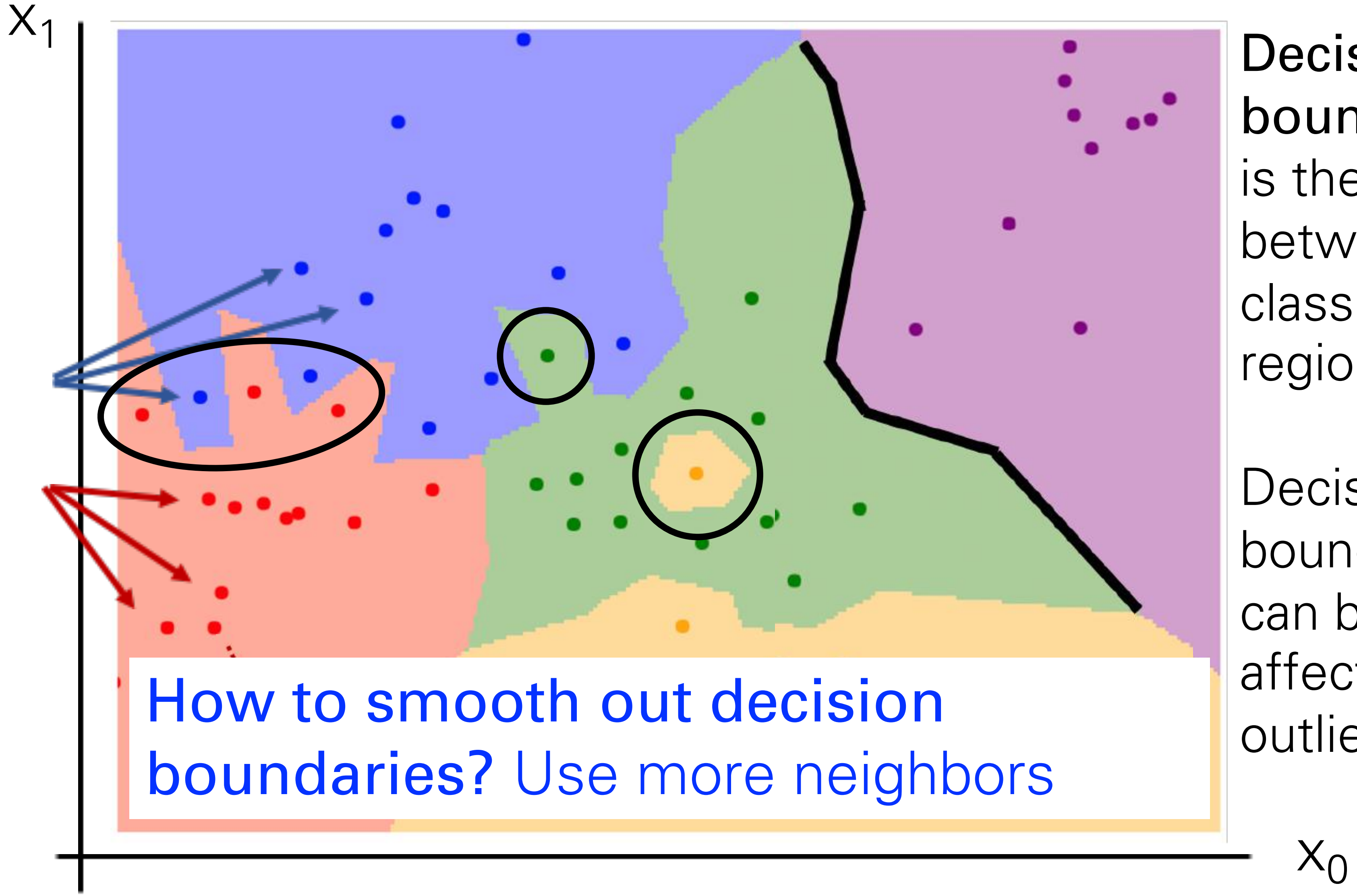


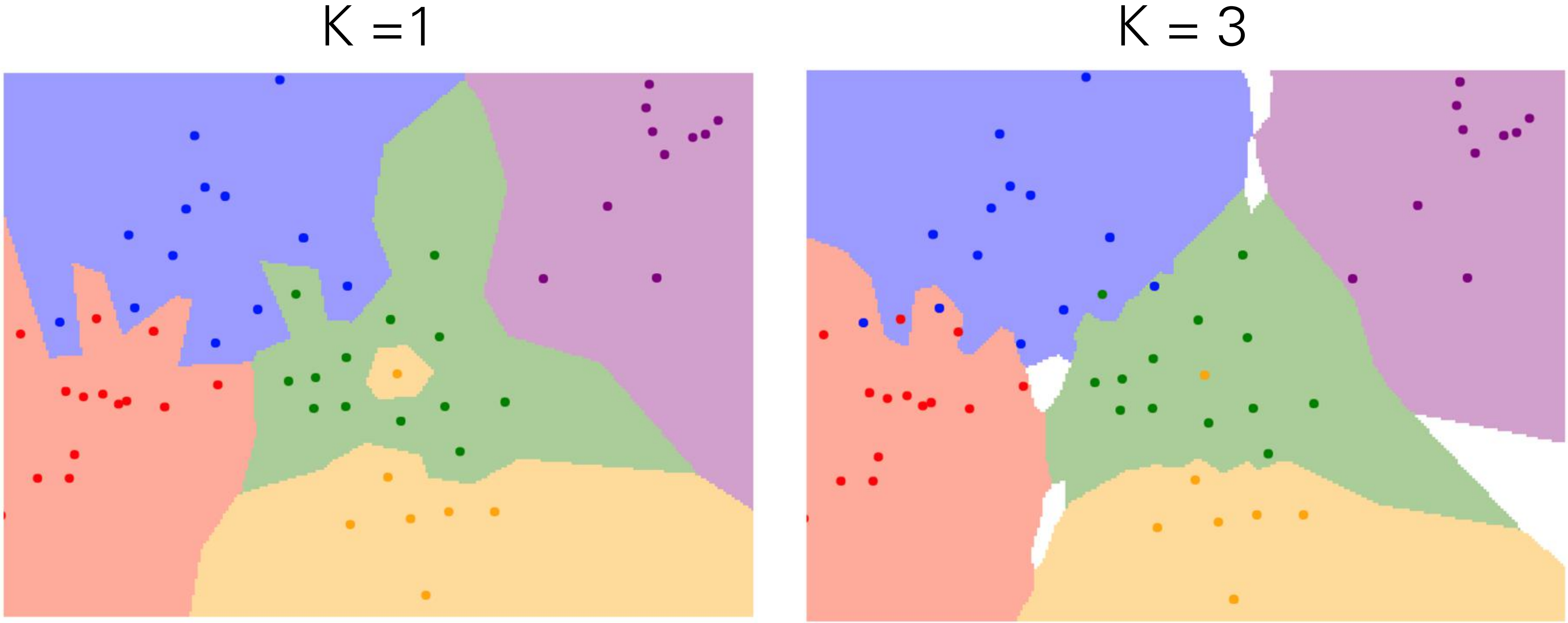
How to smooth out decision boundaries? Use more neighbors

Decision boundary is the boundary between two classification regions

Decision boundaries can be noisy; affected by outliers

K-Nearest Neighbors

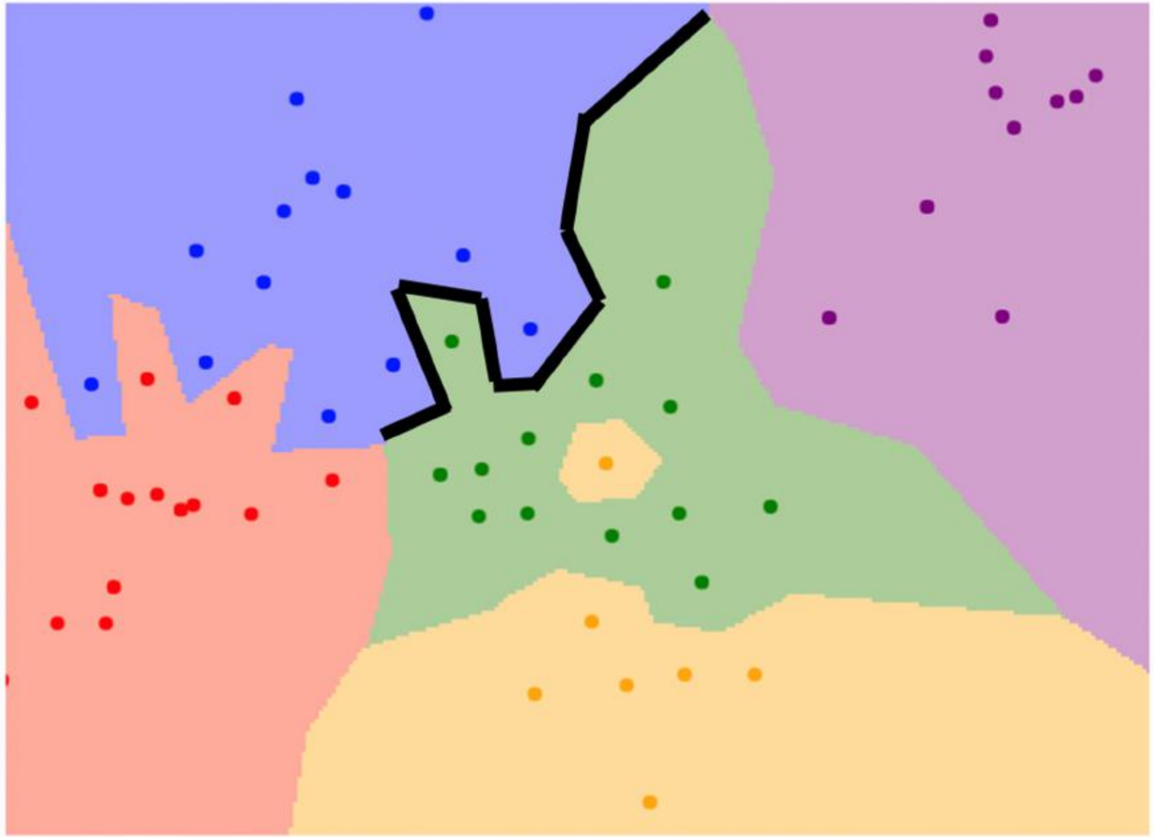
Instead of copying label from nearest neighbor, take **majority vote** from K closest points



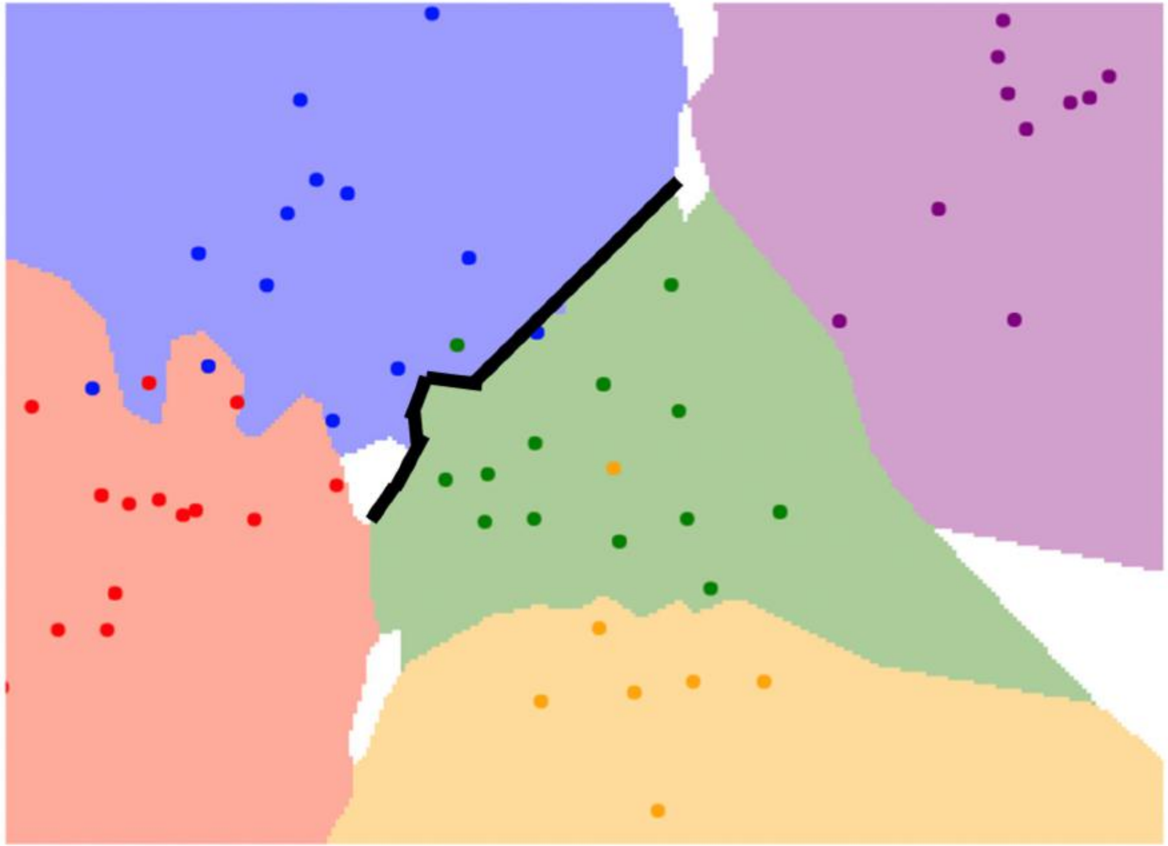
K-Nearest Neighbors

Using more neighbors helps smooth out rough decision boundaries

K =1



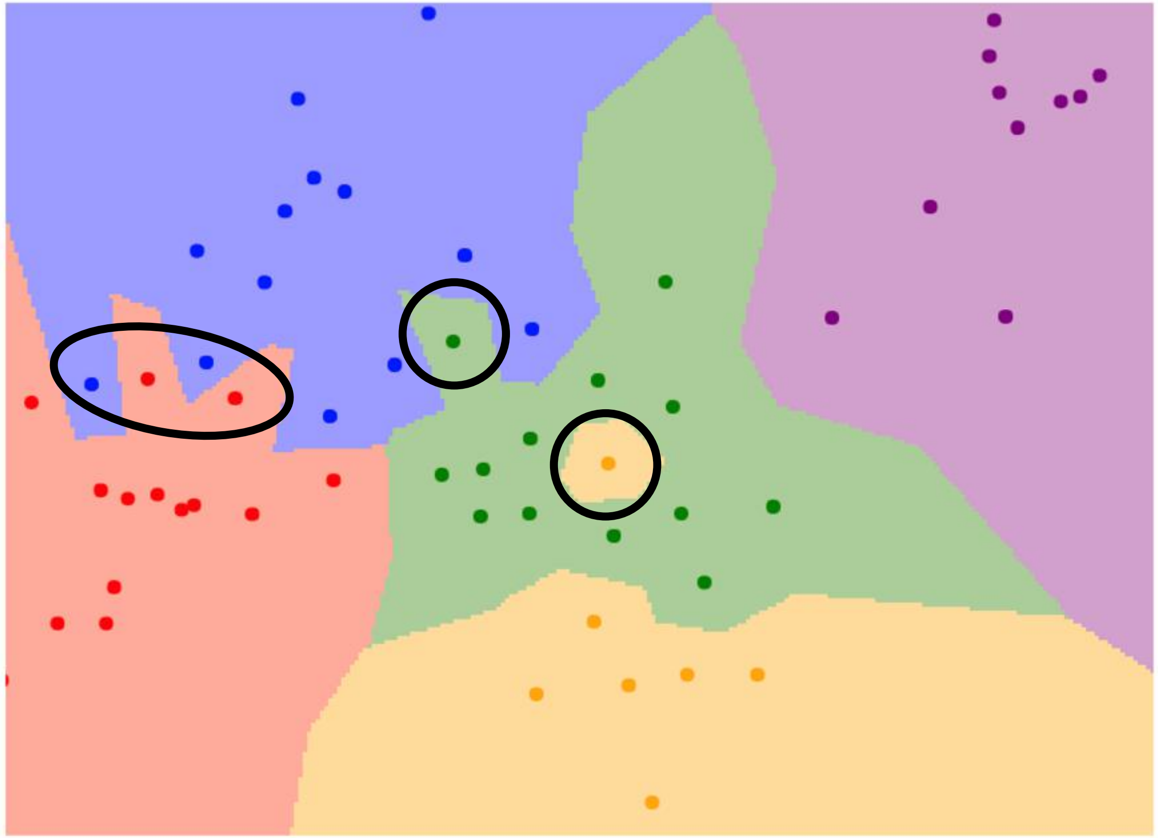
K = 3



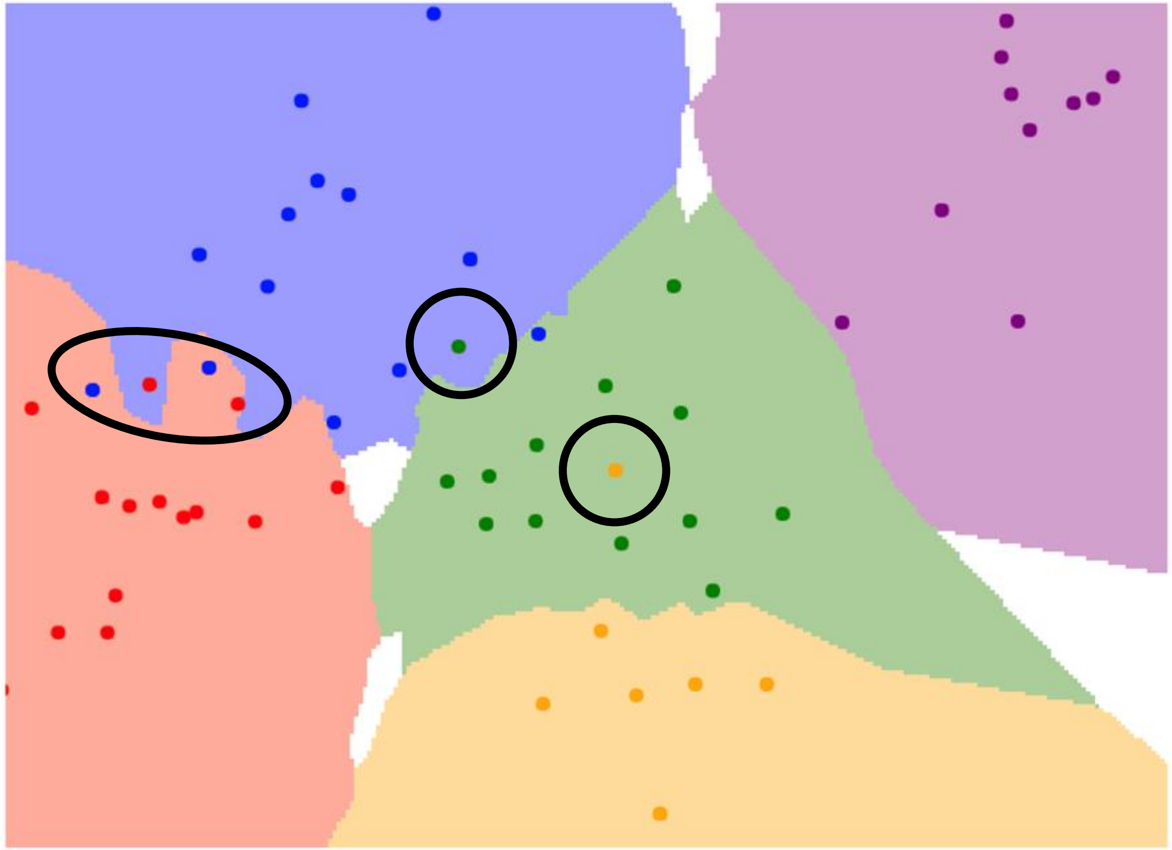
K-Nearest Neighbors

Using more neighbors helps reduce the effect of outliers

K =1



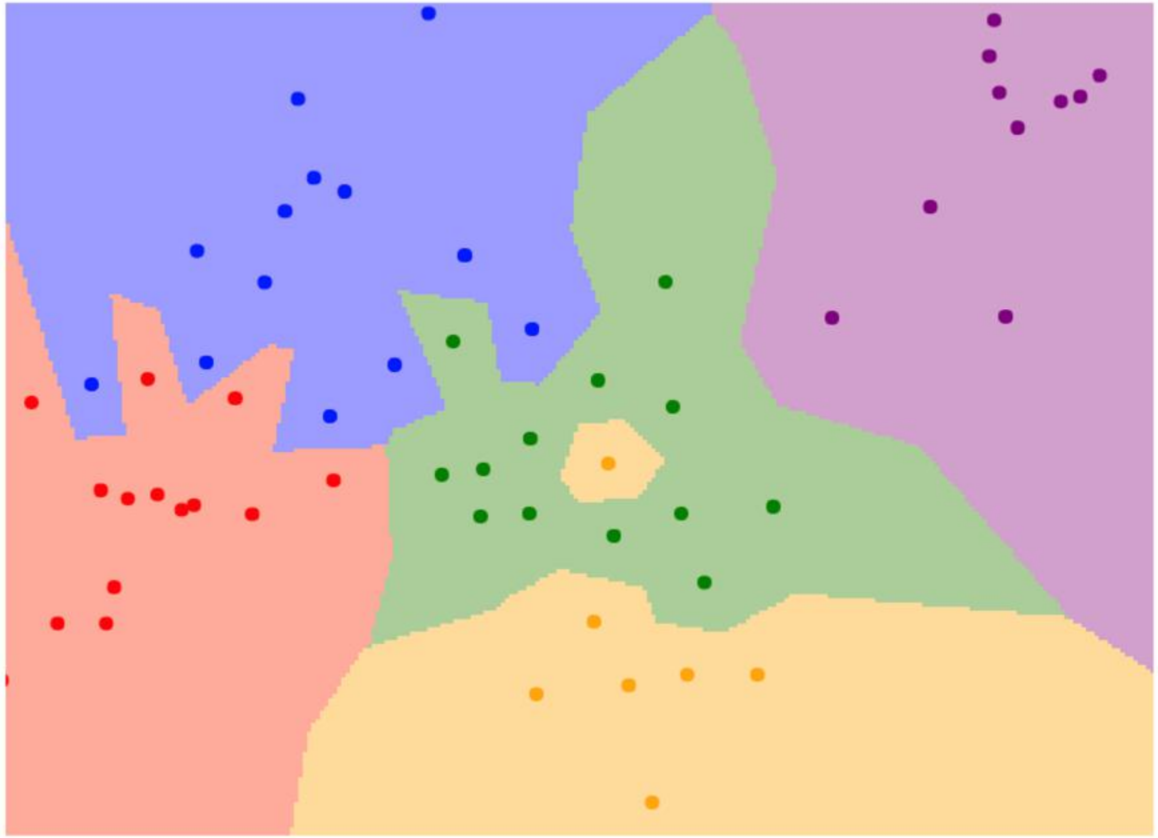
K = 3



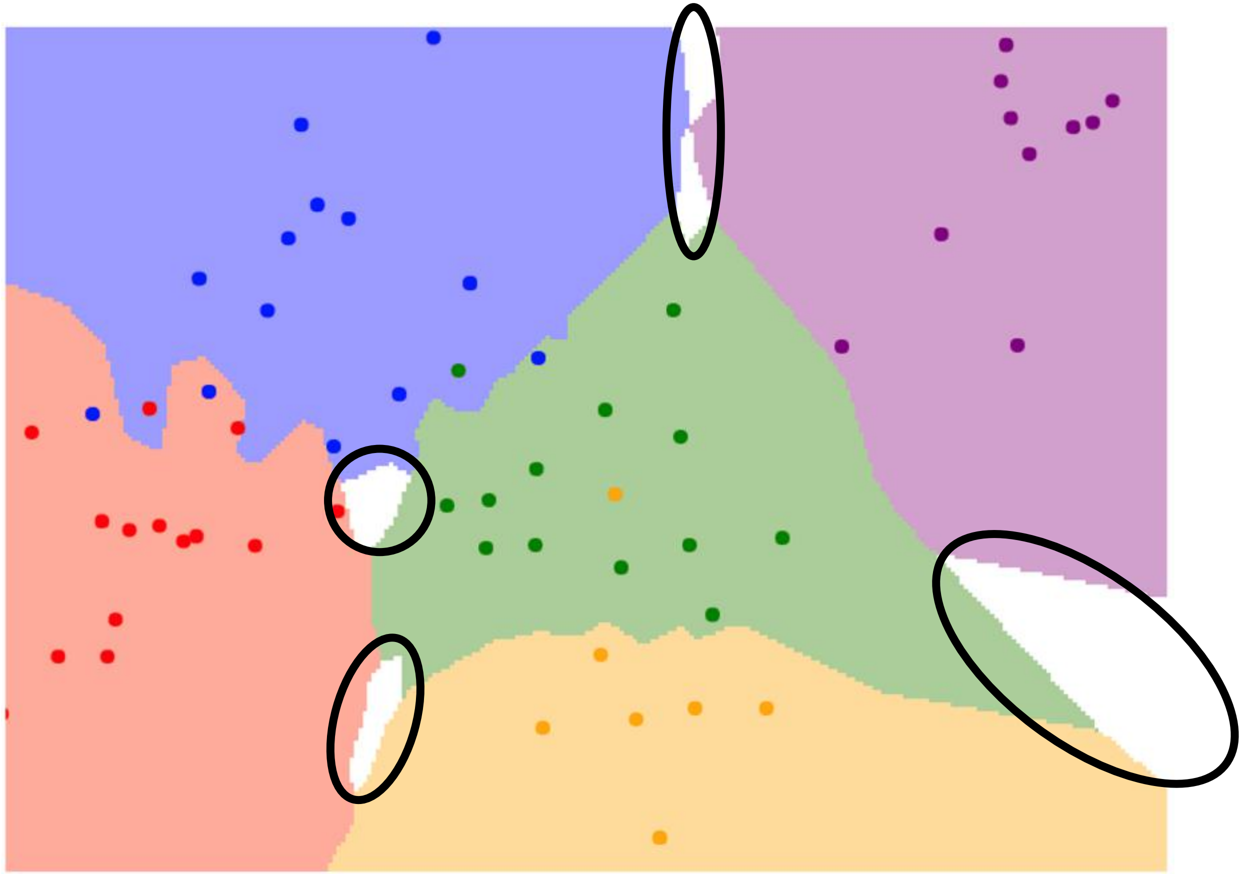
K-Nearest Neighbors

When K > 1 there can be ties between classes. Need to break somehow!

K =1



K = 3



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

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

test image

56	32	10	18
90	23	128	133
24	26	178	200
2	0	255	220

\-

training image

10	20	24	17
8	10	89	100
12	16	178	170
4	32	233	112

=

pixel-wise absolute value differences

46	12	14	1
82	13	39	33
12	10	0	30
2	32	22	108

$\xrightarrow{\text{add}}$ 456

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

L1 (Manhattan) distance

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

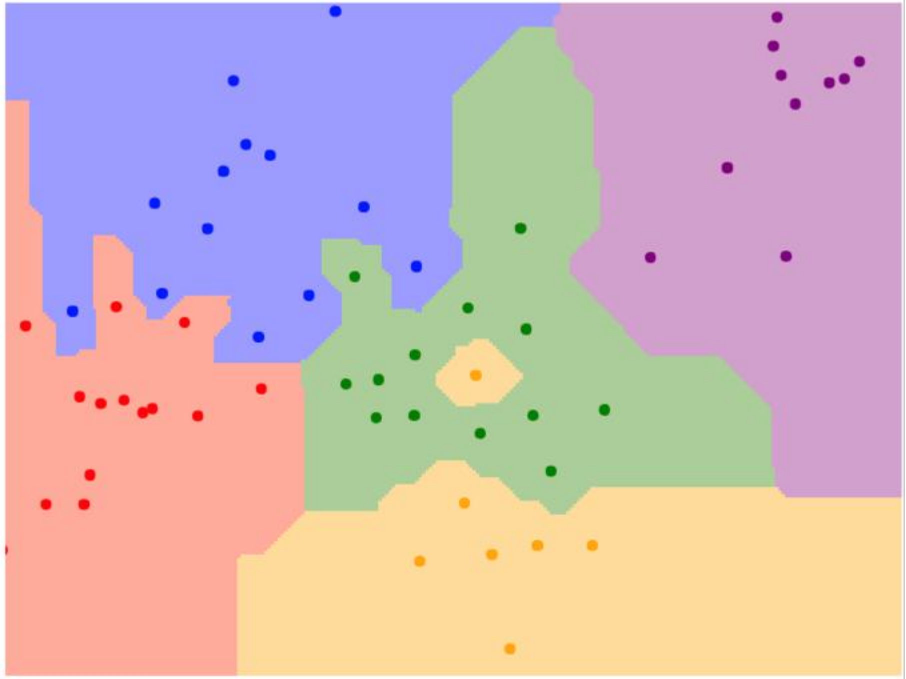
L2 (Euclidean) distance

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

K-Nearest Neighbors: Distance Metric

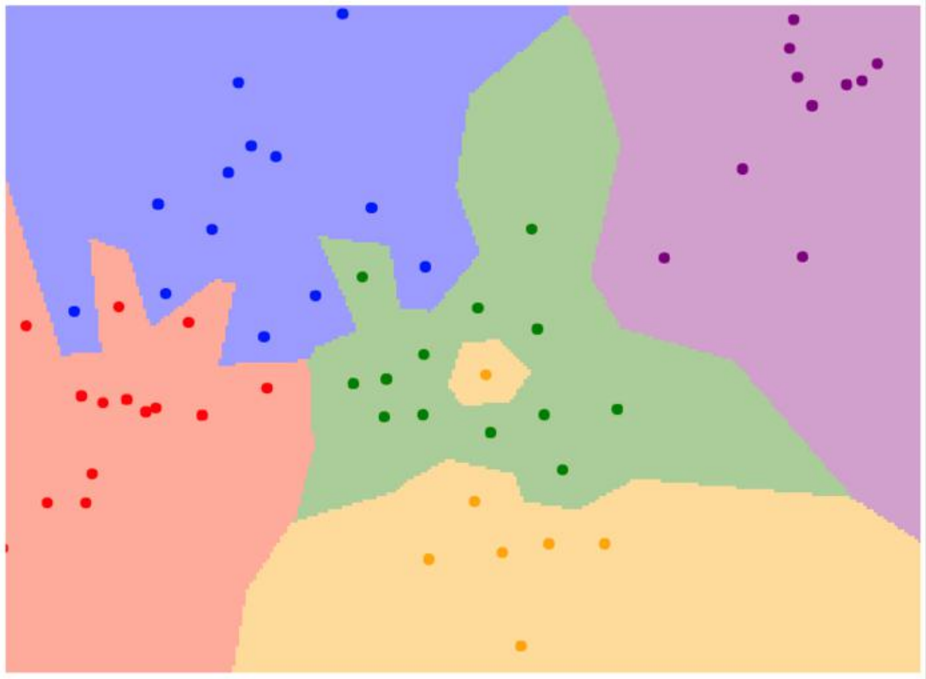
L1 (Manhattan) distance

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



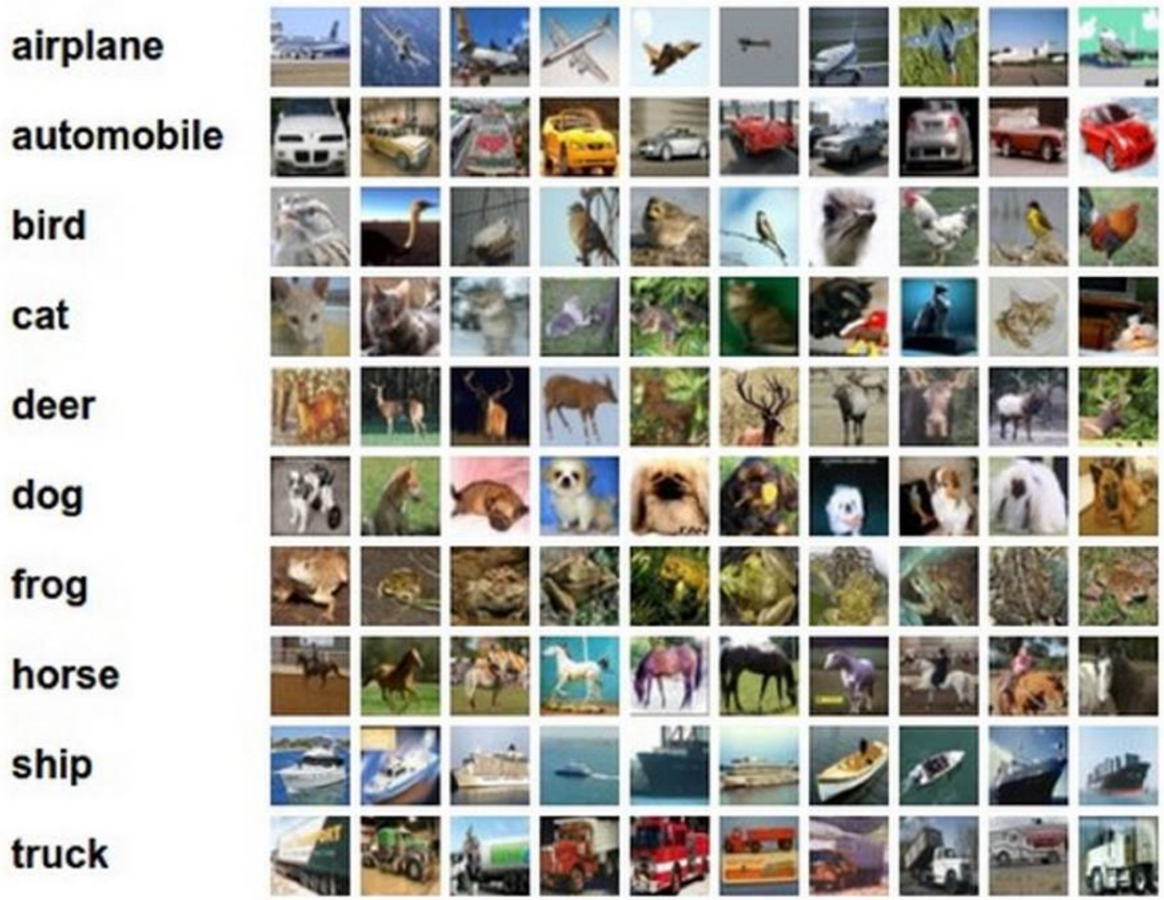
L2 (Euclidean) distance

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

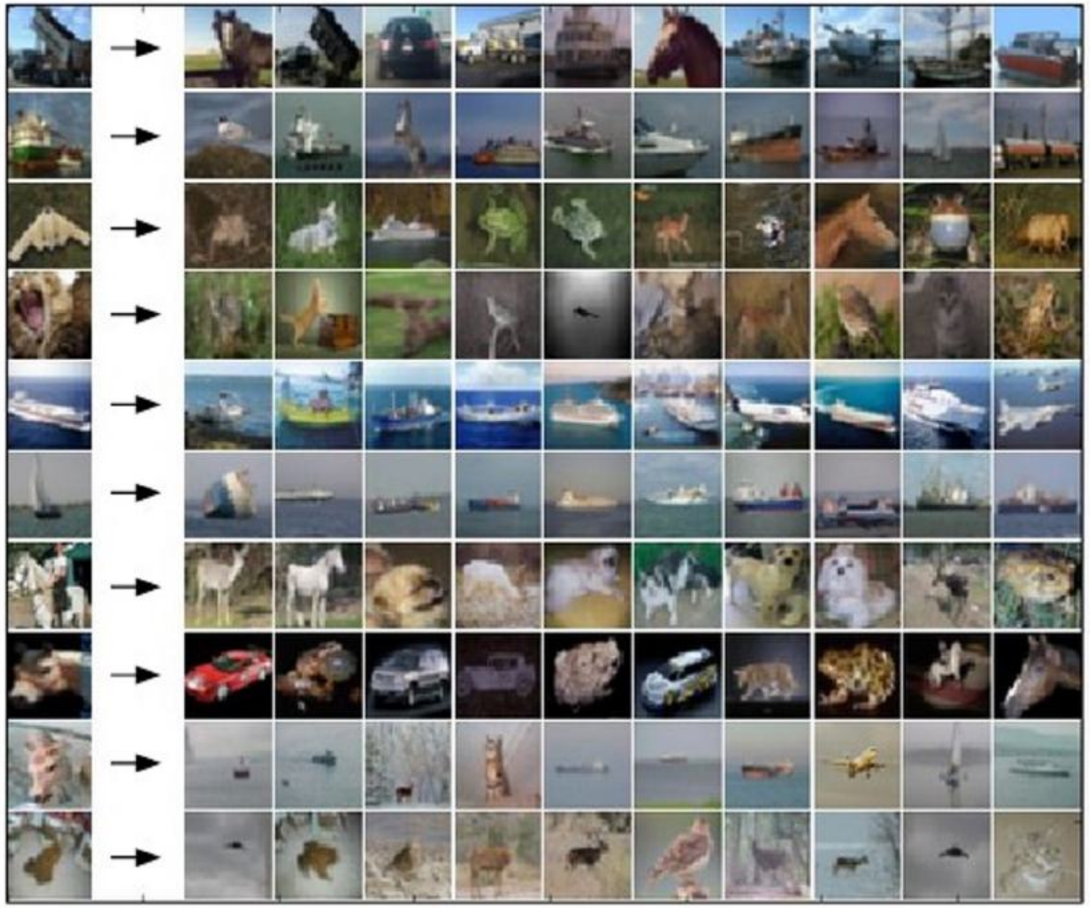


K =1

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



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



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

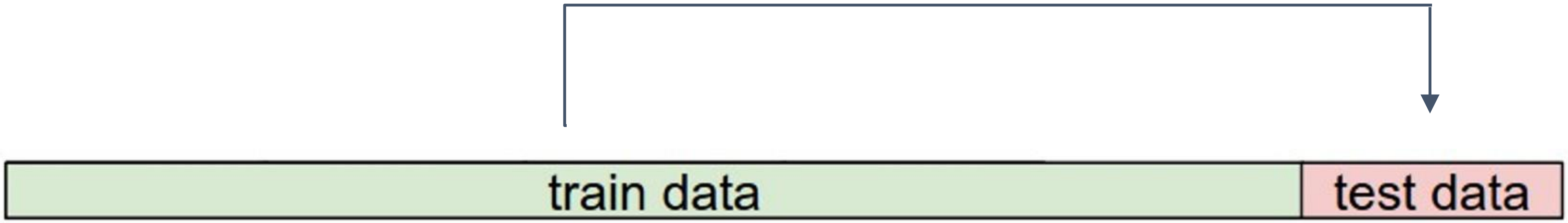
i.e. how do we set the **hyperparameters**?

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.

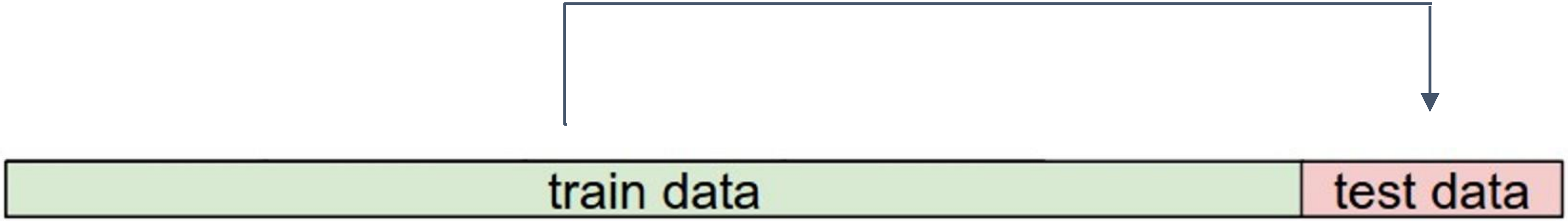
Try out what hyperparameters work best on test set.

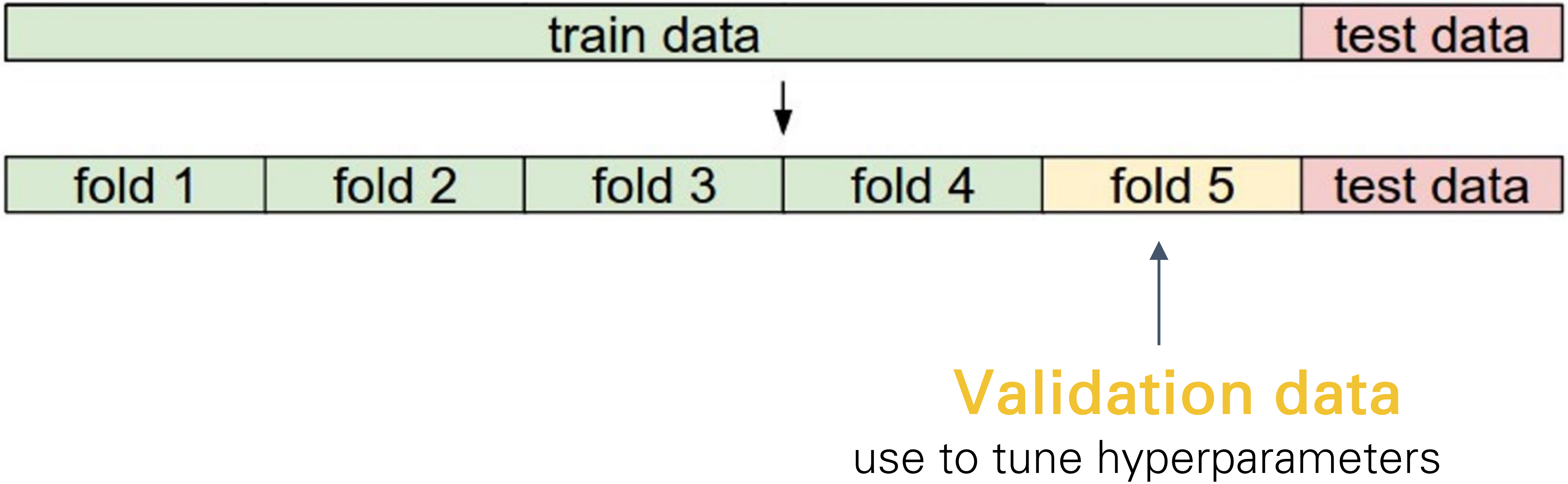


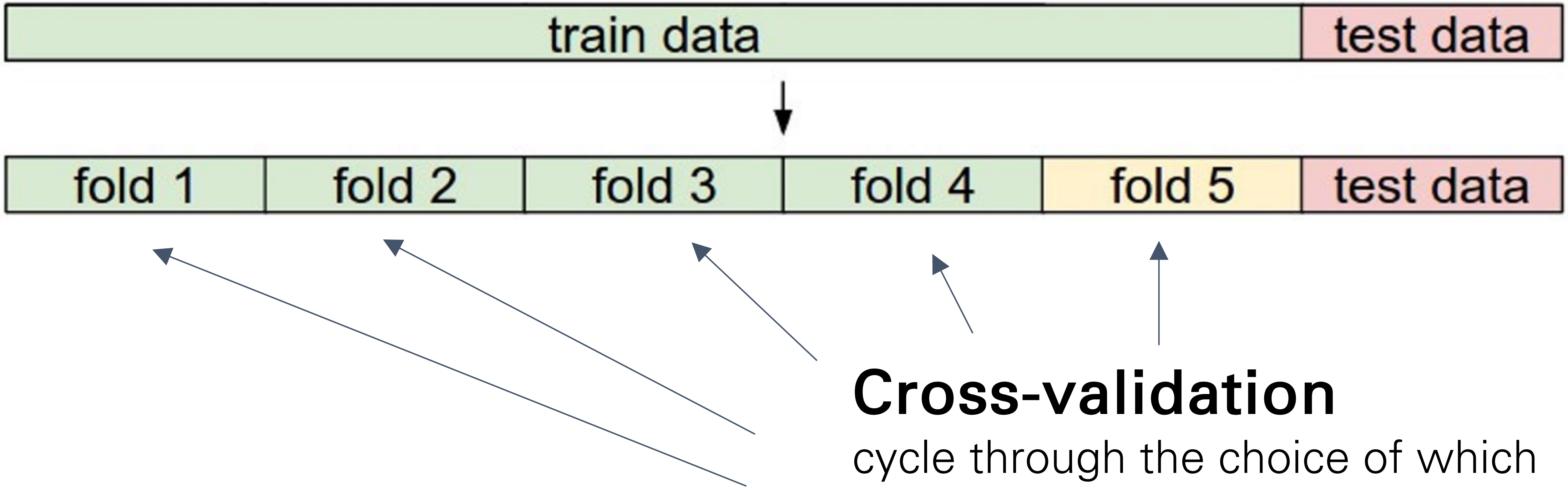
Trying out what hyperparameters work best on test set:

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

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

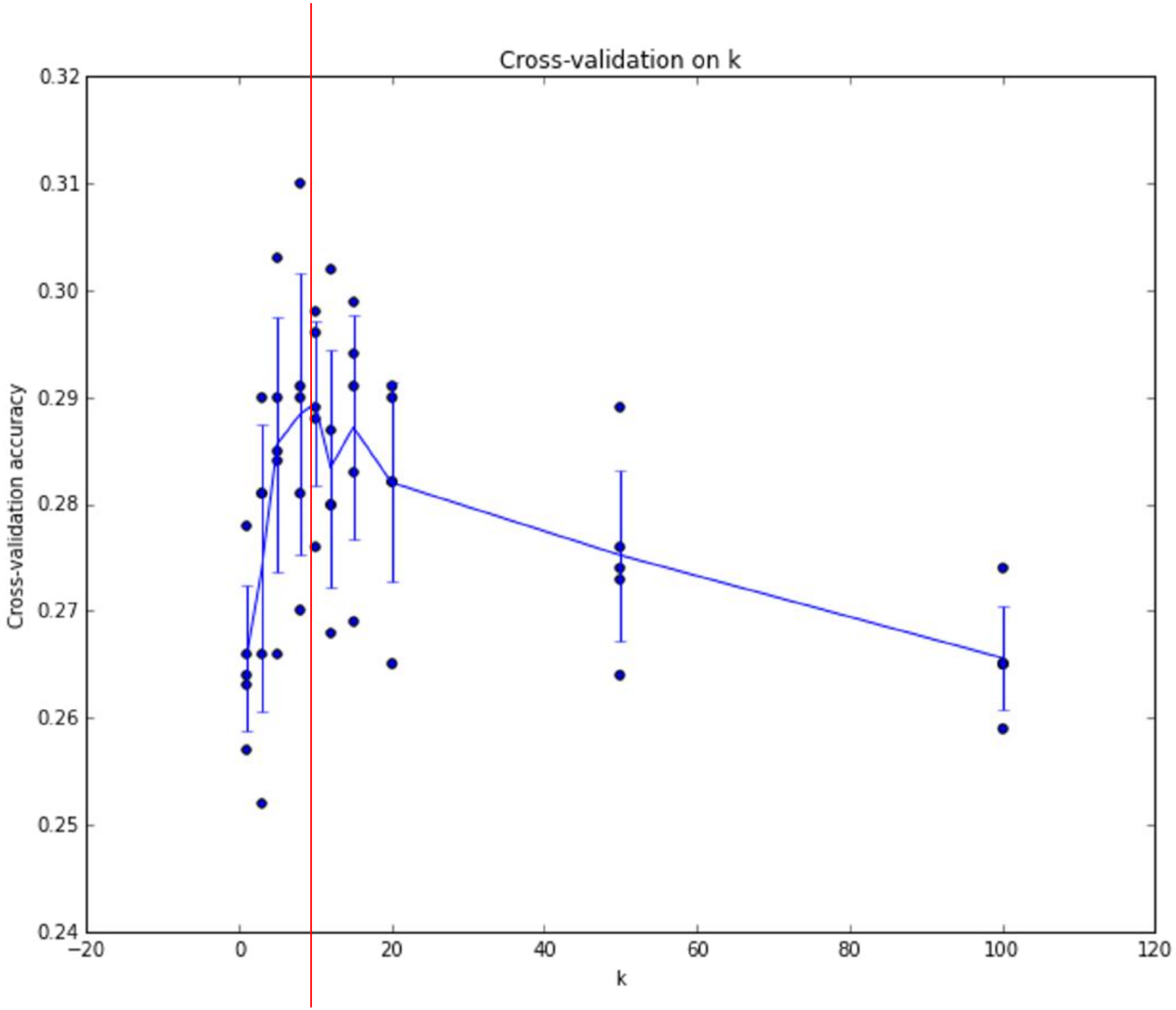



train data
test data
fold 1
fold 2
fold 3
fold 4
fold 5
test data
Validation data
use to tune hyperparameters



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

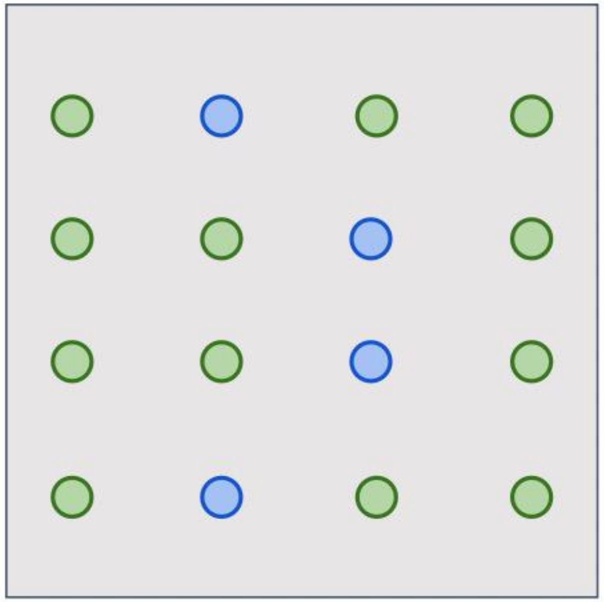
(Seems that k ~= 7 works
the best for this data)

Problem: Curse of Dimensionality

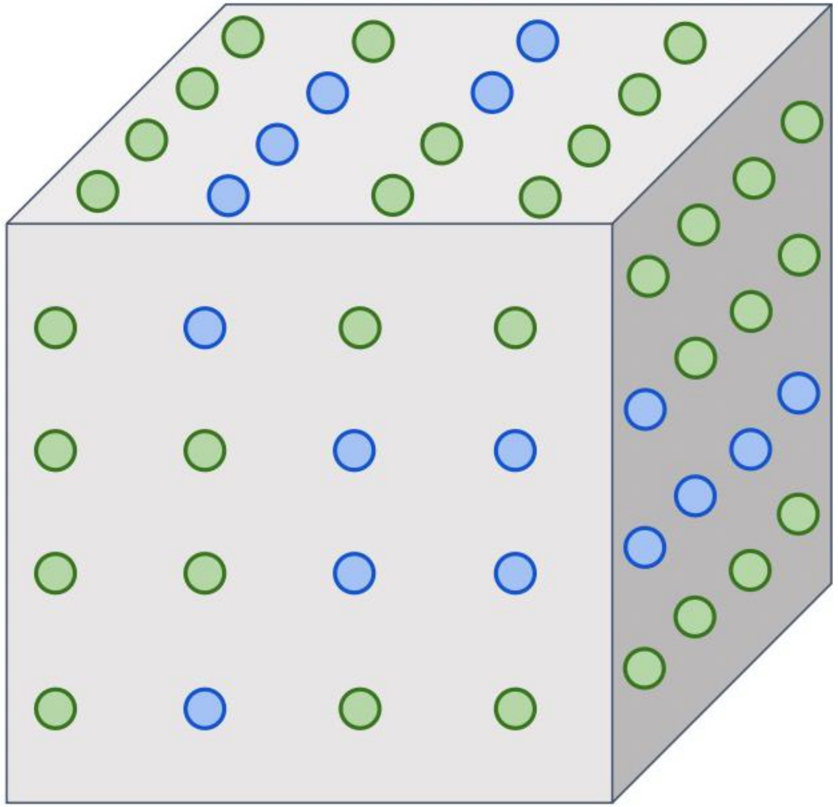
- **Curse of dimensionality:** For uniform coverage of space, number of training points needed grows exponentially with dimension

Dimensions = 1
Points = 4

Dimensions = 3
Points = 4^2



Dimensions = 3
Points = 4^3



Problem: Curse of Dimensionality

- **Curse of dimensionality:** For uniform coverage of space, number of training points needed grows exponentially with dimension

Number of possible
32x32 binary images:

$$2^{32x32} \approx 10^{308}$$

Problem: Curse of Dimensionality

- **Curse of dimensionality:** For uniform coverage of space, number of training points needed grows exponentially with dimension

Number of possible 32x32 binary images:

$$2^{32\text{x}32} \approx 10^{308}$$

Number of elementary particles in the visible universe: (source)

$$\approx 10^{97}$$

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

- Very slow at test time
- Distance metrics on pixels are not informative

Original

Boxed

Shifted

Tinted

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

Nearest Neighbor with ConvNet features works well

Devlin et al, "Exploring Nearest Neighbor Approaches for Image Captioning", 2015

Nearest Neighbor with ConvNet features works well

Example: Image Captioning with Nearest Neighbor

A bedroom with a bed and a couch.

A cat sitting in a bathroom sink.

A train is stopped at a train station.

A wooden bench in front of a building.

Devlin et al, “Exploring Nearest Neighbor Approaches for Image Captioning”, 2015

The learning problem

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

The Learning Problem

Digit Recognition

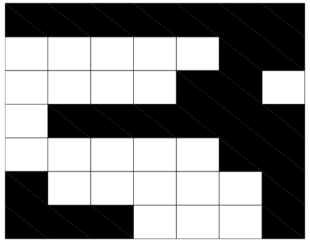


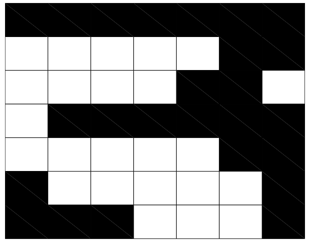
Image Classification

- 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**"

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

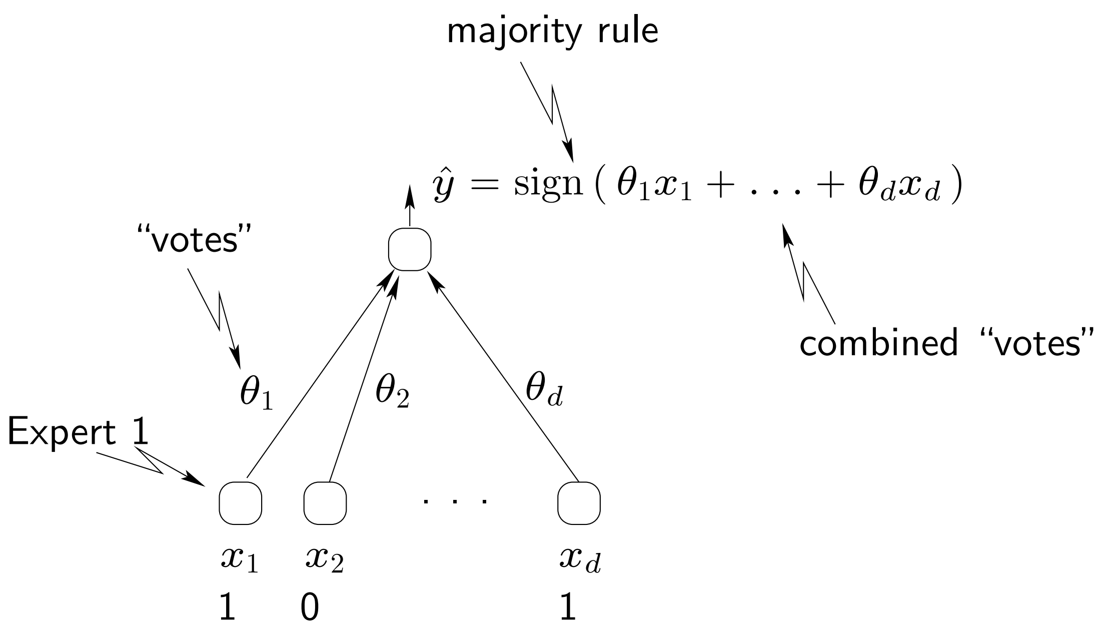
where θ is a vector of **parameters** we have to learn from examples.

Linear classifier/experts

- We can understand the simple linear classifier

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

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



Estimation

$\mathbf{x}$	y
0111111001110010000000100000001001111110111011111001110111110001	+1
0001111100000011000001110000011001111110111111001111111100000011	+1
1111111000000110000011000111111000000111100000111110001101111111	−1
$\cdots$	$\cdots$

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

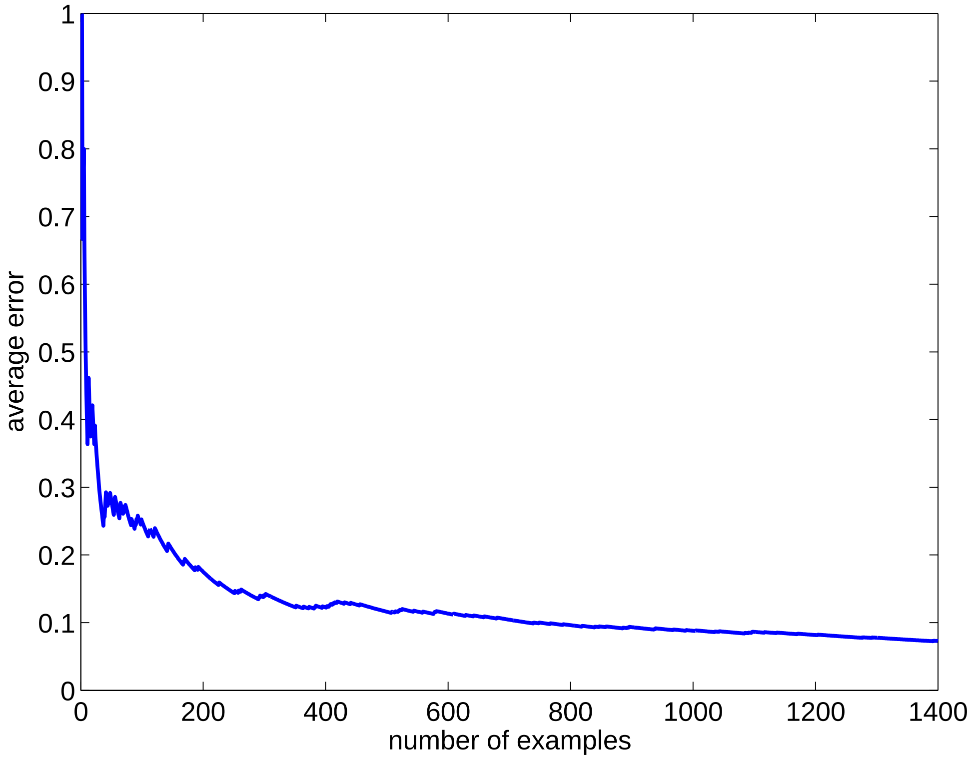
$$\hat{y} = \text{sign}\left(\, \theta \cdot \mathbf{x} \,\right)$$

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

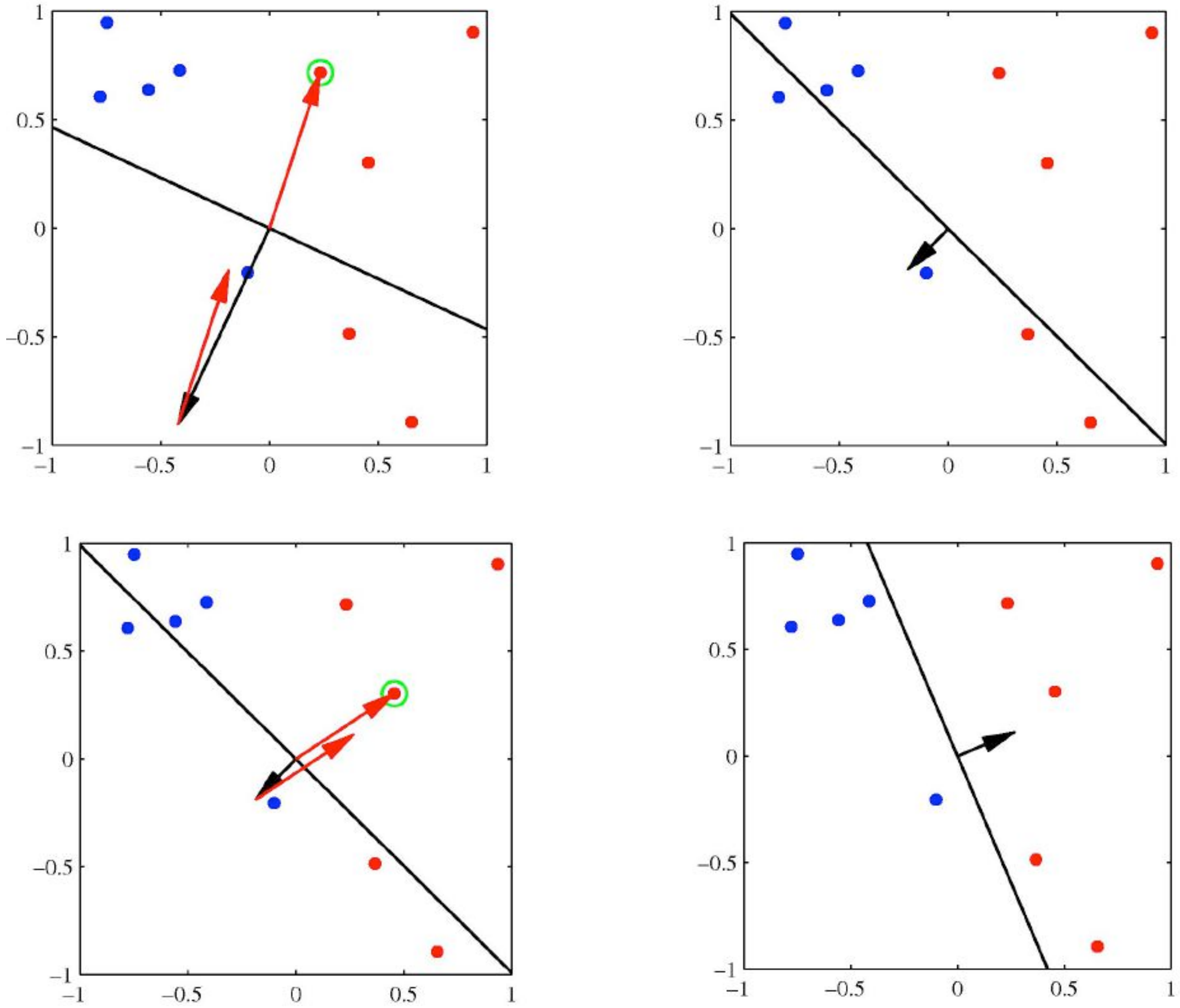
- Does the simple mistake driven algorithm work?



(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



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

$$\boxed{f(x, W)} = \boxed{W}\boxed{x}$$

3072x1

10x1

10x3072

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

10 numbers, indicating class scores

parameters, or "weights"

Linear classifier: image classification

$$\boxed{f(x, W)} = \boxed{W}\boxed{x}$$

10x1 | 10x3072 | 3072x1

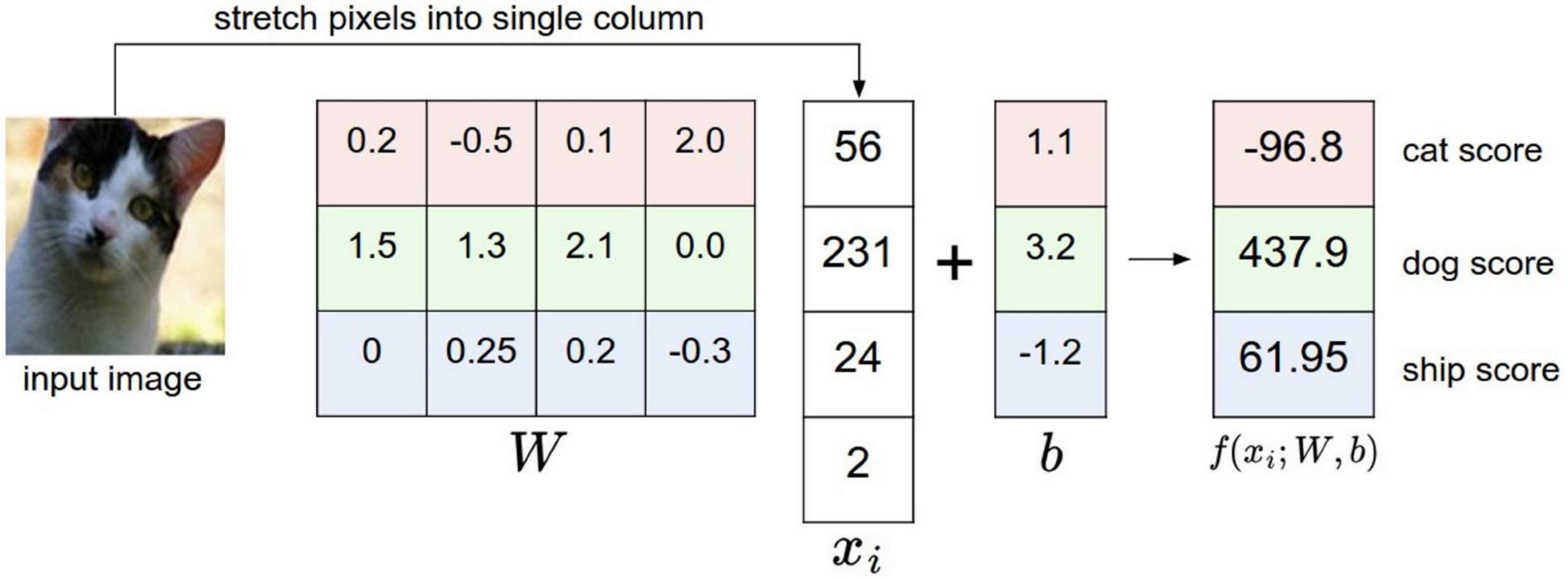
(+b) 10x1

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

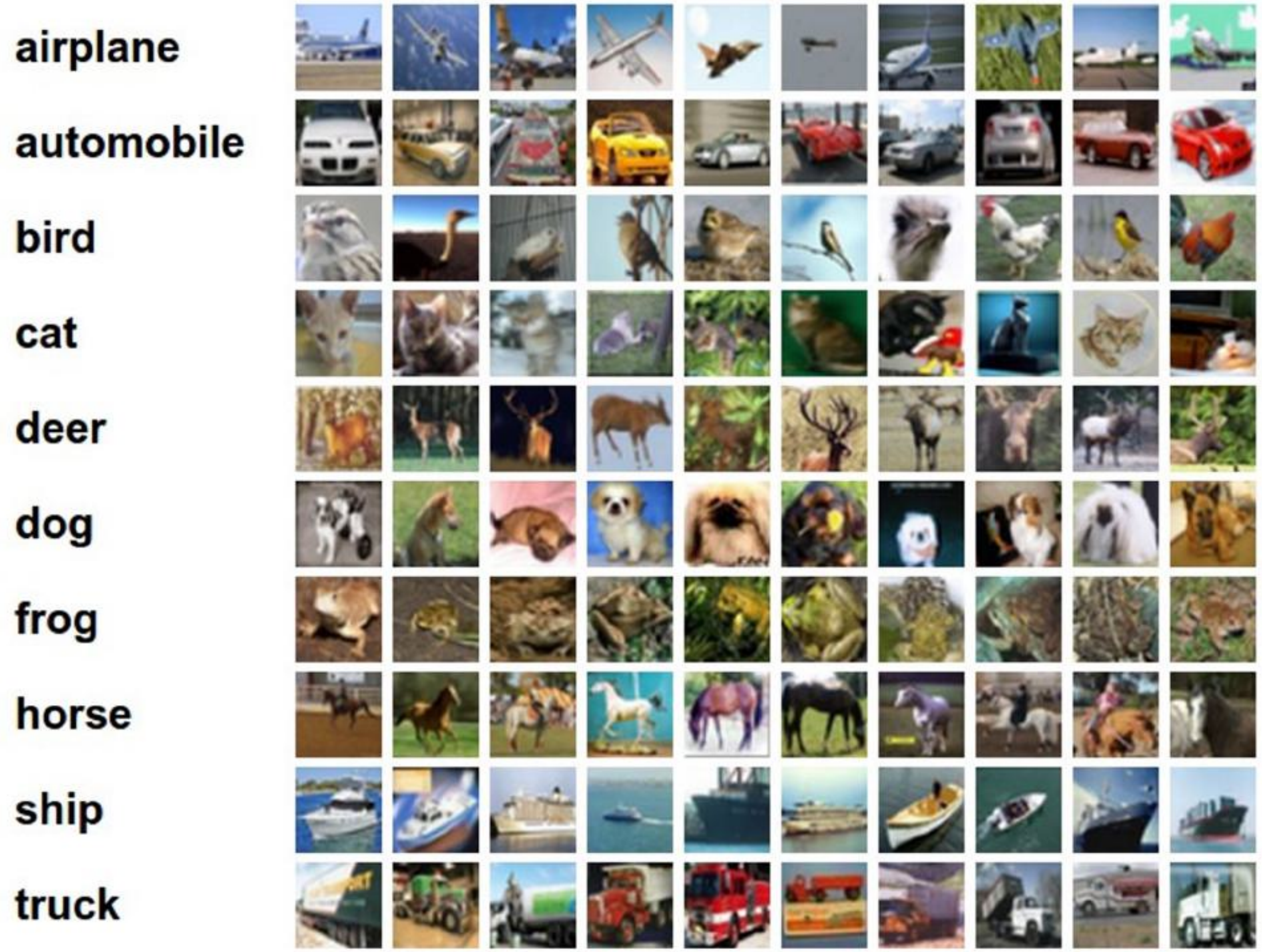
10 numbers, indicating class scores

parameters, or "weights"

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



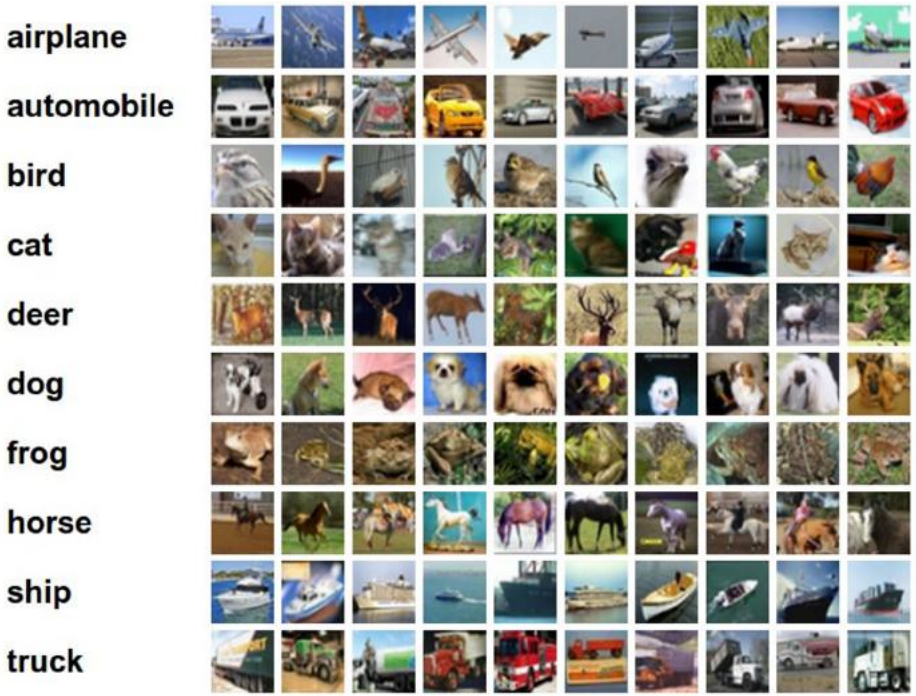
Interpreting a Linear Classifier



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

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

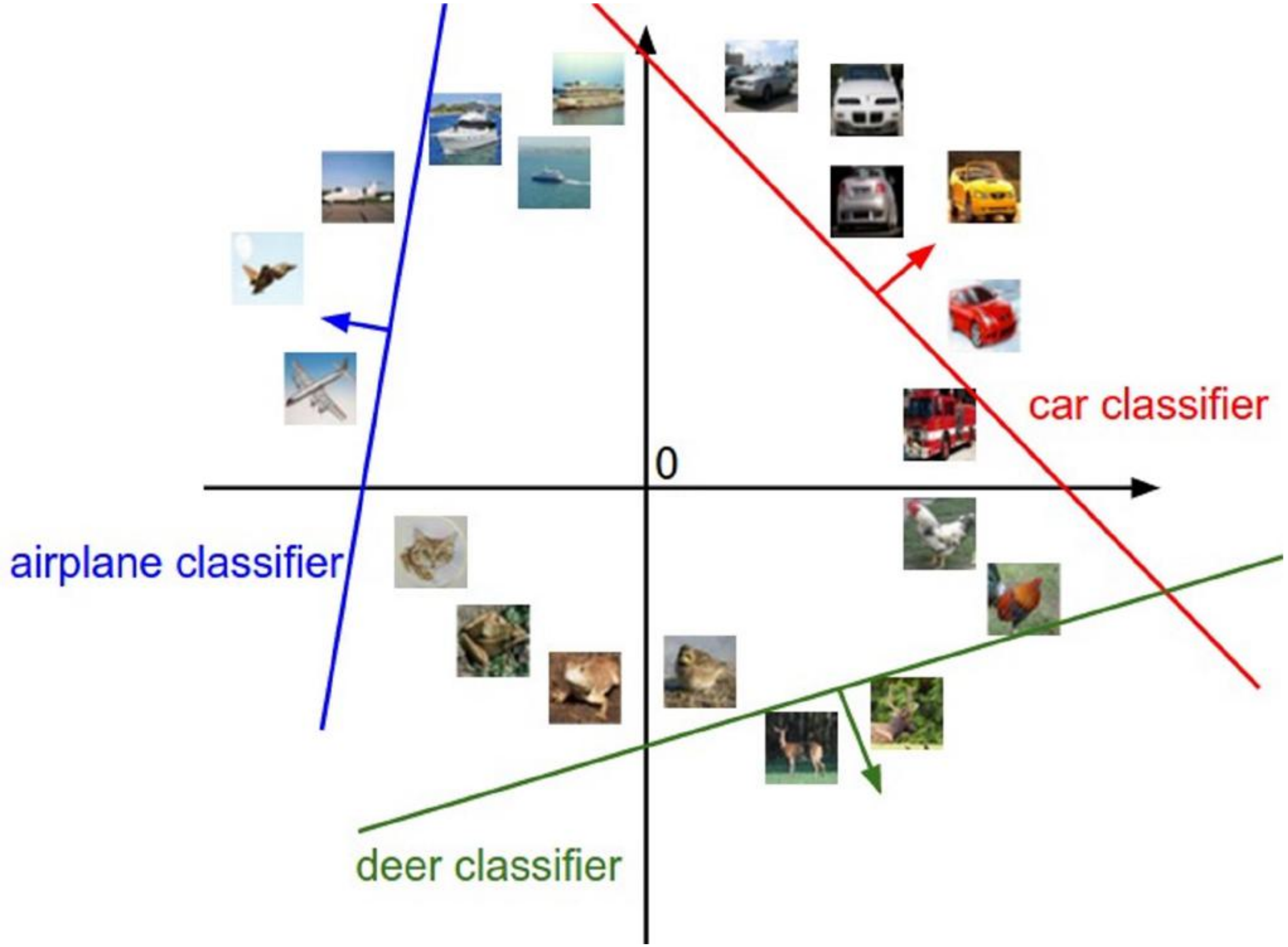
Interpreting a Linear Classifier



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

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

Interpreting a Linear Classifier

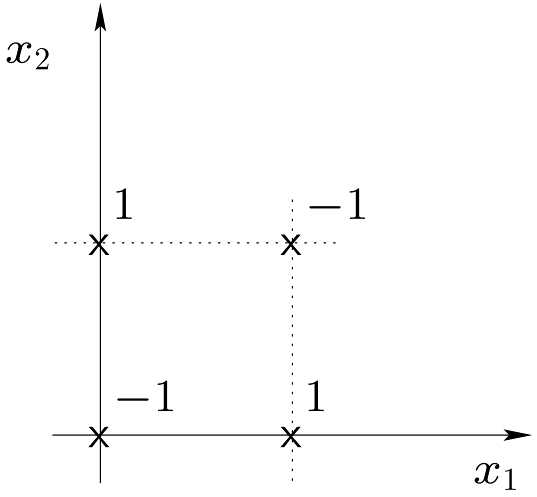


$$f(x_i, W, b) = Wx_i + b$$

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

Model selection

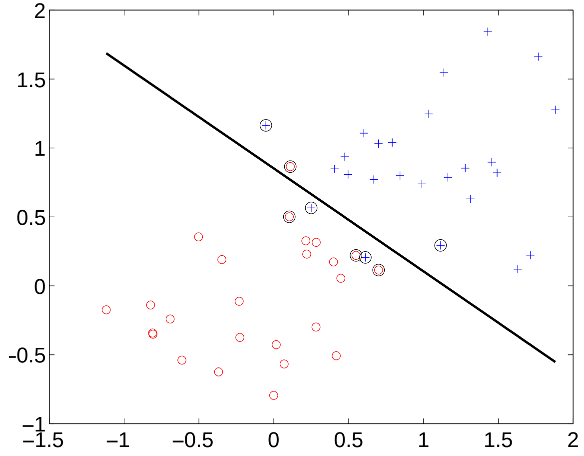
- The simple linear classifier cannot solve all the problems (e.g., XOR)



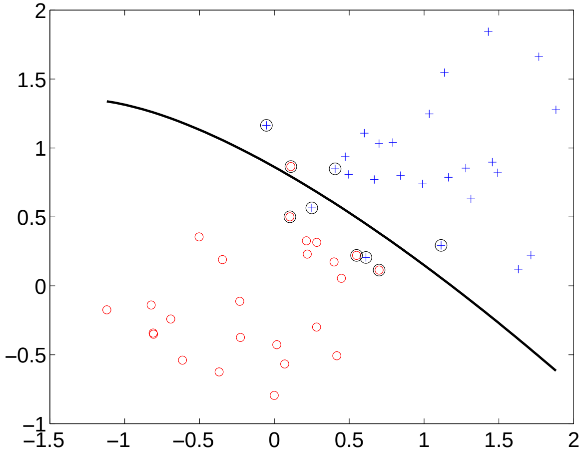
- Can we rethink the approach to do even better?
- We can, for example, add "polynomial experts"

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

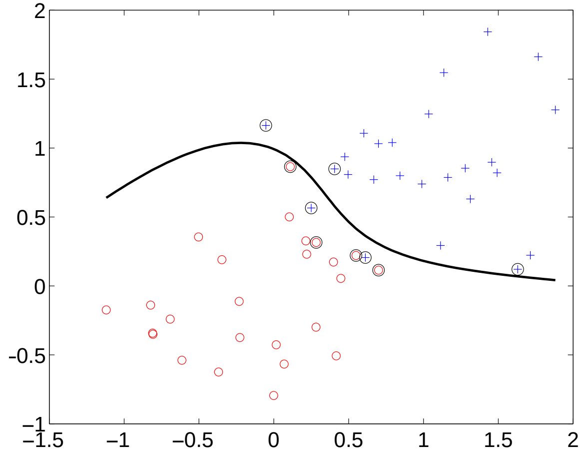
Model selection (cont'd)



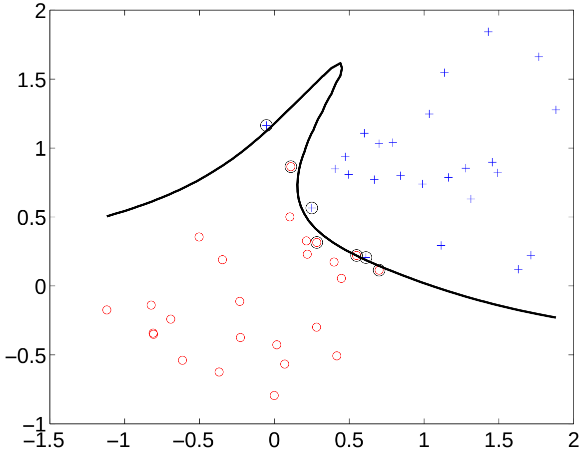
linear



2^{nd} order polynomial



4^{th} order polynomial



8^{th} 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):

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

  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:

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

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car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9		

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the SVM loss has the form:

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

= 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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Losses:	2.9	0	

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the SVM loss has the form:

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

= 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

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:

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

= 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
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:

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

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

Suspose: 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	

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

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)

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

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

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

—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

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

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

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

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

- 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

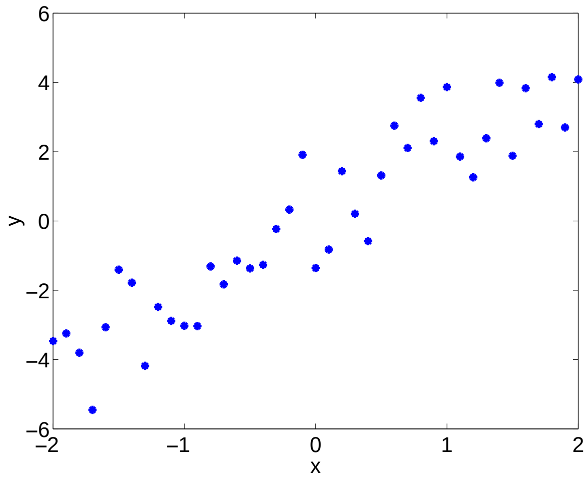
Regression

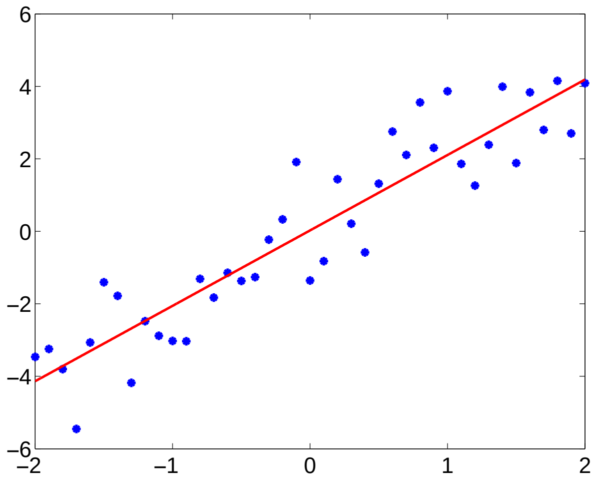
- The goal is to make quantitative (real valued) predictions on the basis of a (vector of) features or attributes
- Example: predicting vehicle fuel efficiency (mpg) from 8 attributes

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





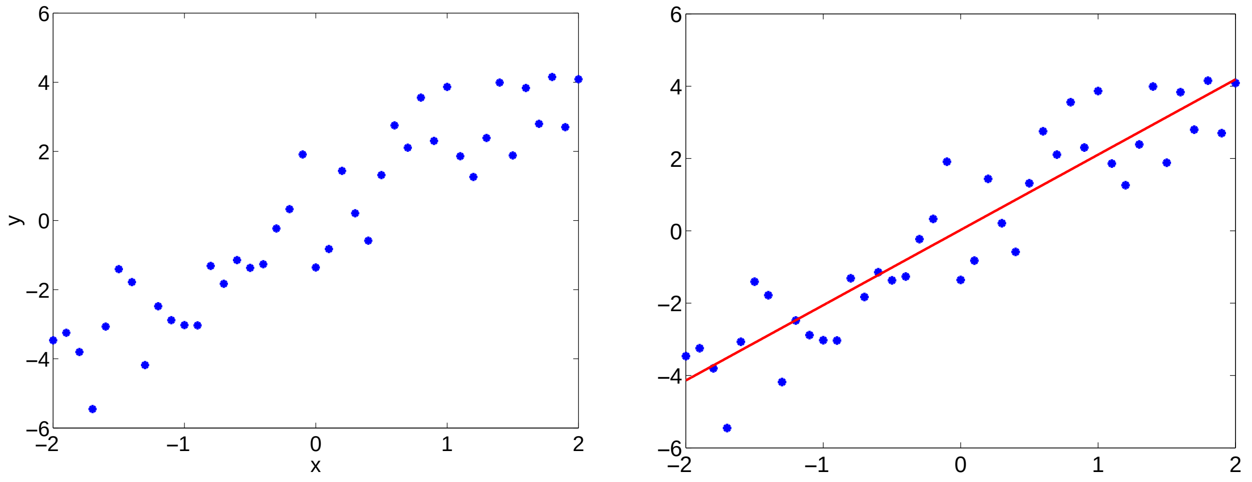
- We begin by considering linear regression (easy to extend to more complex predictions later on)

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

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

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, Loss$(y, \hat{y}) = (y - \hat{y})^2$, so that the empirical loss on n training samples becomes mean squared error

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

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

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

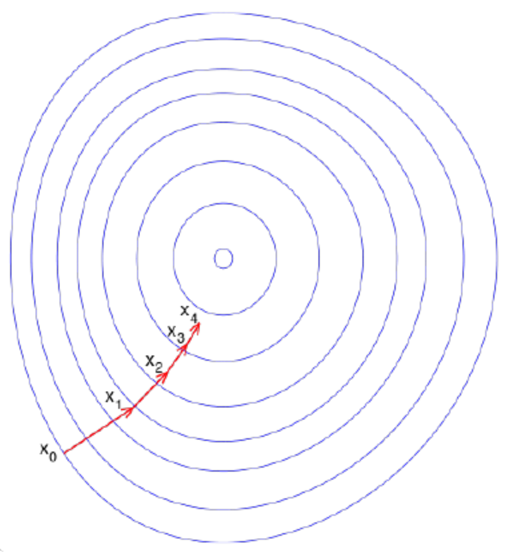
- The solution is a linear function of the outputs y

Alternative: Gradient Descent Algorithm

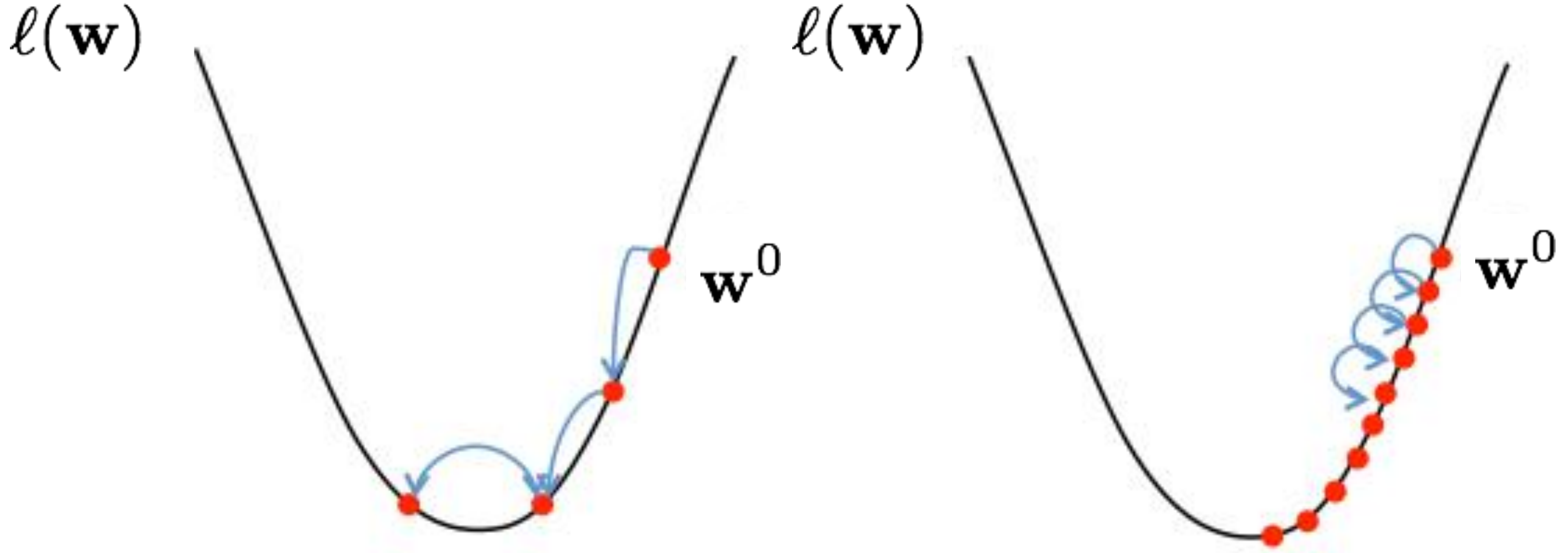
- One straightforward method: **gradient descent**
  - initialize $\boldsymbol{\theta}$ (e.g., randomly)
  - repeatedly update $\boldsymbol{\theta}$ based on the gradient

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

- α is the **learning rate**



Effect of learning rate λ

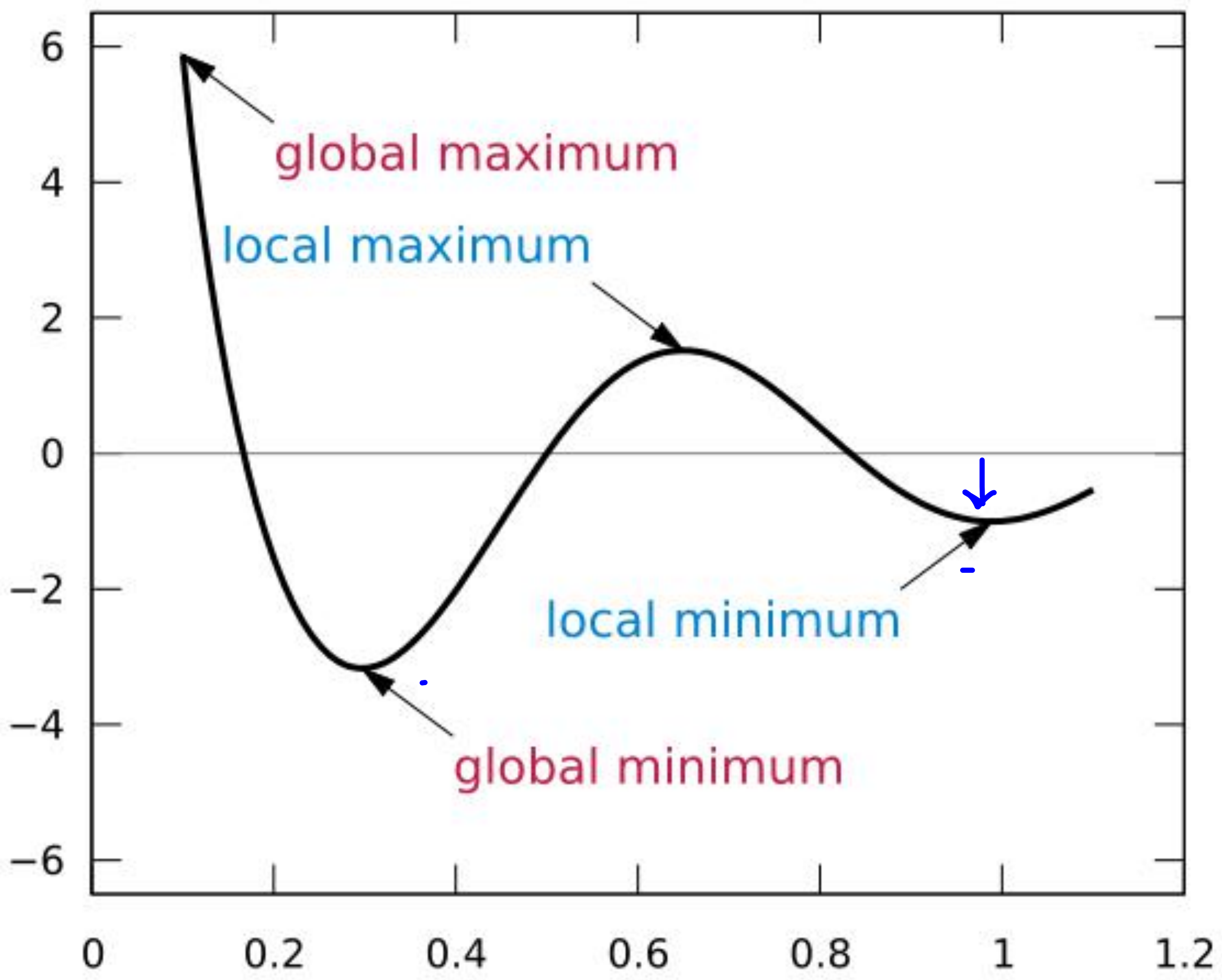


- Large λ => Fast convergence but larger residual error
  Also possible oscillations

- Small λ => Slow convergence but small residual error

Slide credit: Erik Sudderth

Local and Global Optima



Stochastic Gradient Descent

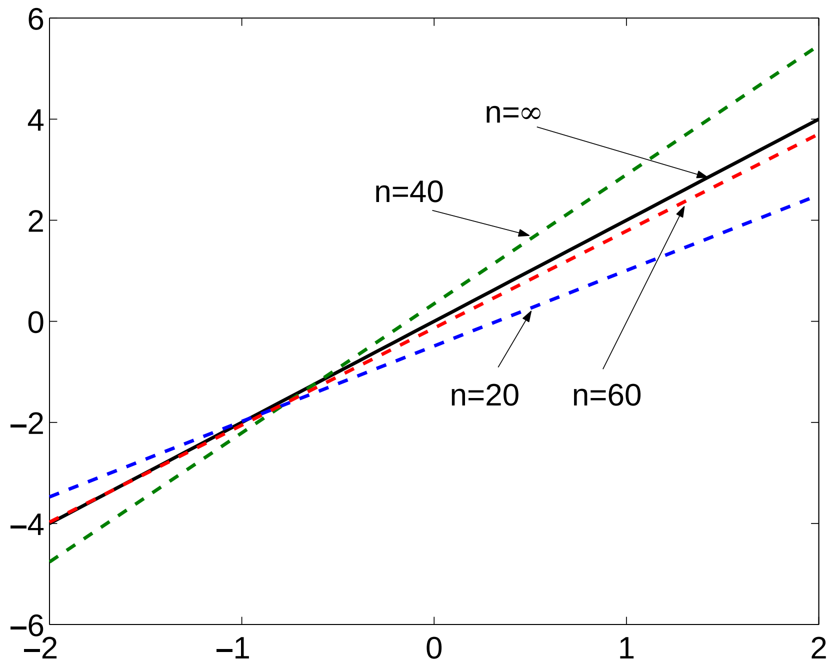
- Two ways to generalize this for all examples in training set:
  1. **Batch updates:** sum or average updates across every example n, then change the parameter values
  2. **Stochastic/online updates:** update the parameters for each training case in turn, according to its own gradients

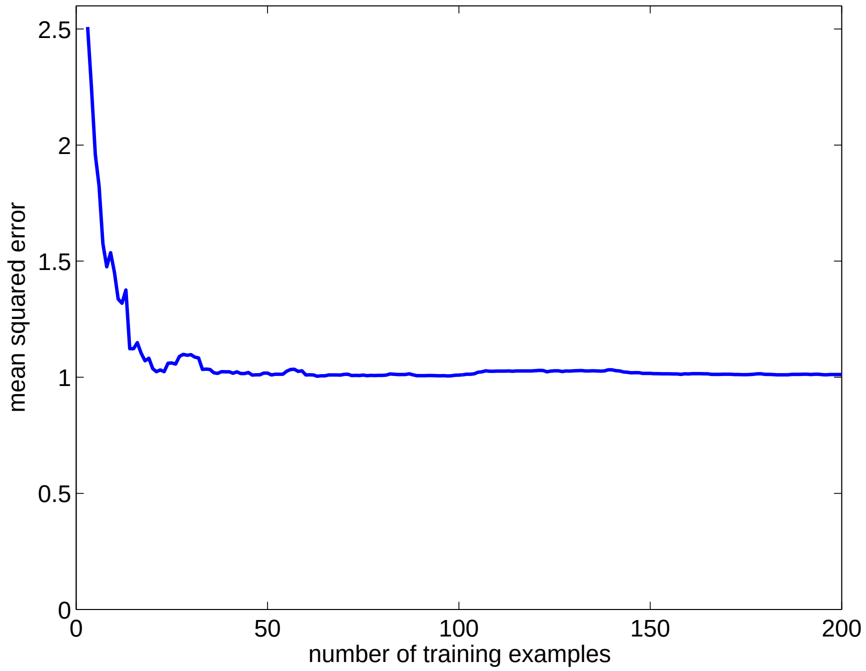
$$\Delta = -\nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$$

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

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:

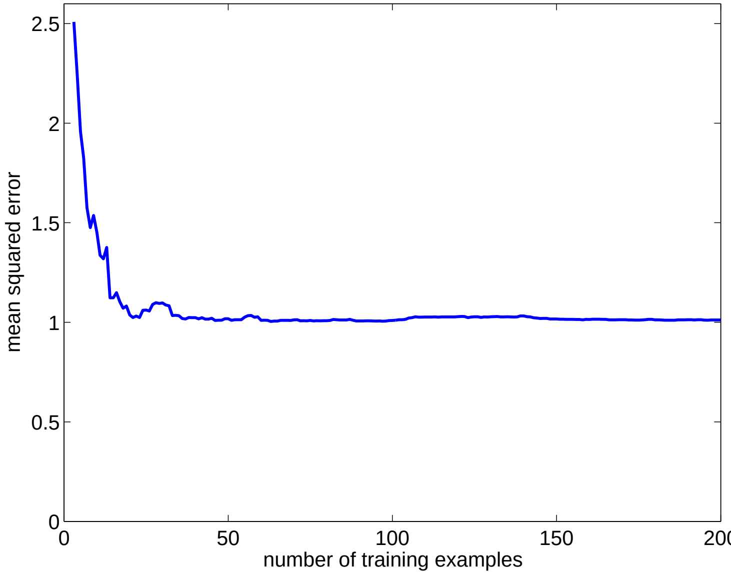
$$E_{(x,y)\sim P}\left(w_0^* + w_1^* x - \hat{w}_0 - \hat{w}_1 x\right)^2$$

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

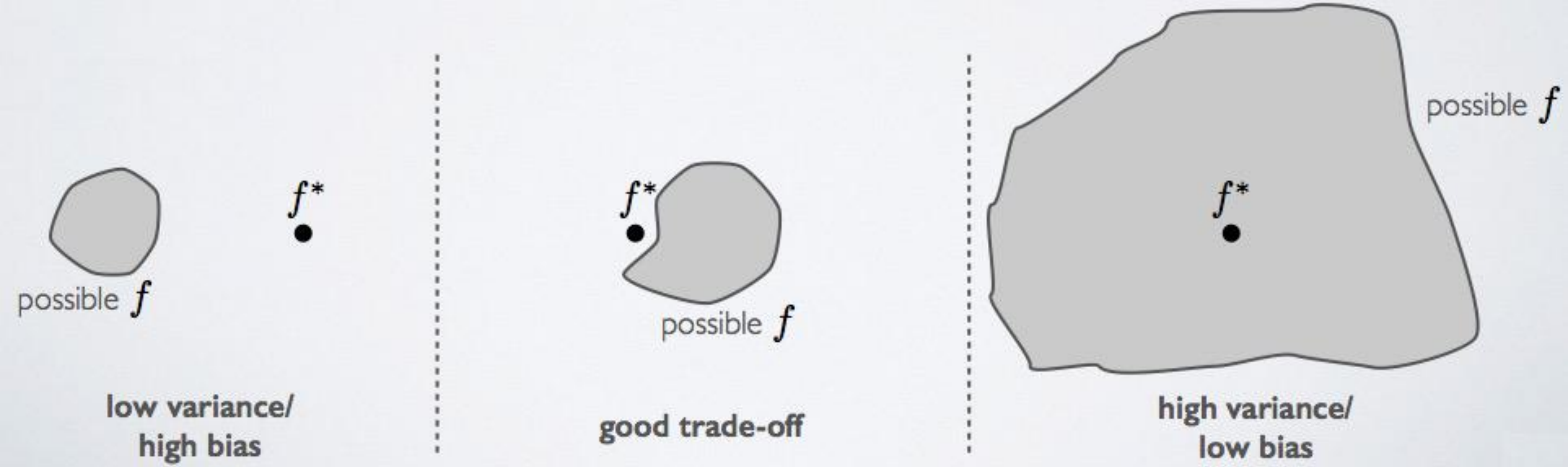
- The expected error of our linear regression function decomposes into the sum of structural and approximation errors

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



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

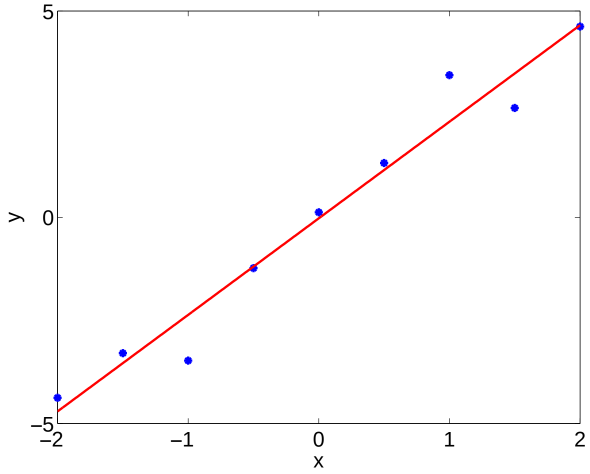
—solution as before

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

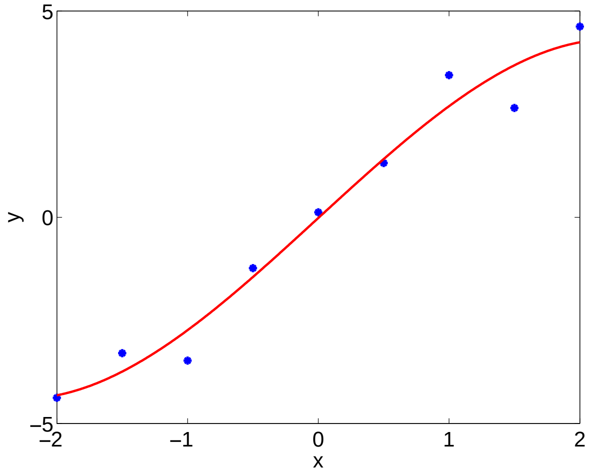
where

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

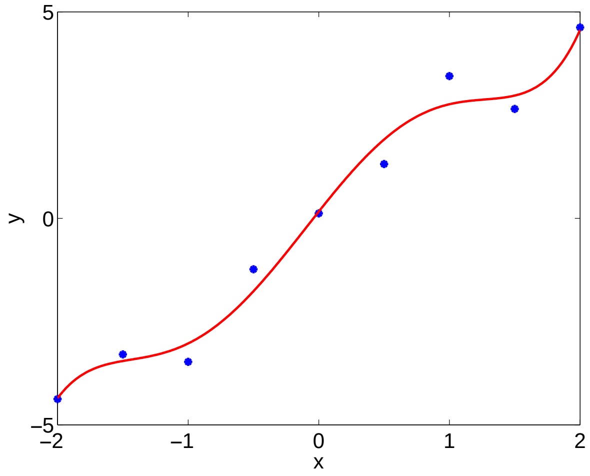
Polynomial regression



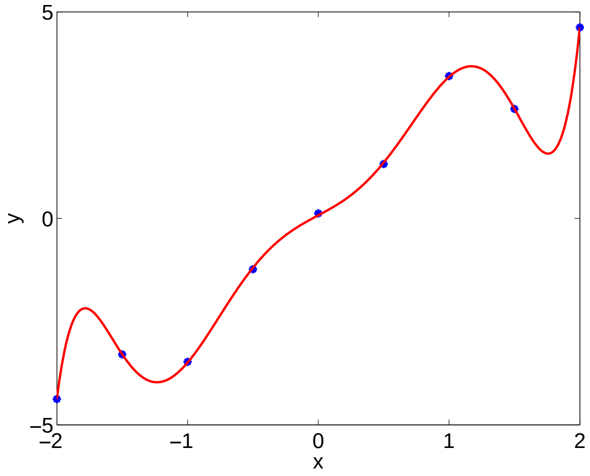
degree $= 1$



degree $= 3$



degree $= 5$



degree $= 7$

Underfitting and Overfitting

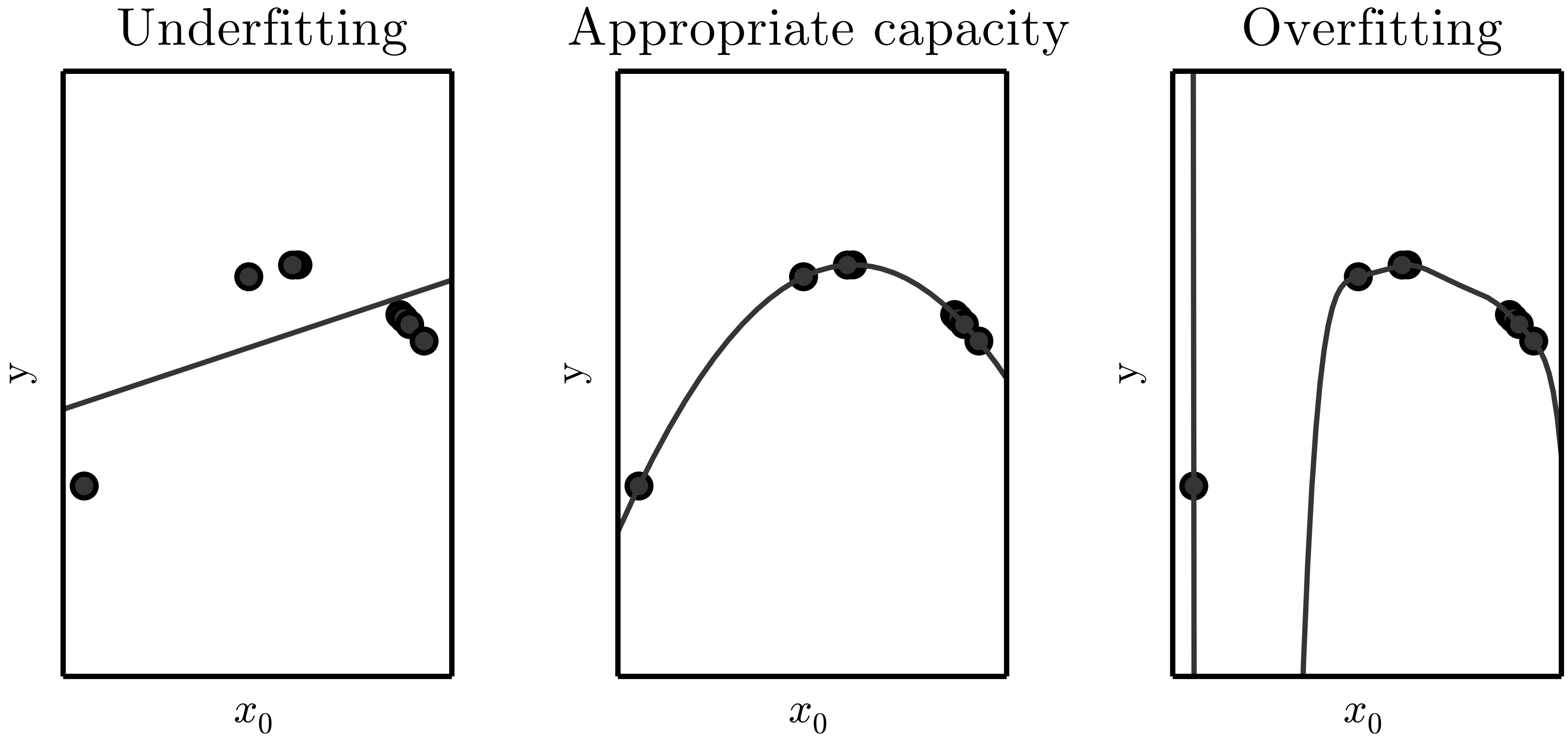
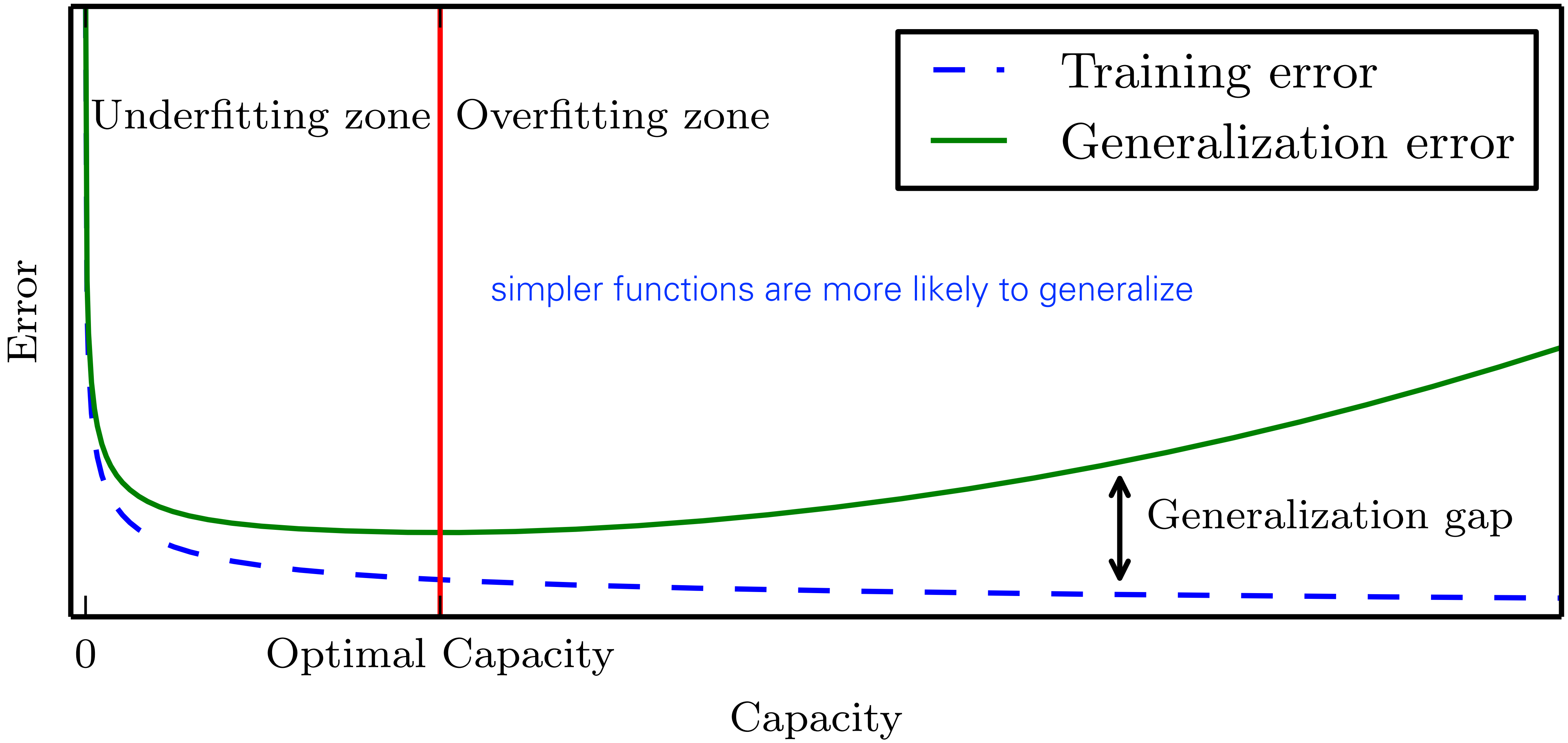


Image credit: Ian Goodfellow

Generalization and Capacity



simpler functions are more likely to generalize

Image credit: Ian Goodfellow

Bias and Variance

sufficiently simpler models are more likely to generalize

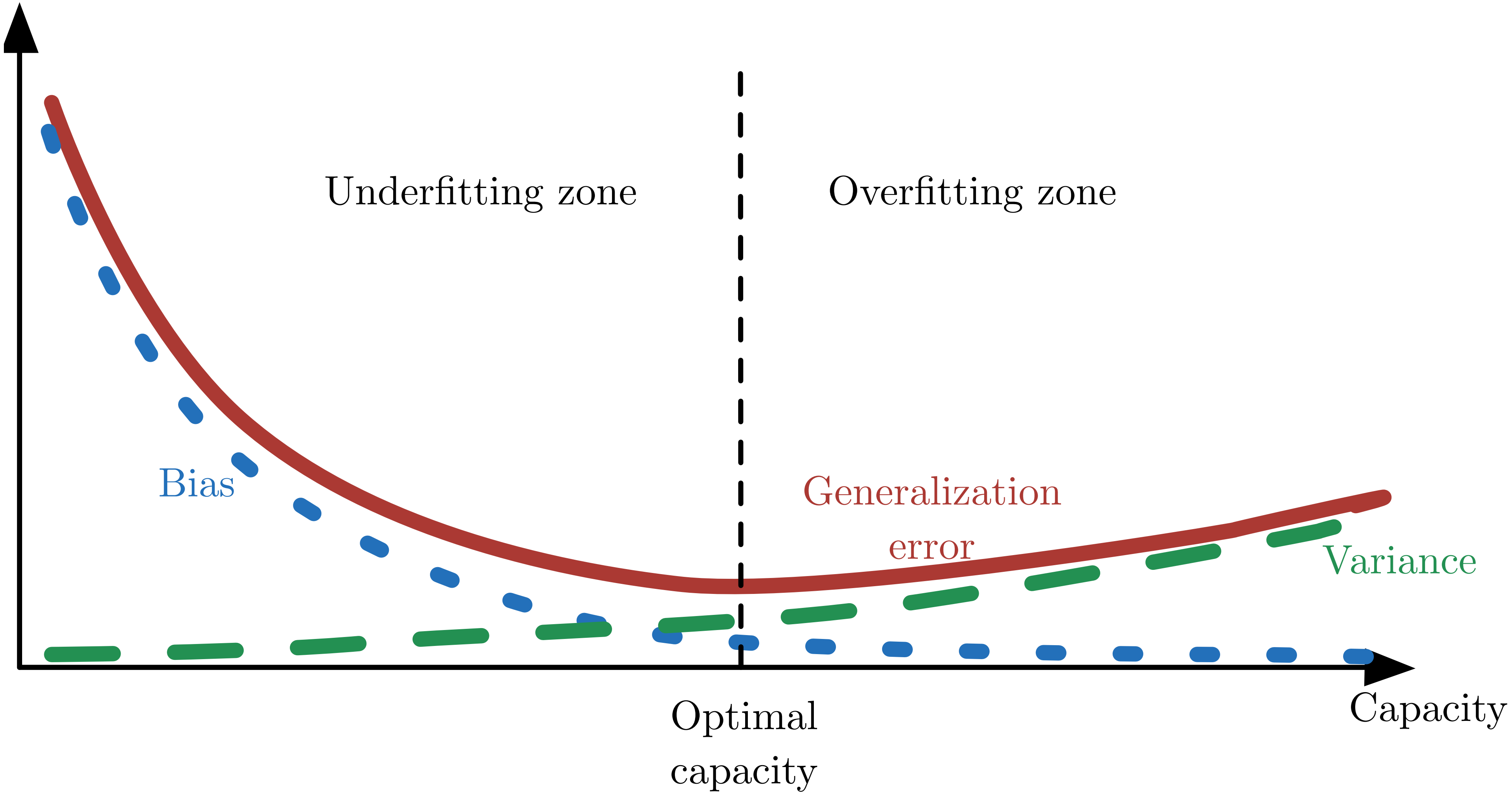


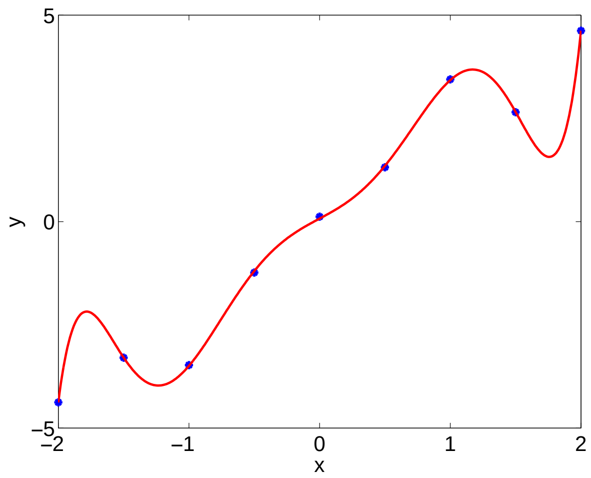
Image credit: Ian Goodfellow

Complexity and overfitting

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

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

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



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

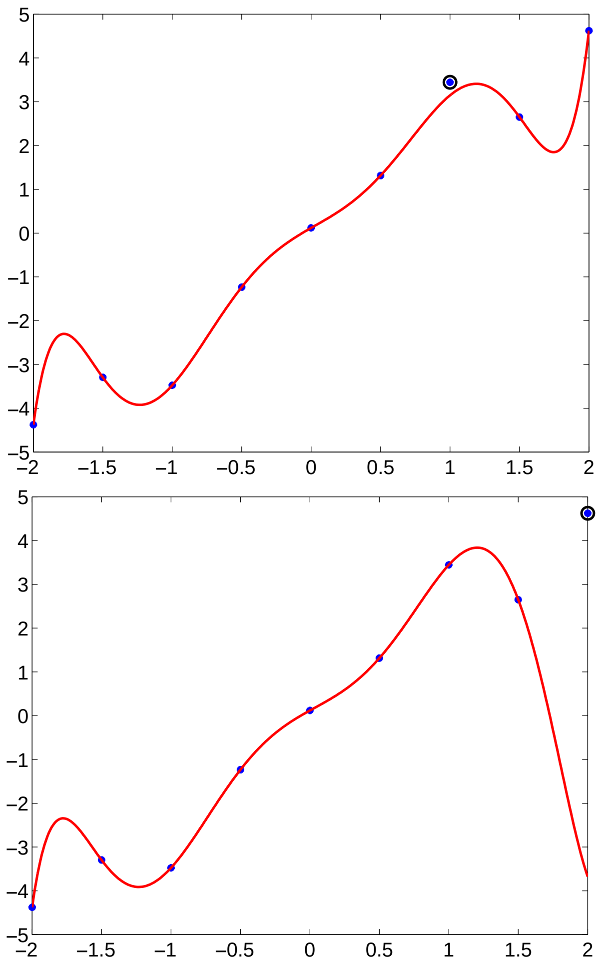
Avoiding overfitting: cross-validation

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

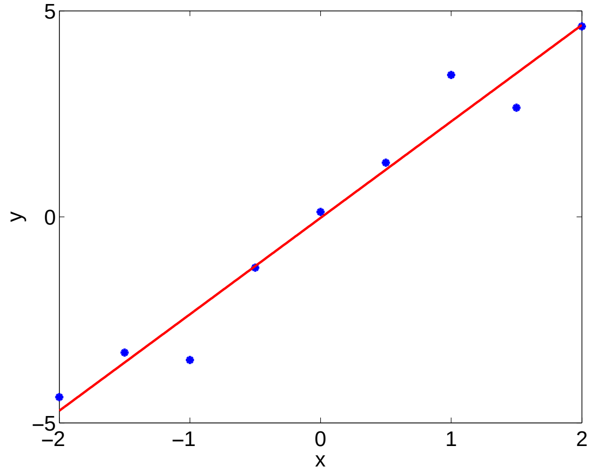
  Leave-one-out cross-validation treats each training example in turn as a test example:

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

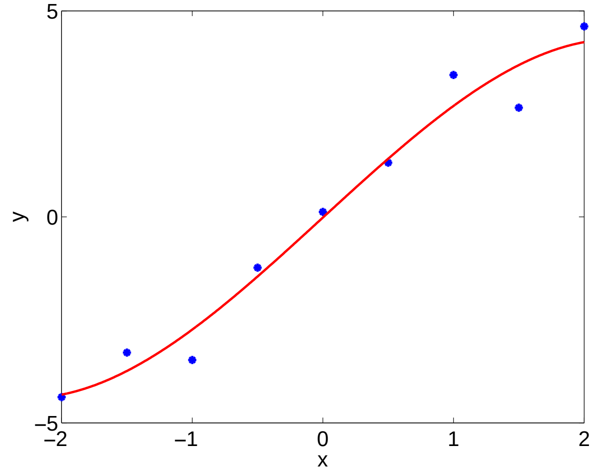
  where $\hat{\mathbf{w}}^{-i}$ are the least squares estimates of the parameters without the i^{th} training example.



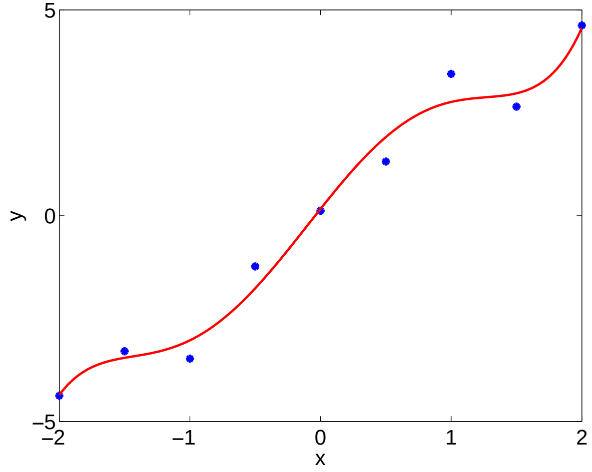
Polynomial regression: example (cont'd)



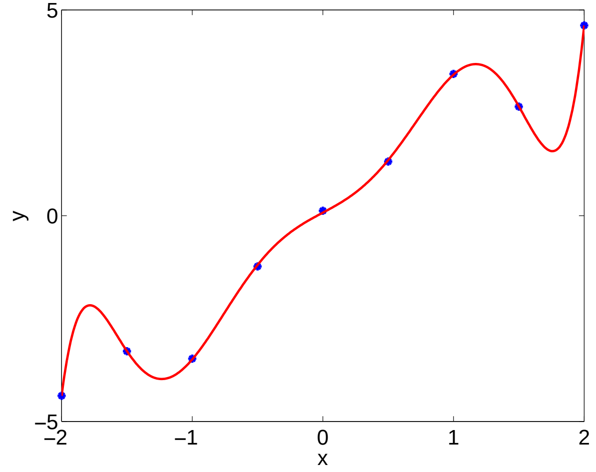
degree $= 1$, CV $= 0.6$



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

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

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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)

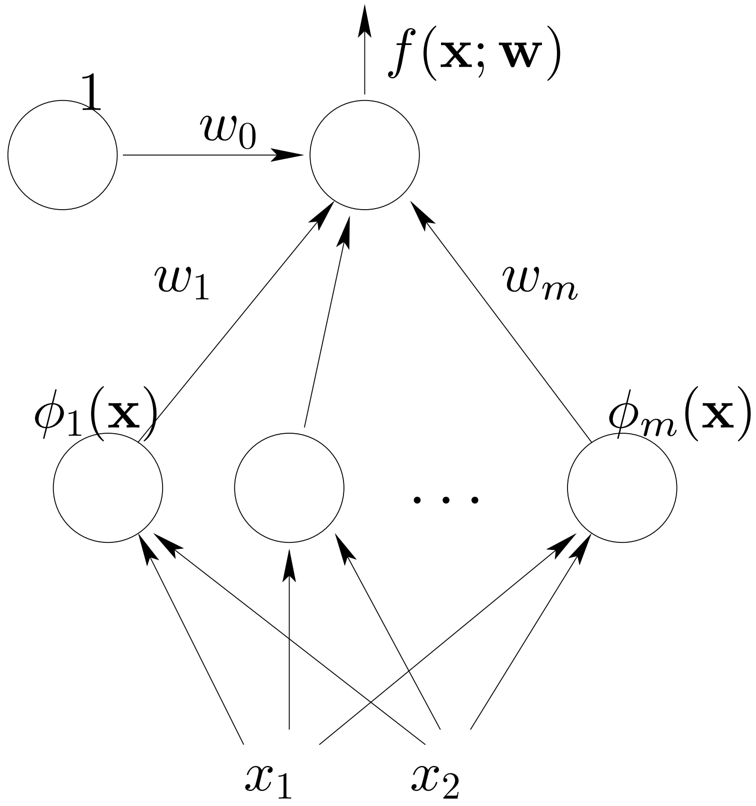
- The basis functions can capture various (e.g., qualitative) properties of the inputs.

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

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

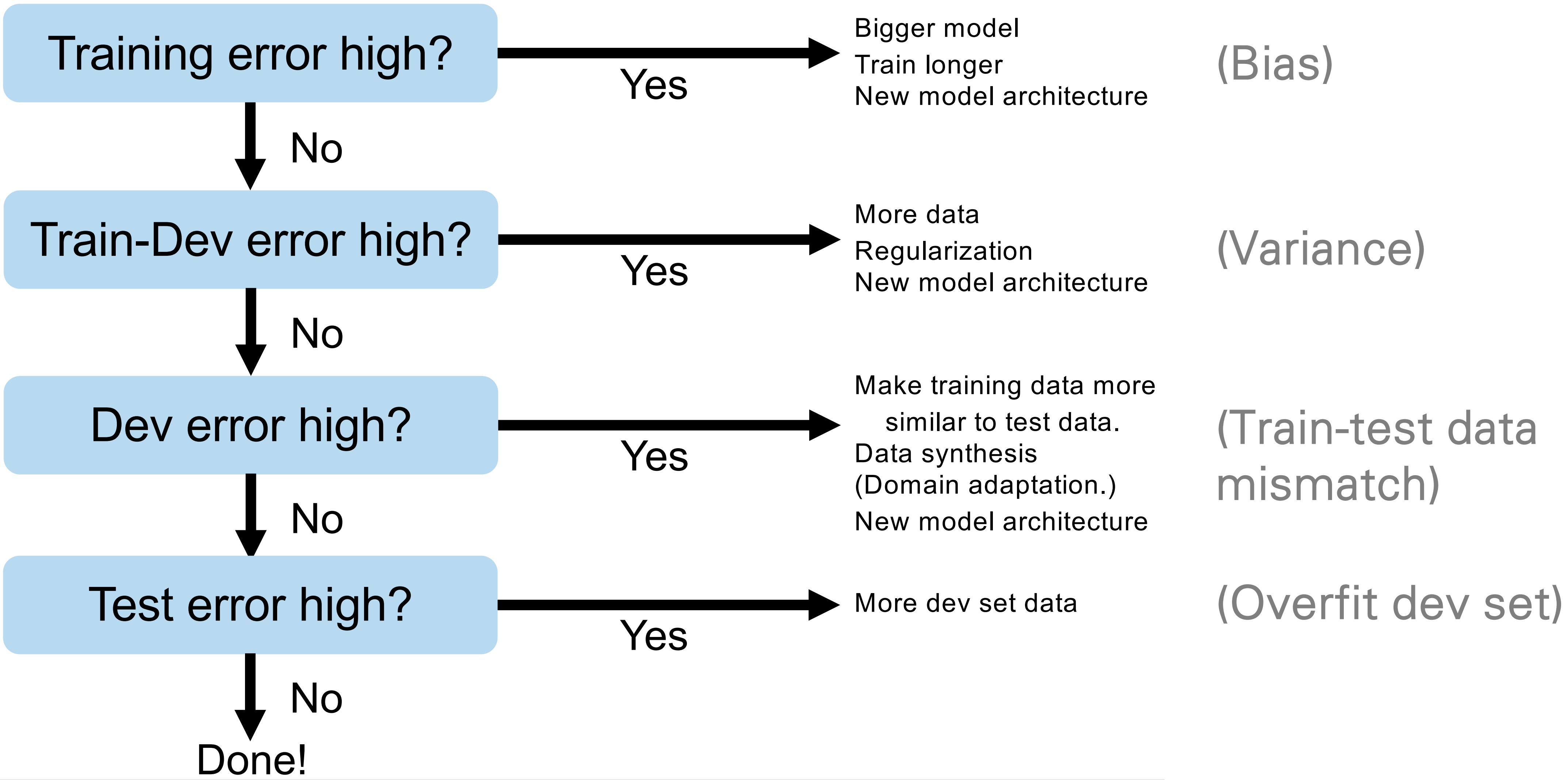
Additive models (cont'd)

- 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



Slide credit: Andrew Ng

Statistical regression models

— model formulation, motivation
— maximum likelihood estimation

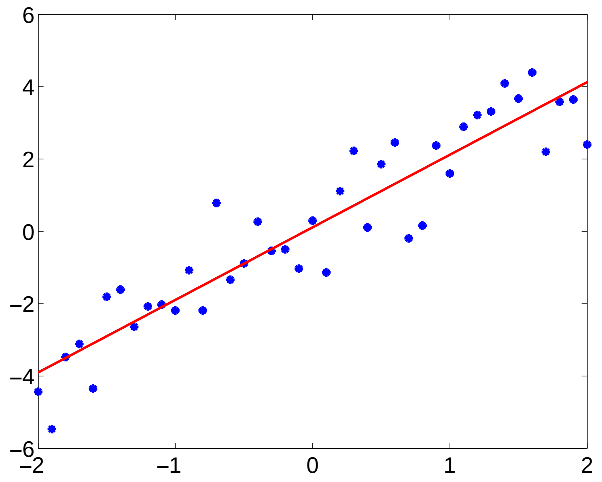
Statistical view of linear regression

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

$$\begin{aligned}\textbf{Observed output} &= \textbf{function} + \textbf{noise}\\ y &= f(\mathbf{x}; \mathbf{w}) + \epsilon\end{aligned}$$

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

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

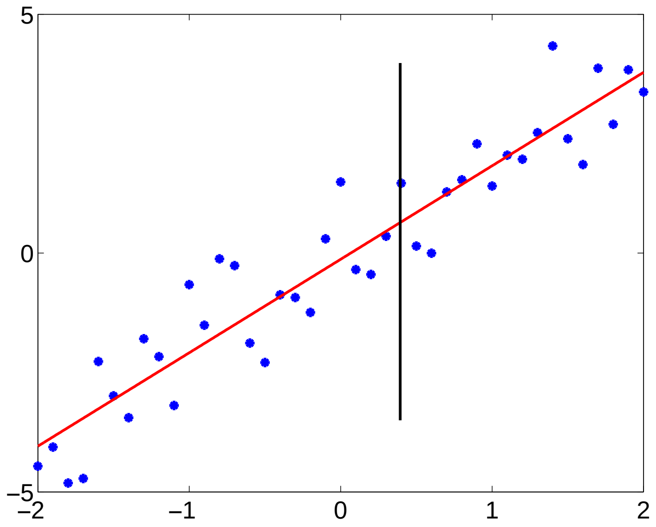


Statistical view of linear regression

- $f(\mathbf{x}; \mathbf{w})$ 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?

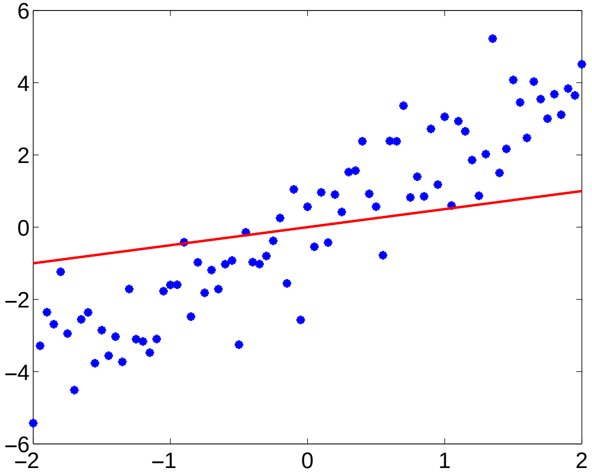
Maximum likelihood estimation

- 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

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



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:

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

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

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

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

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

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

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

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

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

Recap: Lecture overview

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

Next Lecture:

Multi-layer Perceptrons