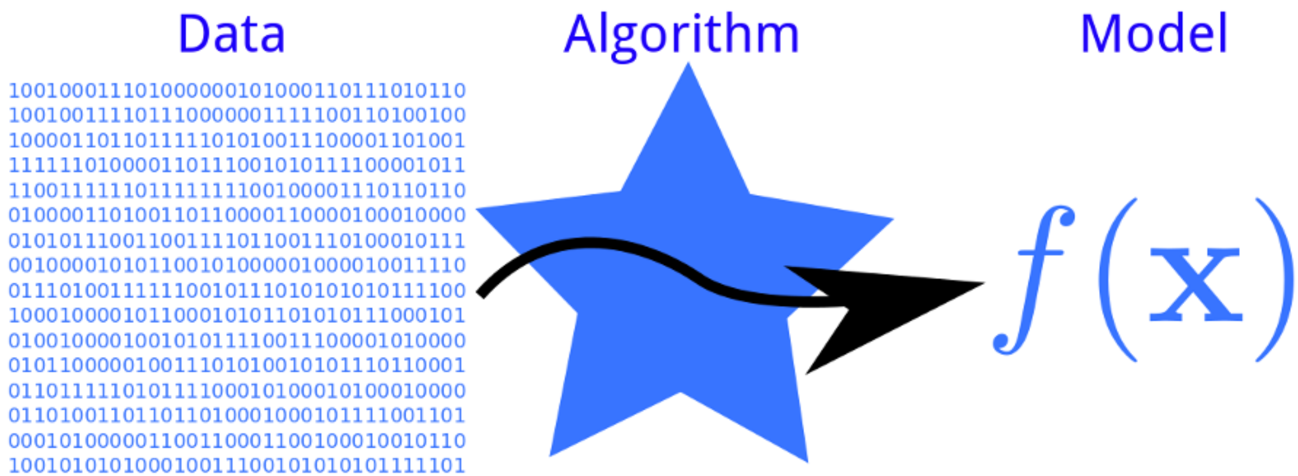
Introduction to Machine Learning



Lecture 1: Introduction and Linear Regression

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Lecture outline

Introduction to the course

Introduction to Machine Learning

Least squares

Machine Learning

Principles, methods, and algorithms for learning and prediction based on past evidence

Goal: Machines that perform a task based on experience, instead of explicitly coded instructions

Why?

- Crucial component of every intelligent/autonomous system
- Important for a system's adaptability
- Important for a system's generalization capabilities
- Attempt to understand human learning

Machine Learning variants

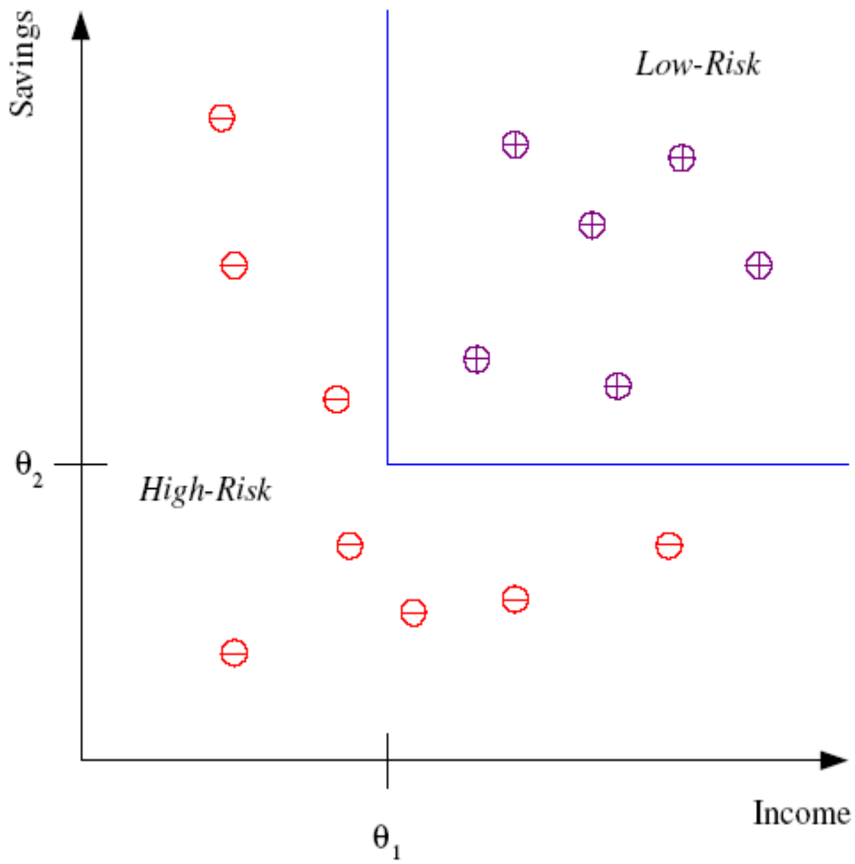
- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised/semi-supervised

  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: sparse reward for a sequence of decisions

Classification

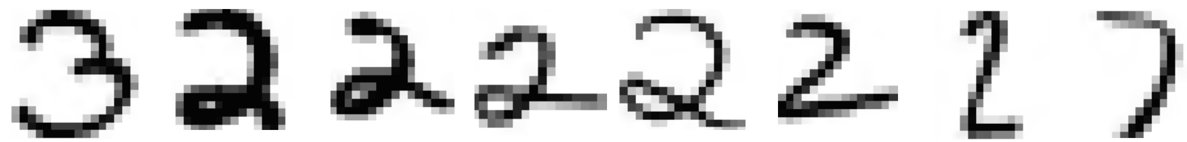
- Based on our experience, should we give a loan to this customer?
  - Binary decision: yes/no



Decision boundary

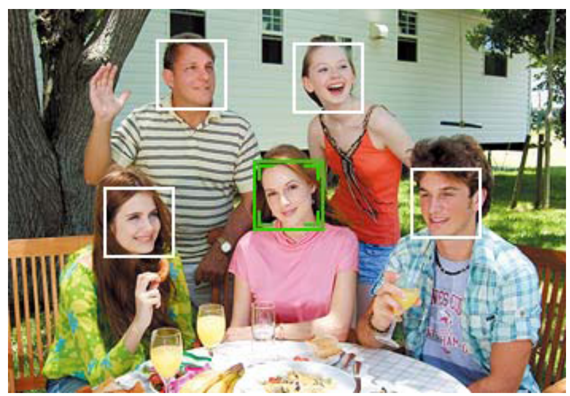
Classification examples

- Digit Recognition

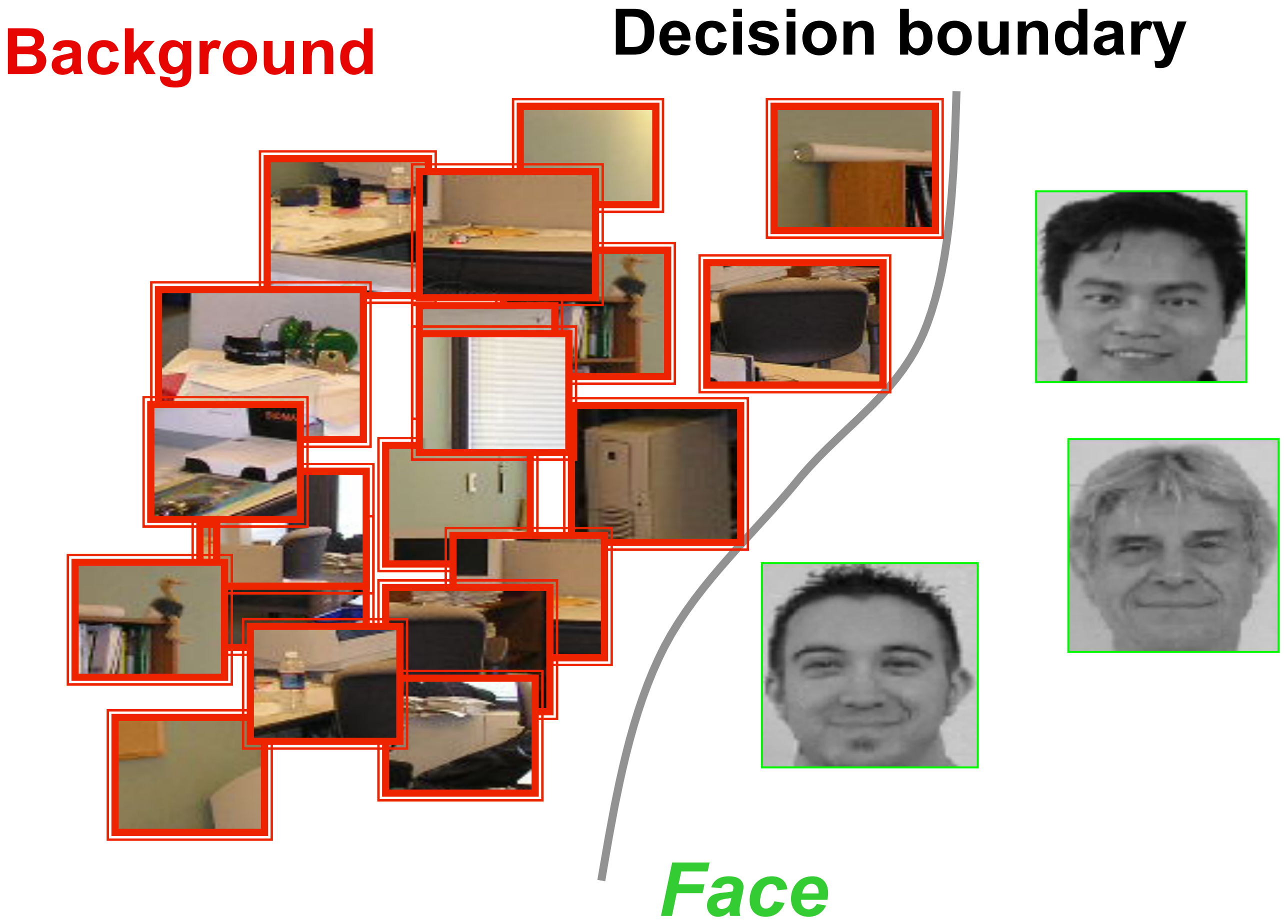


- Spam Detection

- Face detection



`Faceness function': classifier



Test time: deploy the learned function

- Scan window over image
  - Multiple scales
  - Multiple orientations
- Classify window as either:
  - Face
  - Non-face

Machine Learning variants

- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised

  Some data supervised, some unsupervised
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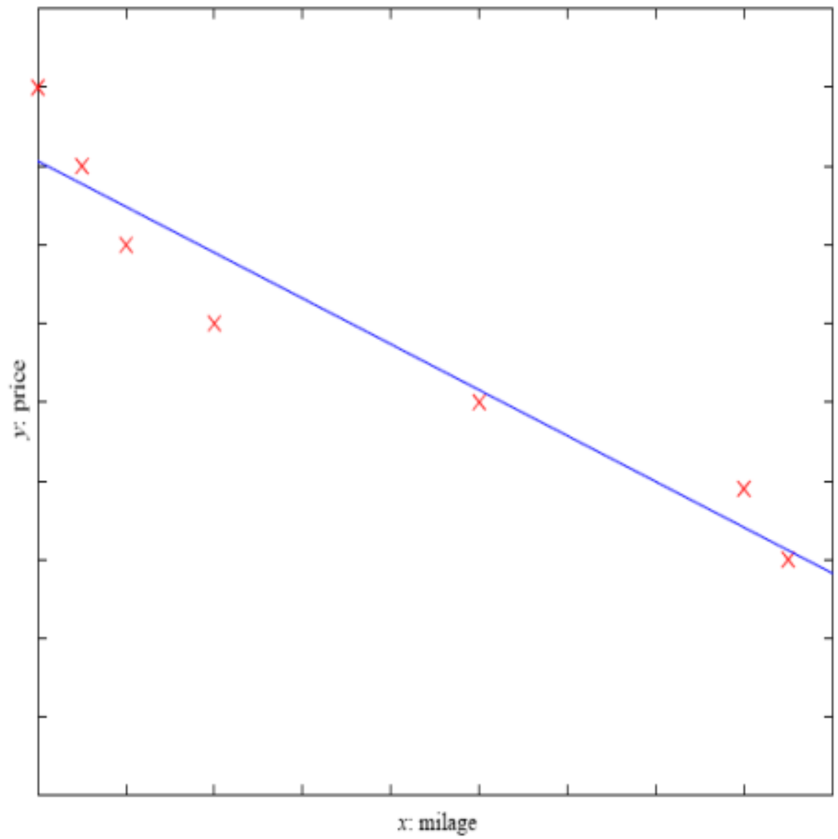
  Supervision: reward for a sequence of decisions

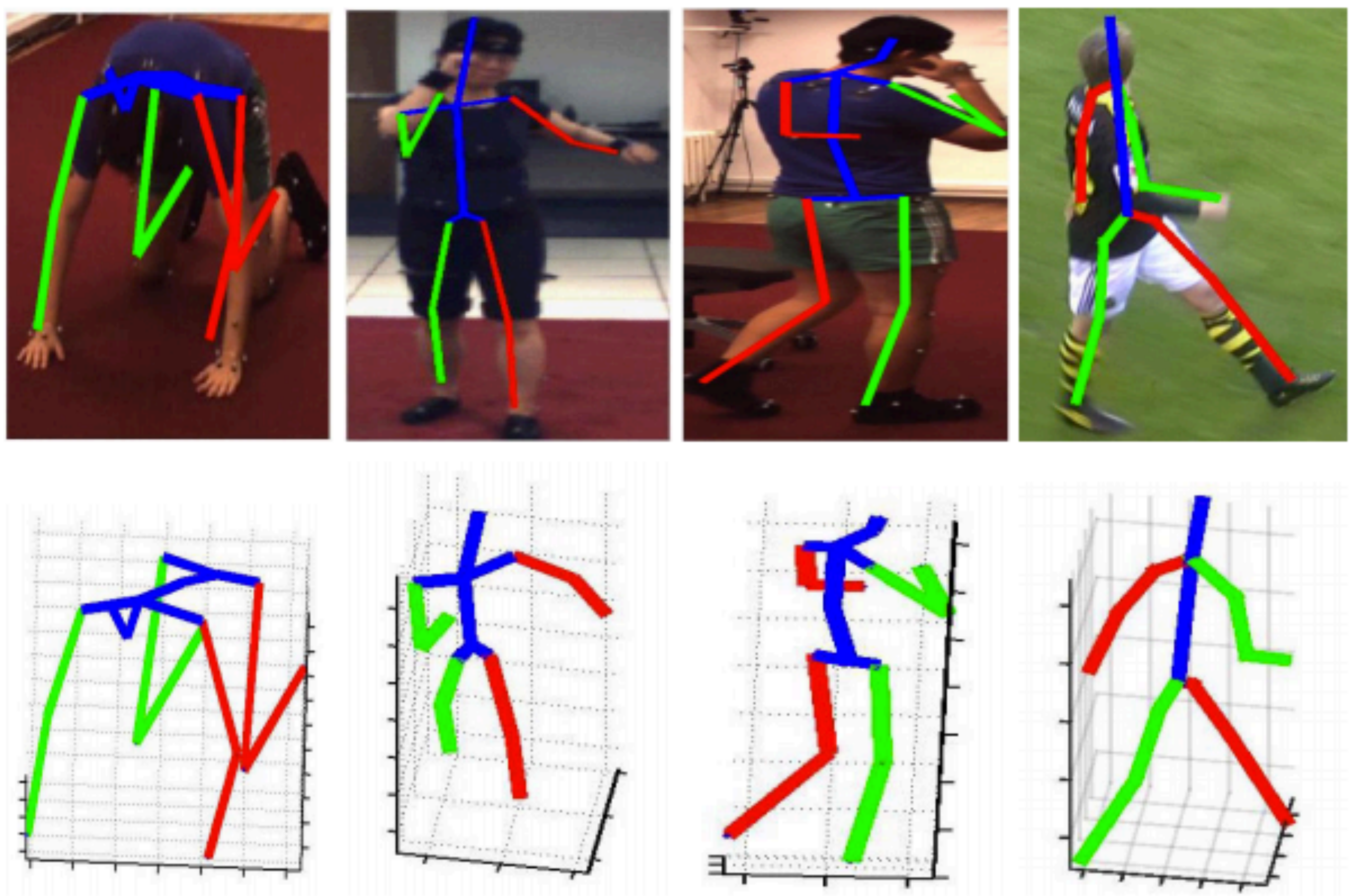
Regression

- Output: Continuous
  - E.g. price of a car based on years, mileage, condition,…



Computer vision example

- Human estimation: from image to vector-valued pose estimate



Machine Learning variants

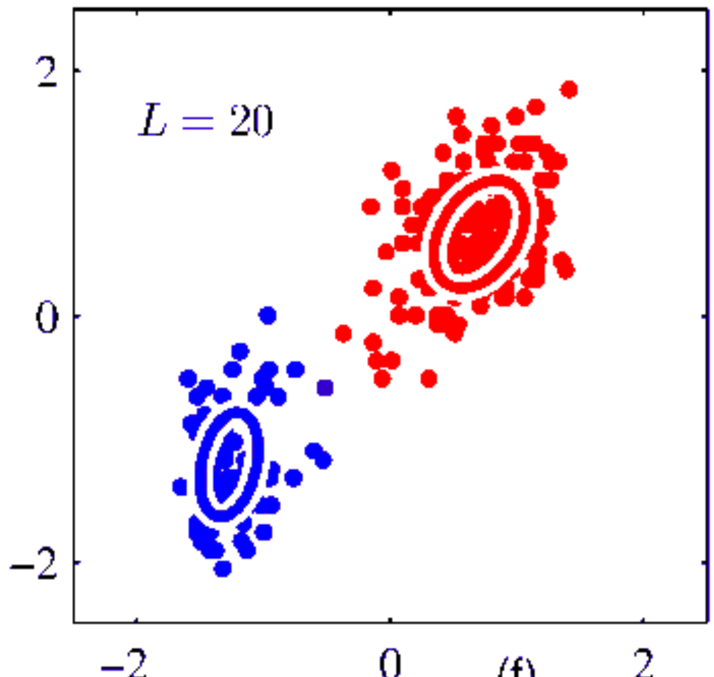
- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised

  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: reward for a sequence of decisions

Clustering

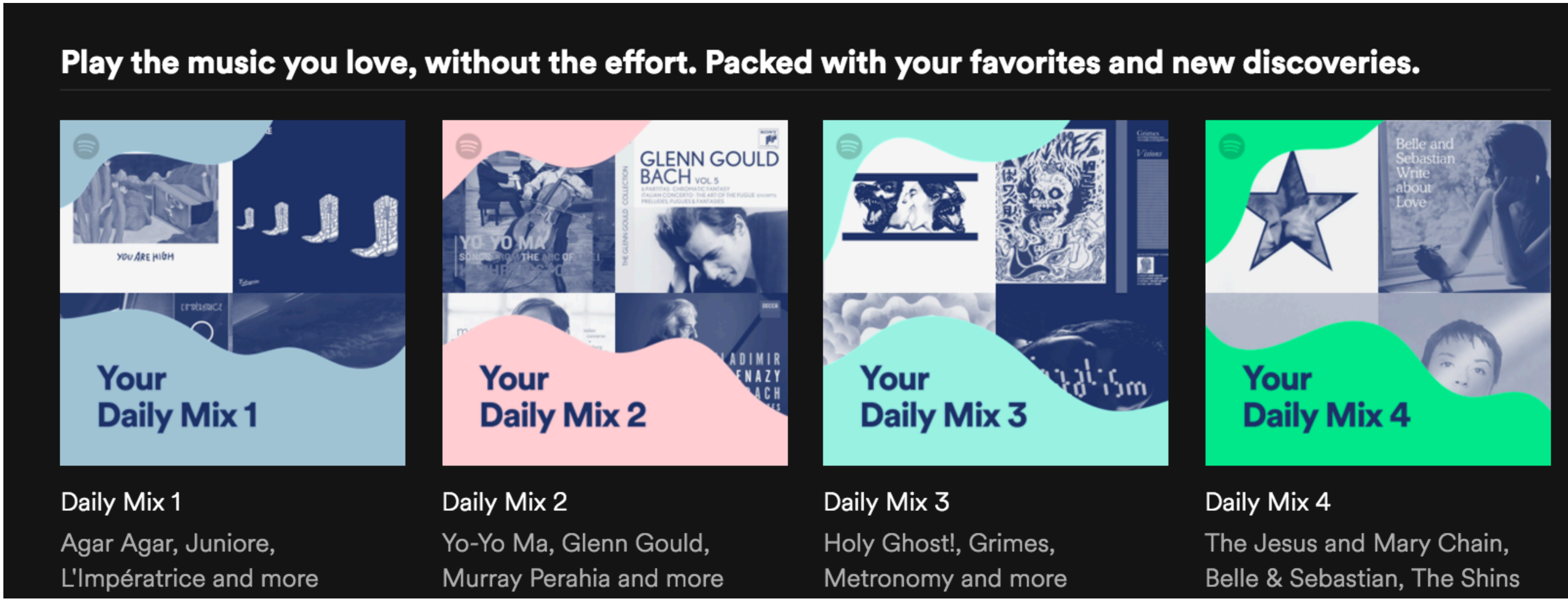
- Break a set of data into coherent groups
  - Labels are `invented'



(f)

Clustering examples

- Spotify recommendations



Clustering examples

- Image segmentation

Machine Learning variants

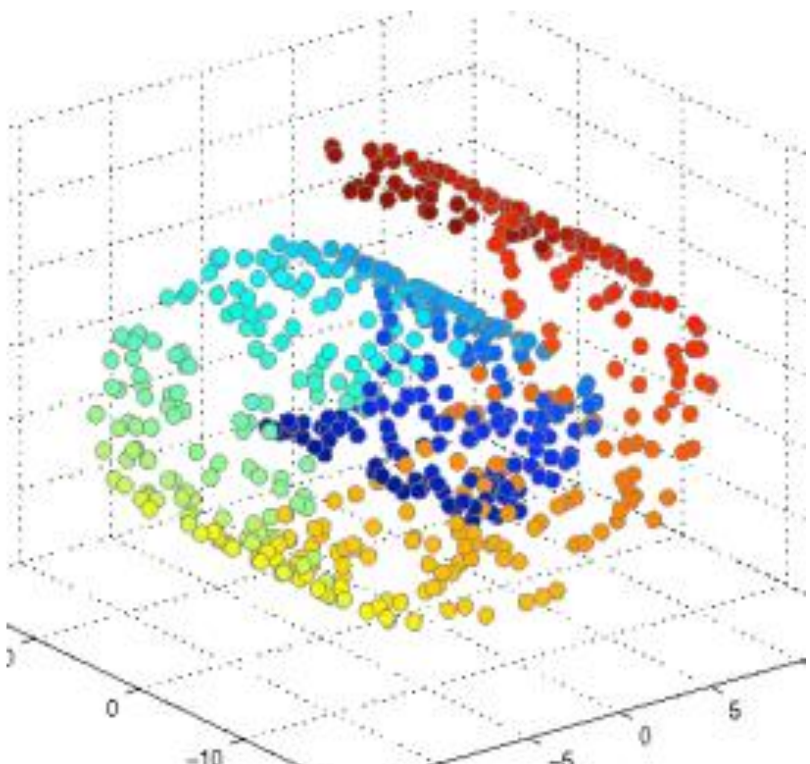
- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised

  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: reward for a sequence of decisions

Dimensionality reduction & manifold learning

- Find a low-dimensional representation of high-dimensional data
  - Continuous outputs are `invented'



Example of nonlinear manifold: faces

Average of two faces is not a face

$$\mathbf{x}_1$$

$$\frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2)$$

$$\mathbf{x}_2$$

Moving along the learned face manifold

Trajectory along the "male" dimension

Trajectory along the "young" dimension

Lample et. al. Fader Networks, NIPS 2017

Machine Learning variants

- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised/semi supervised

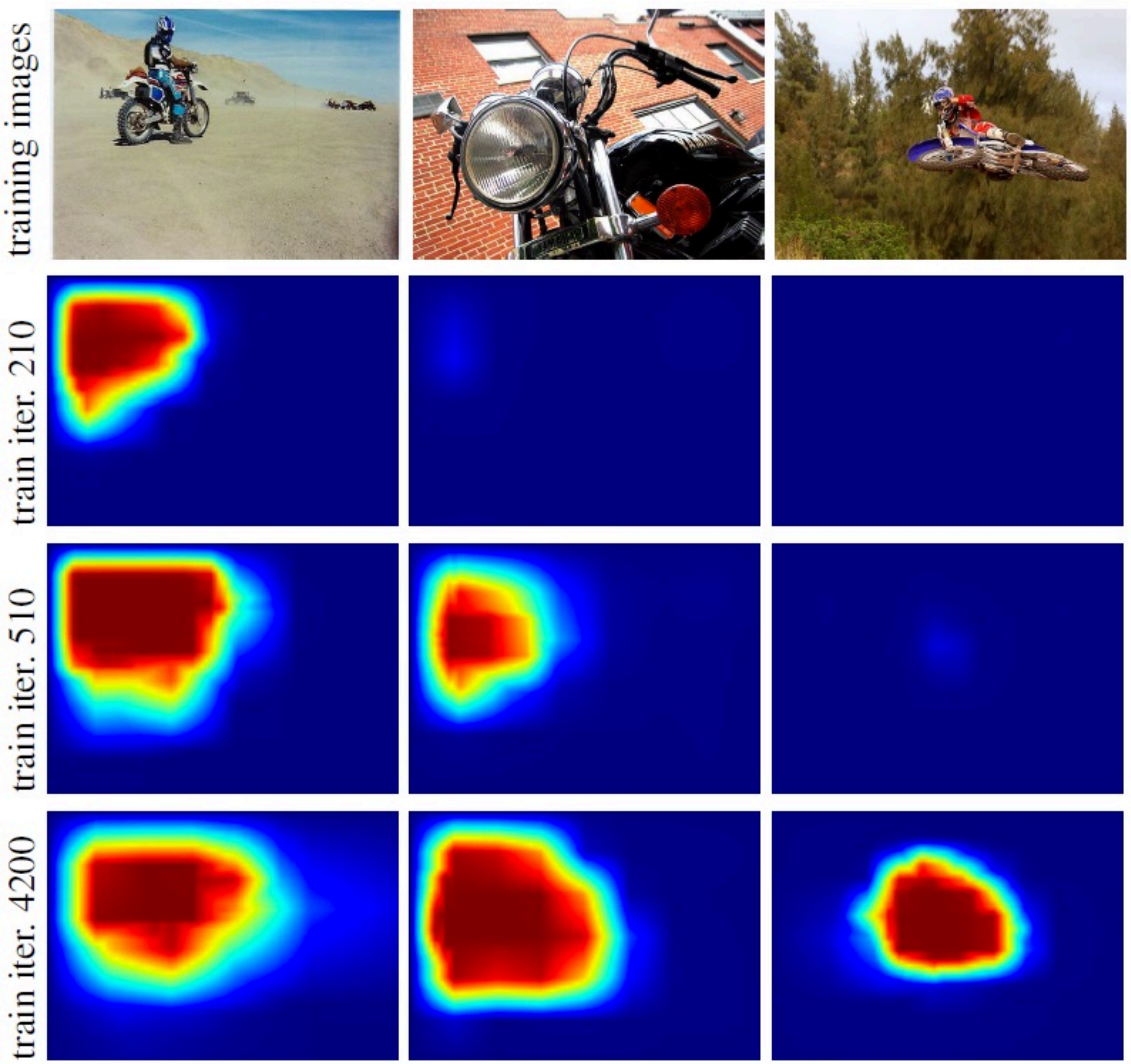
  Partially supervised
- Reinforcement learning

  Supervision: reward for a sequence of decisions

Weakly supervised learning: only part of the supervision signal

Supervision signal: "motorcycle"

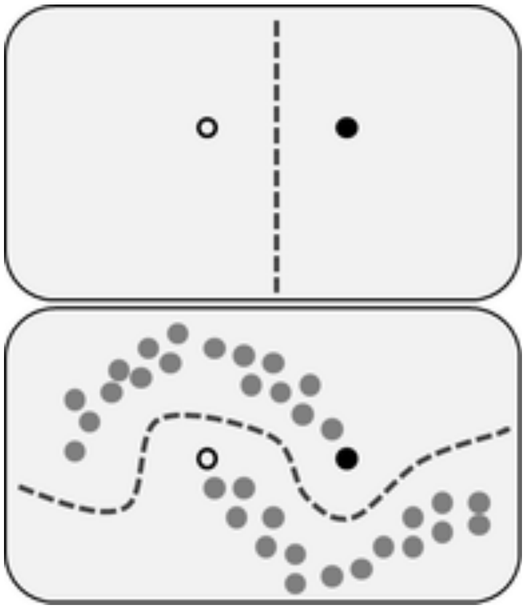
Weakly supervised learning: only part of the supervision signal



Supervision signal: “motorcycle”

Inferred localization information

Semi-supervised learning: only part of the data labelled



Labelled data

Labelled + unlabelled data

Machine Learning variants

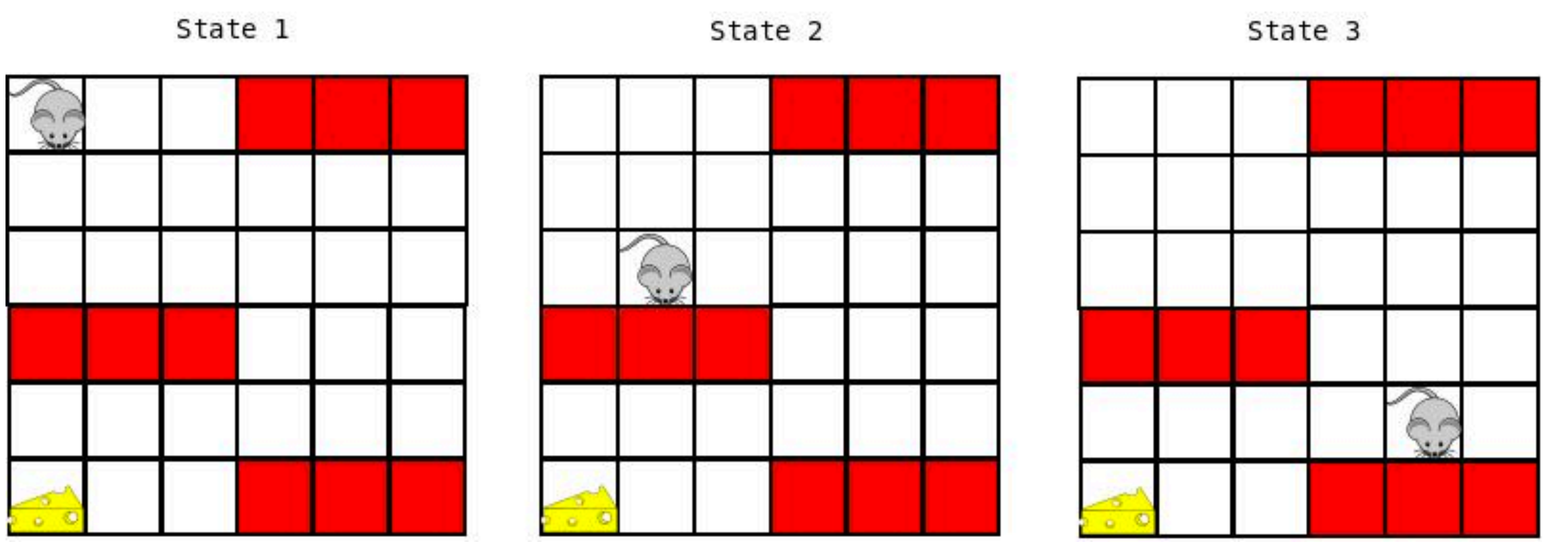
- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction
- Weakly supervised/semi supervised learning

  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: reward for a sequence of decisions

Reinforcement learning

- Agent interacts with environment repeatedly
  - Take actions, based on state
  - (occasionally) receive rewards
  - Update state
  - Repeat
- Goal: maximize cumulative reward



Reinforcement learning examples

- Beat human champions in games

Backgammon, 90's

GO, 2015

- Robotics

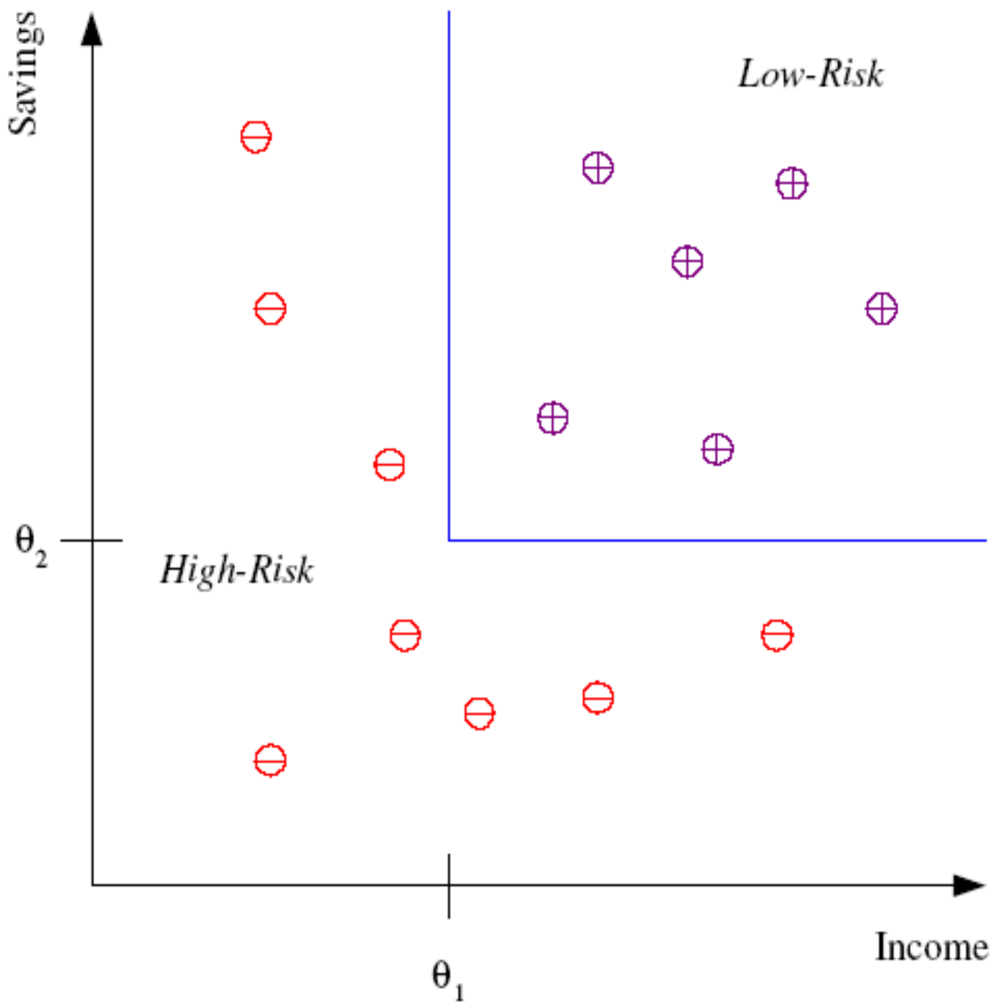
Focus of first part: supervised learning

- Supervised
  - Classification
  - Regression
- Unsupervised
  - Clustering
  - Dimensionality Reduction, Manifold Learning
- Weakly supervised

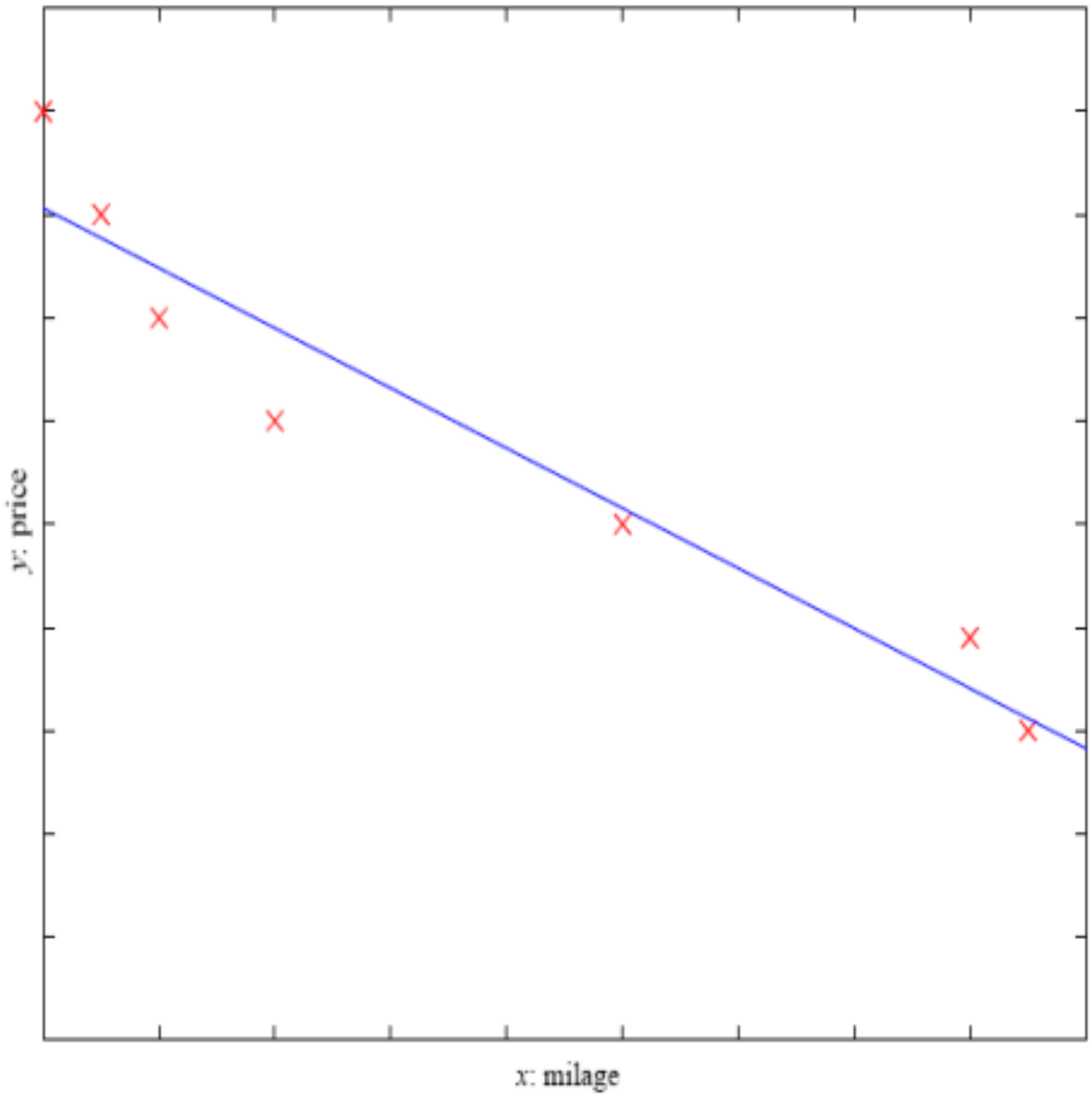
  Some data supervised, some unsupervised
- Reinforcement learning

  Supervision: reward for a sequence of decisions

Classification: yes/no decision



Regression: continuous output



What we want to learn: a function

- Input-output mapping

$$y = f_w(x)$$

What we want to learn: a function

- Input-output mapping

method

prediction

$$y = f_w(x)$$

parameters **Input**

What we want to learn: a function

method

prediction

$$y = f_w(x)$$

parameters **Input**

Calculus $x \in \mathbb{R}$

Vector calculus $\mathbf{x} \in \mathbb{R}^D$

Machine learning: can work also for discrete inputs, strings, trees, graphs,…

What we want to learn: a function

method

prediction

$$y = f_w(x)$$

parameters

Input

Classification: $y \in \{0, 1\}$

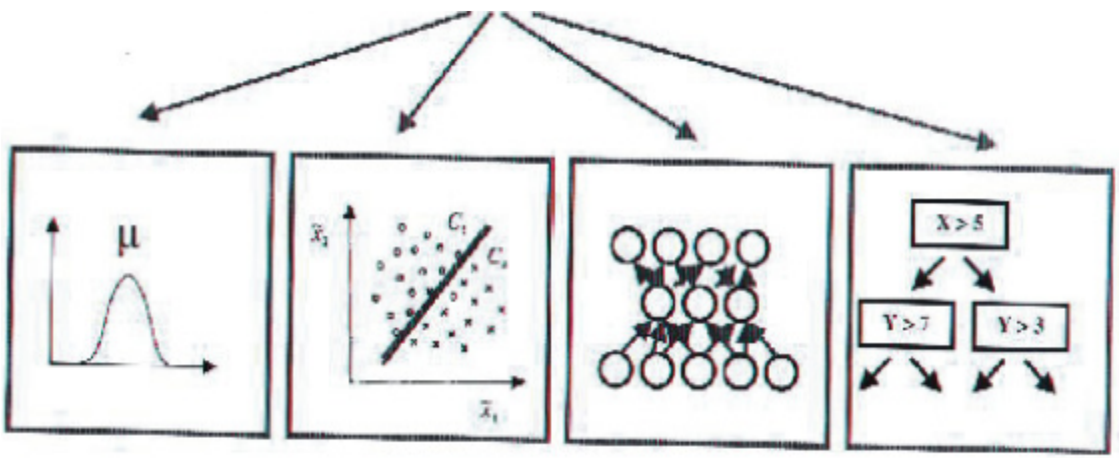
Regression: $y \in \mathbb{R}$

What we want to learn: a function

method

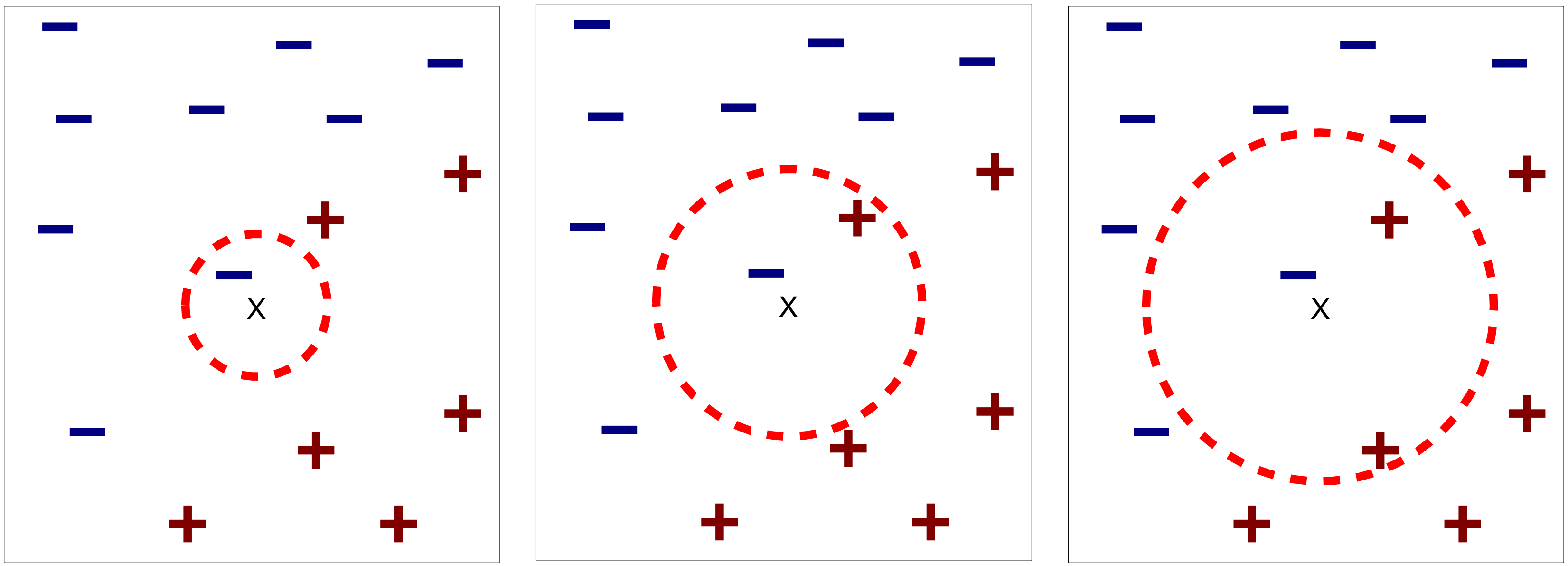
prediction

$$y = f_w(x)$$



Linear classifiers, neural networks, decision trees, ensemble models, probabilistic classifiers, …

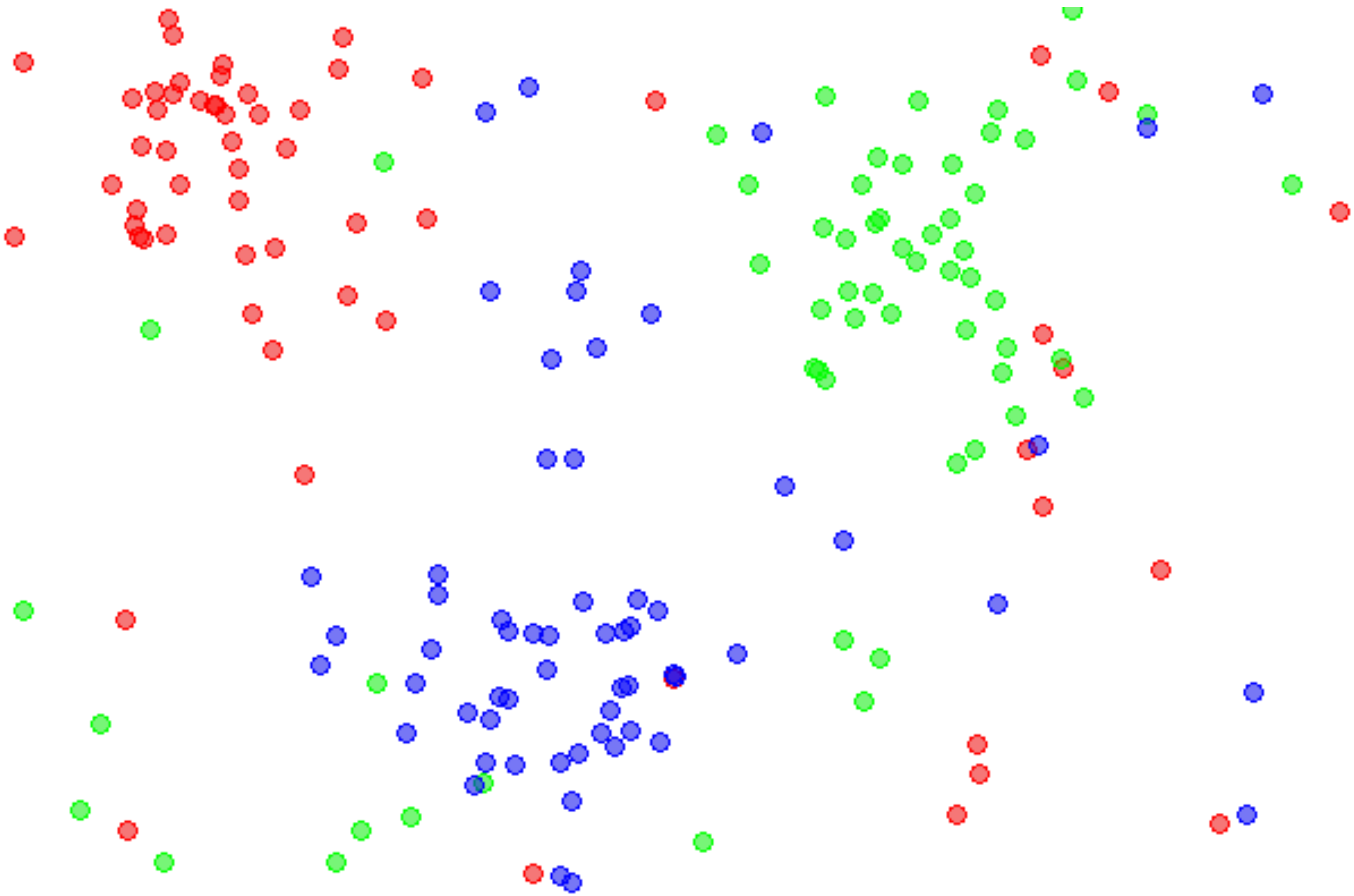
Example of method: K-nearest neighbor classifier



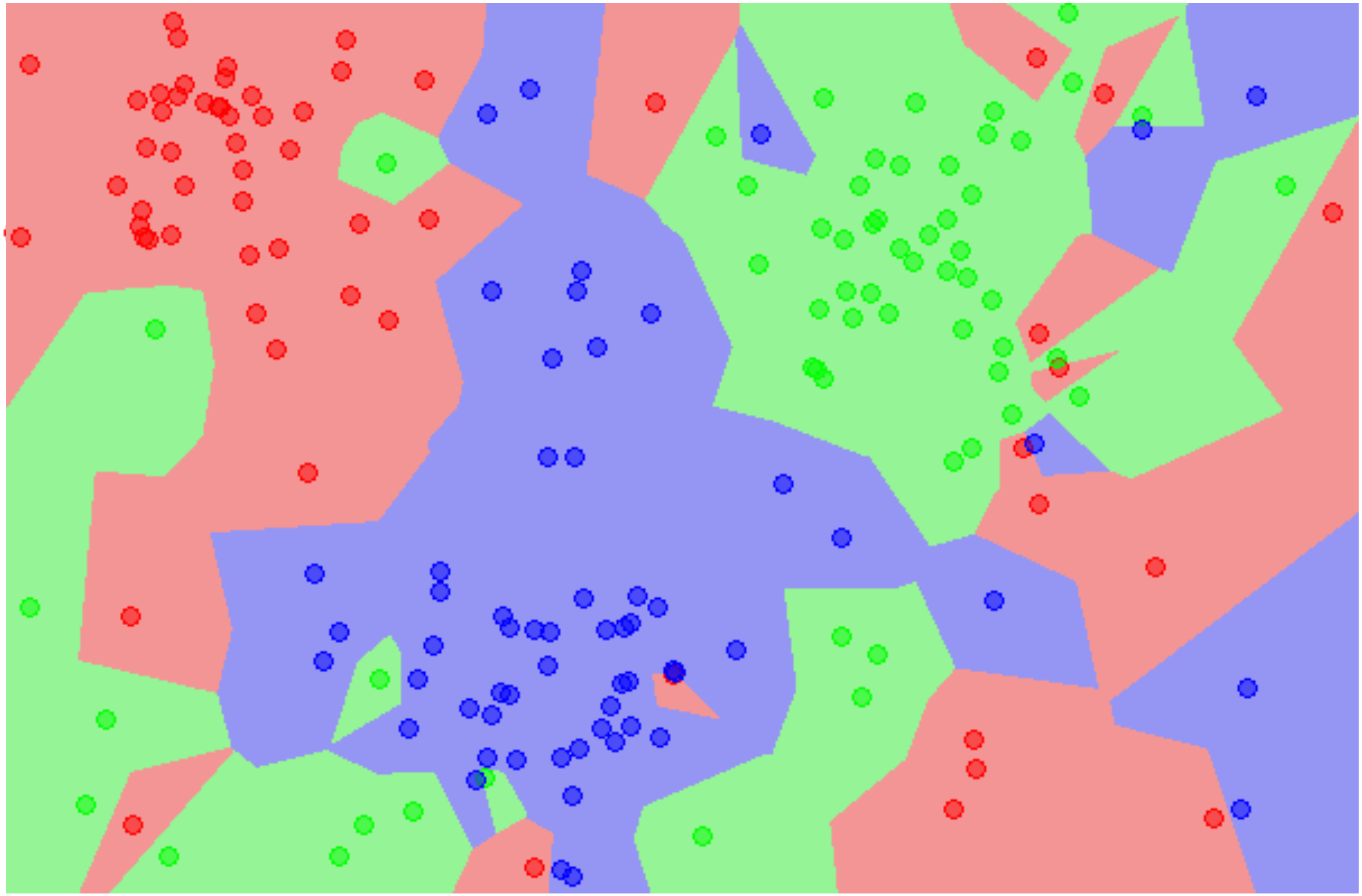
(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

– **Compute distance to other training records**
– **Identify *K* nearest neighbors**
– **Take majority vote**

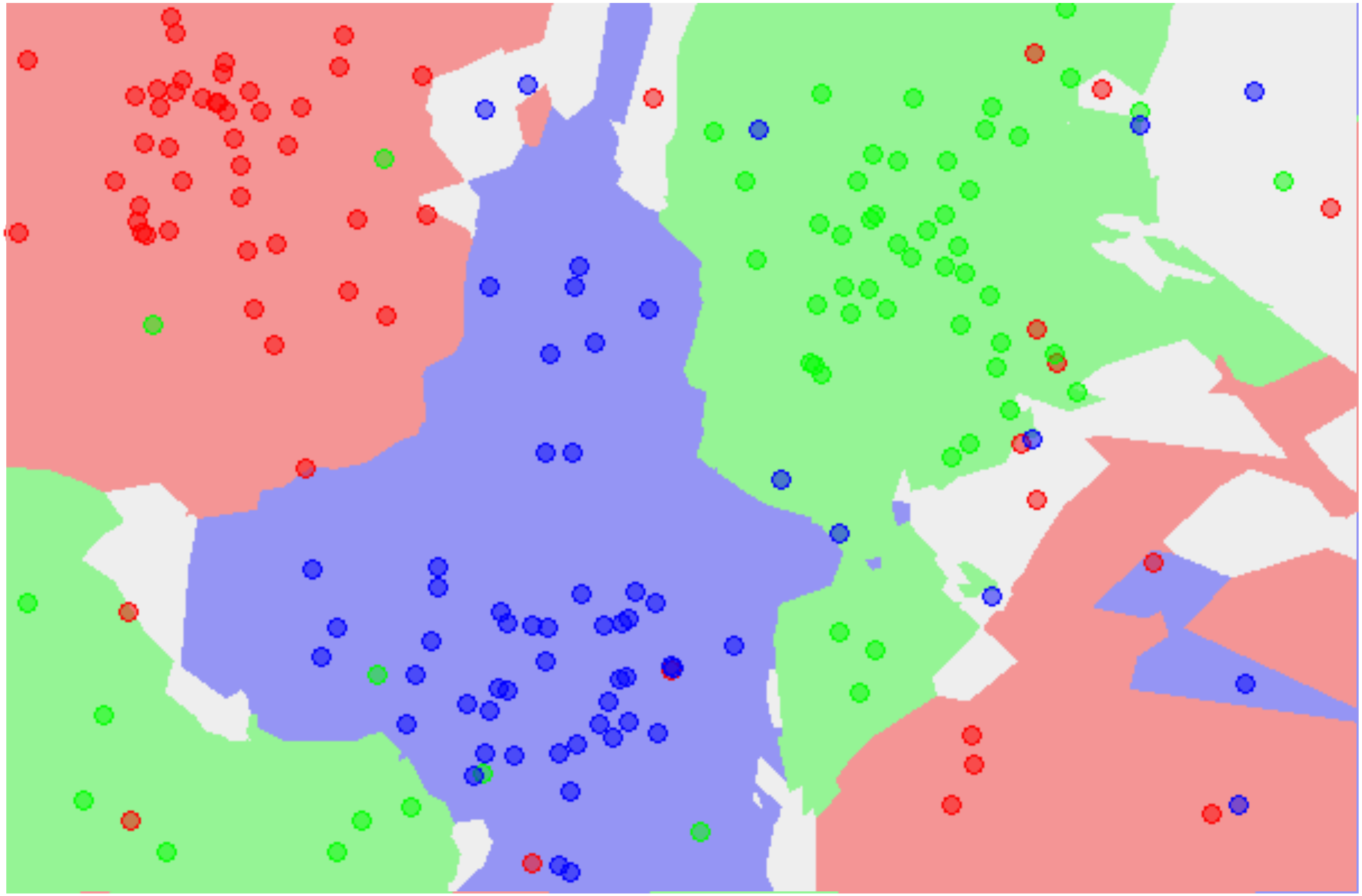
Training data for NN classifier (in R^2)



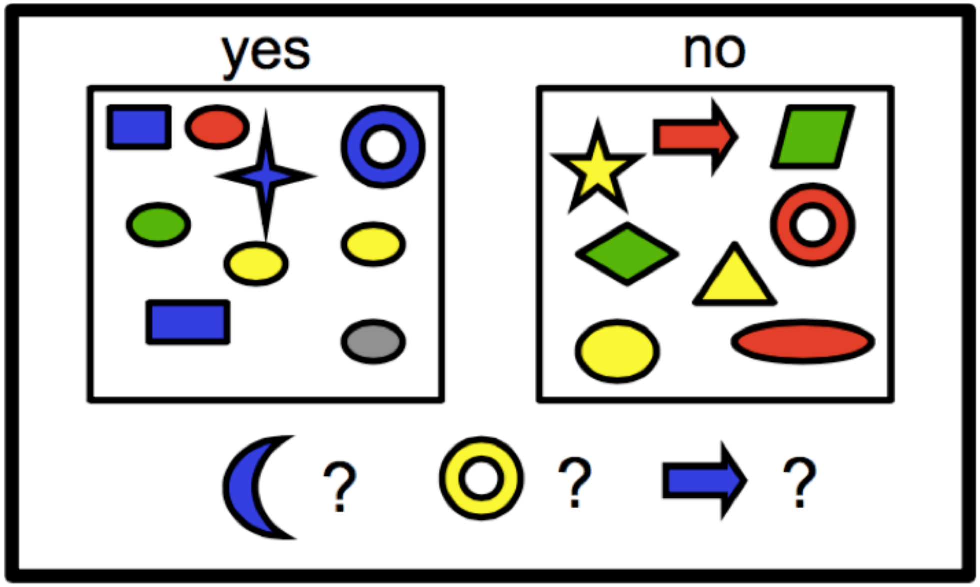
1-nn classifier prediction (in R^2)



3-nn classifier prediction



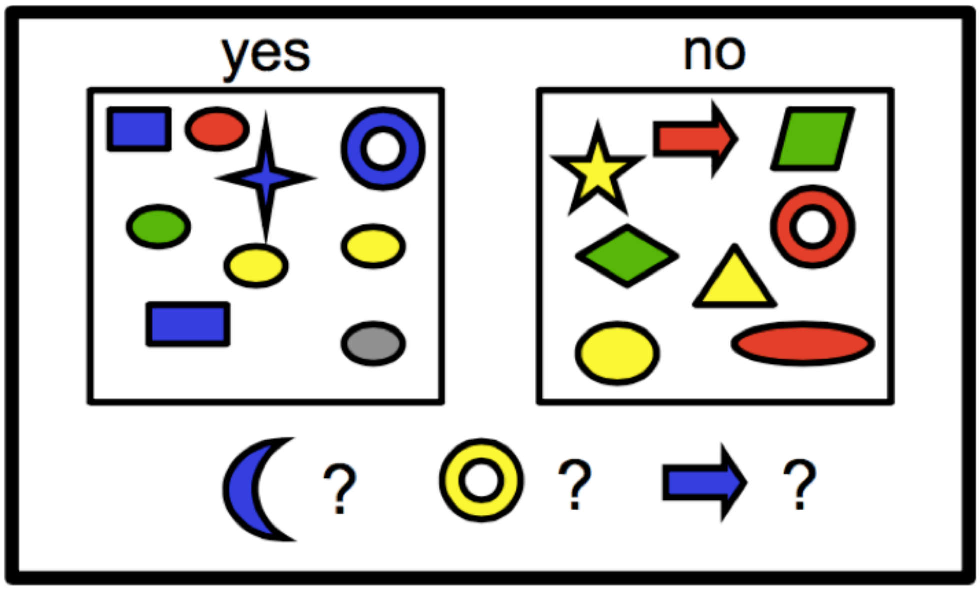
Method example: decision tree



Features: color, shape, size

Machine learning: can work also for discrete inputs, strings, trees, graphs,…

Method example: decision tree



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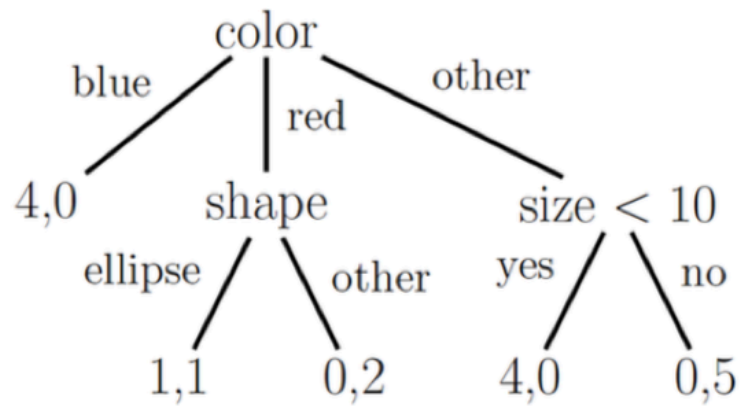
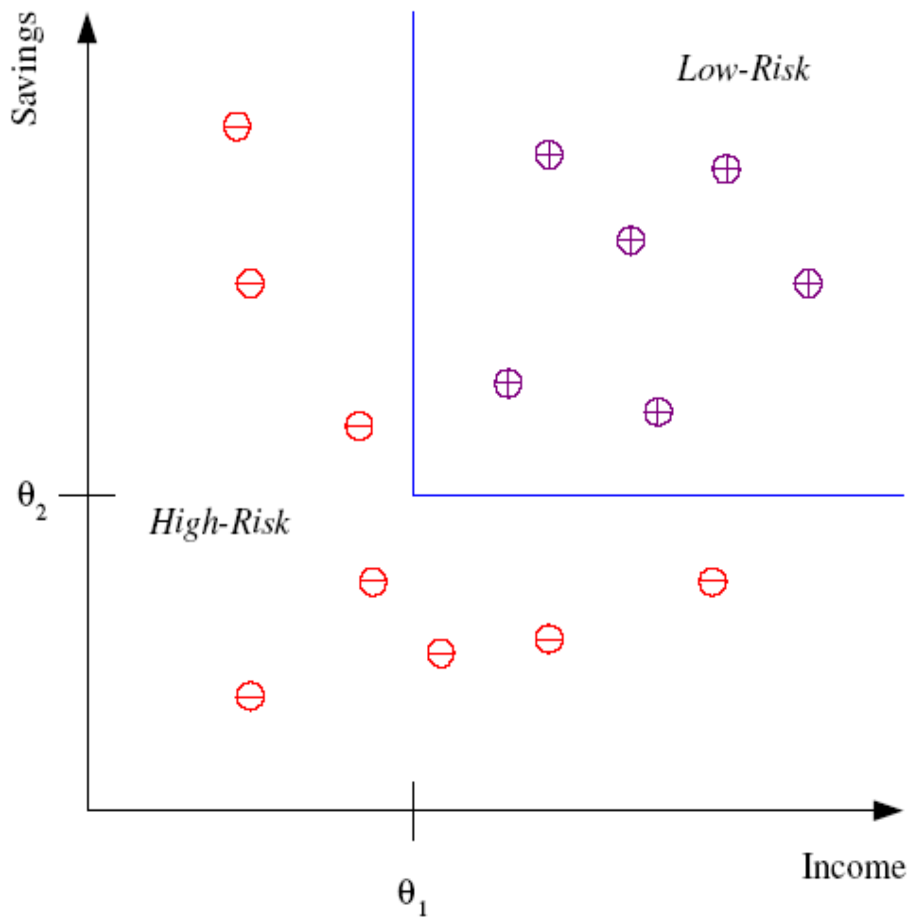
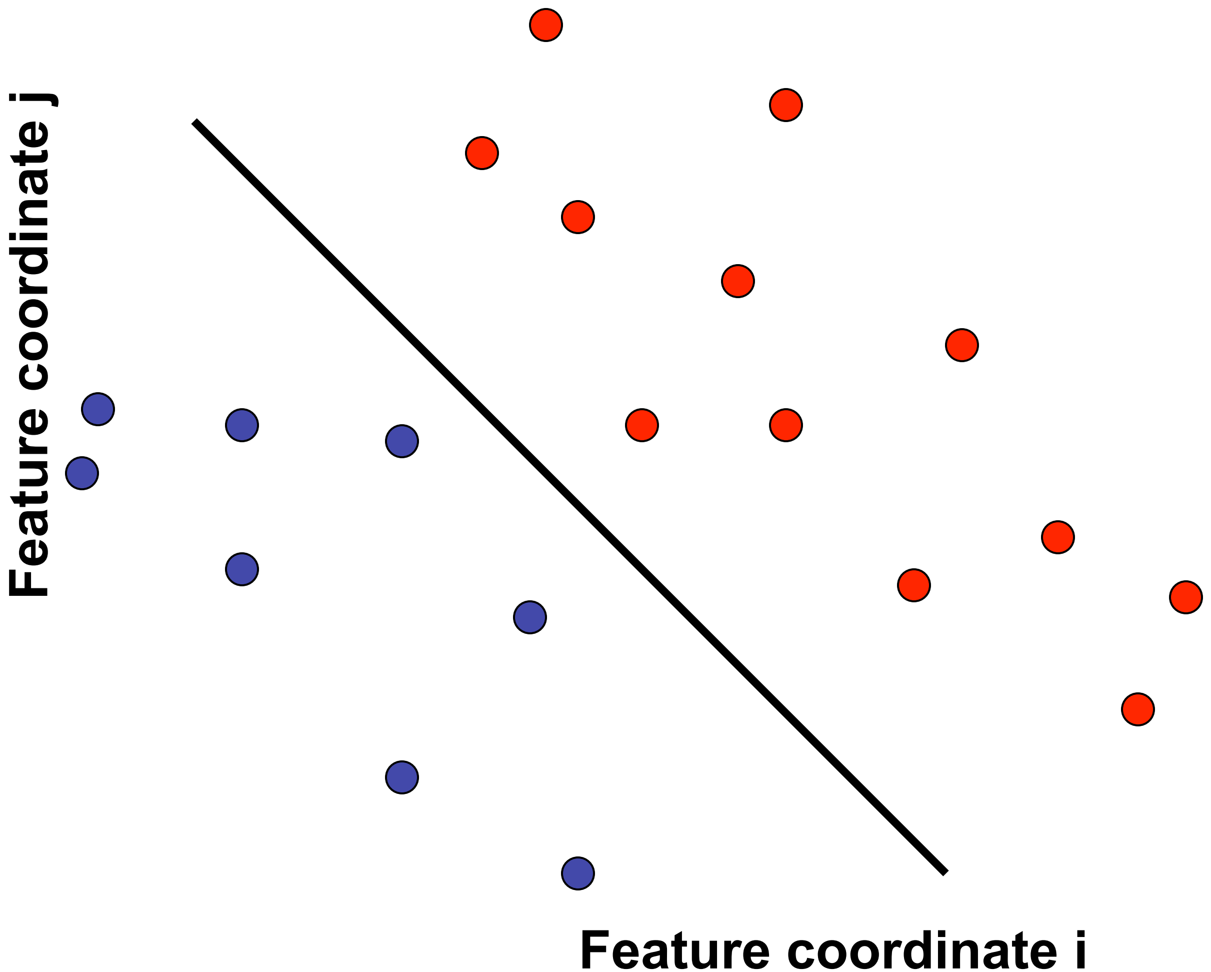


Method example: decision tree

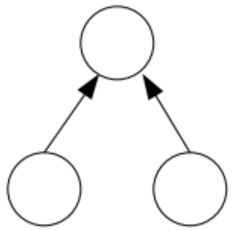
What is the depth of the decision tree for this problem?

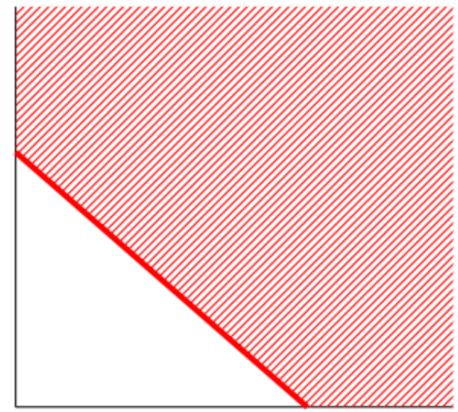


Method example: linear classifier



Method example: neural network

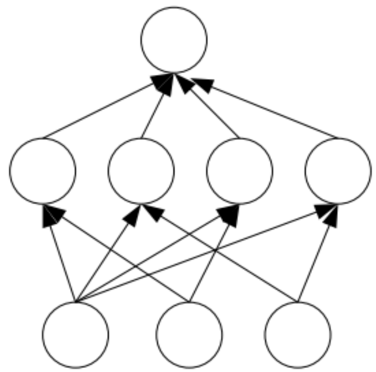


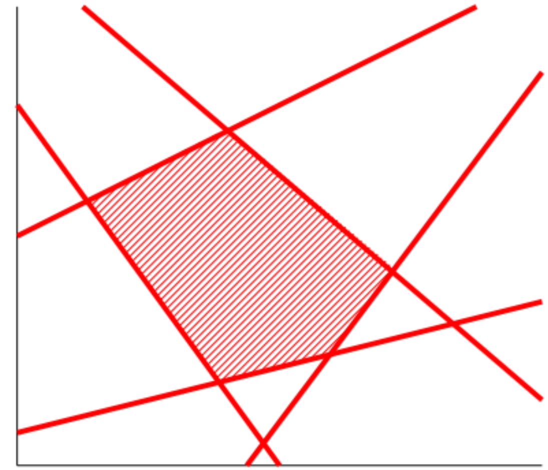


separating hyperplane

Method example: neural network

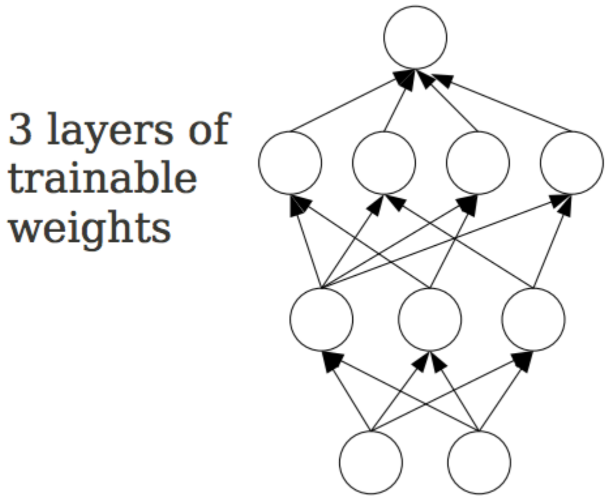
2 layers of trainable weights

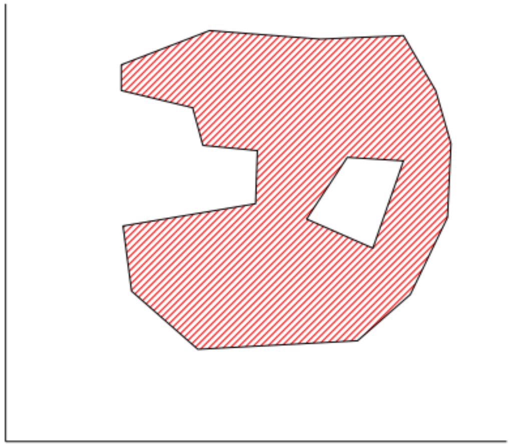




convex polygon region

Method example: neural network





composition of polygons:
convex regions

We have two centuries of material to cover!

https://en.wikipedia.org/wiki/Least_squares

The first clear and concise exposition of the method of least squares was published by Legendre in **1805.**

The technique is described as an **algebraic procedure** for **fitting linear equations to data** and Legendre demonstrates the new method by analyzing the same data as Laplace for the shape of the earth.

The value of Legendre's method of least squares was immediately recognized by leading astronomers and geodesists of the time

What we want to learn: a function

- Input-output mapping

method

prediction

$$y = f_w(x) = f(x; w)$$

parameters

Input

$$w \in \mathbb{R}$$

$$\mathbf{w} \in \mathbb{R}^K$$

Assumption: linear function

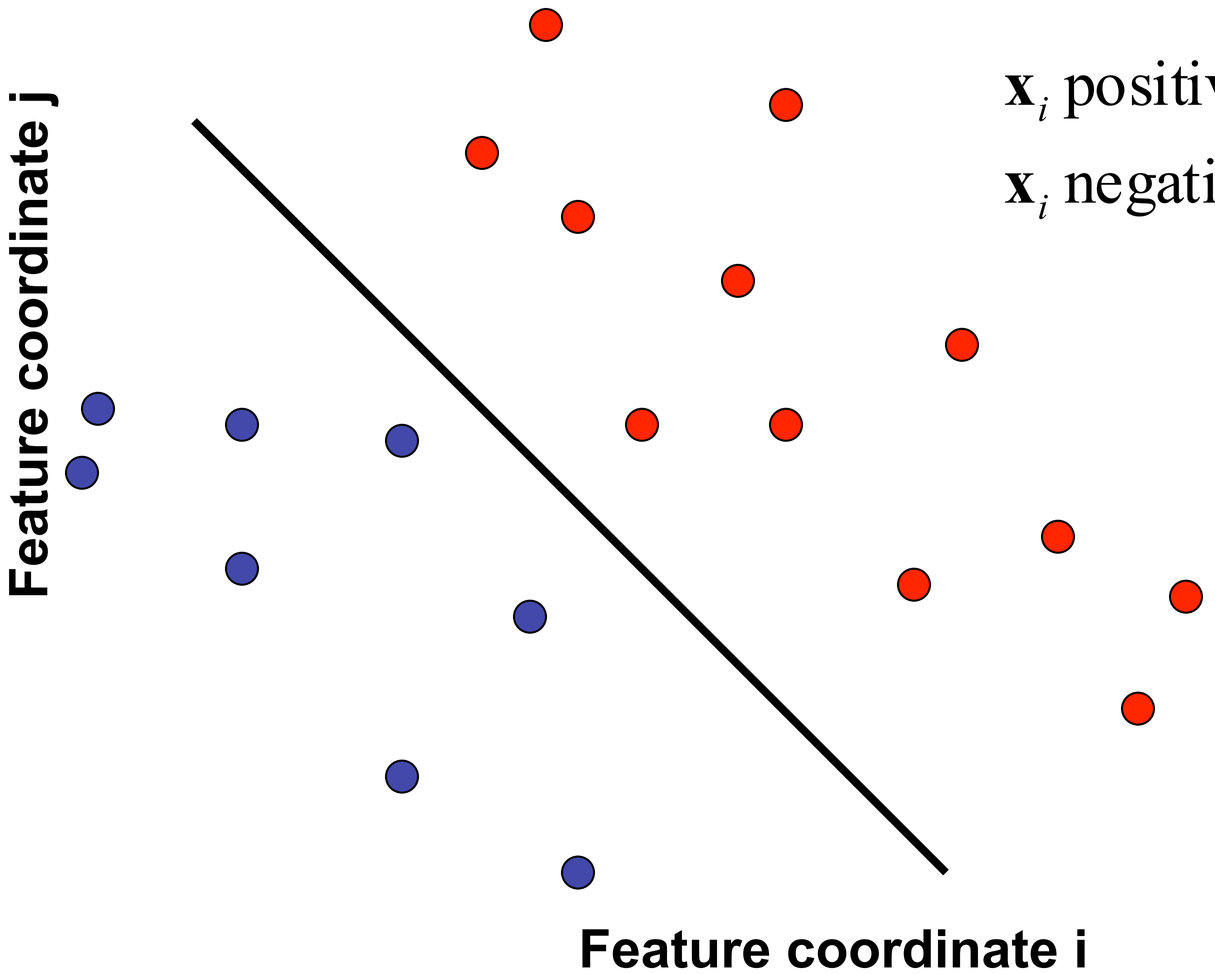
$$y = f_{\mathbf{w}}(\mathbf{x}) = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x}$$

Inner product:

$$\mathbf{w}^T \mathbf{x} = \langle \mathbf{w}, \mathbf{x} \rangle = \sum_{d=1}^{D} \mathbf{w}_d \mathbf{x}_d$$

$$\mathbf{x} \in \mathbb{R}^D, \mathbf{w} \in \mathbb{R}^D$$

Reminder: linear classifier



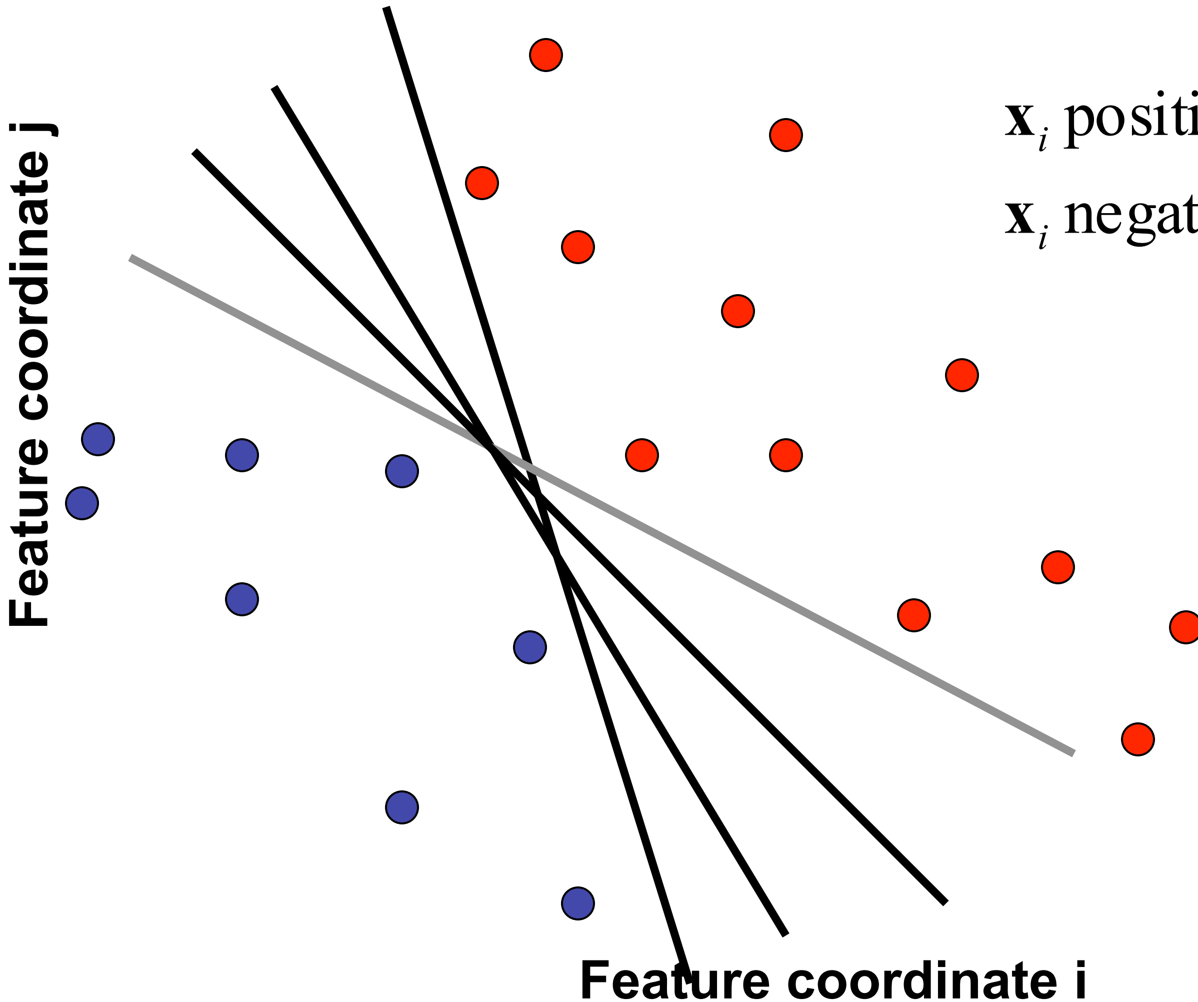
$$\mathbf{x}_i \text{ positive}: \quad \mathbf{x}_i \cdot \mathbf{w} + b \geq 0$$

$$\mathbf{x}_i \text{ negative}: \quad \mathbf{x}_i \cdot \mathbf{w} + b < 0$$

Each data point has a class label:

$$y_t = \begin{cases} +1 \ (\ ) \\ -1 \ (\ ) \end{cases}$$

Question: which one?



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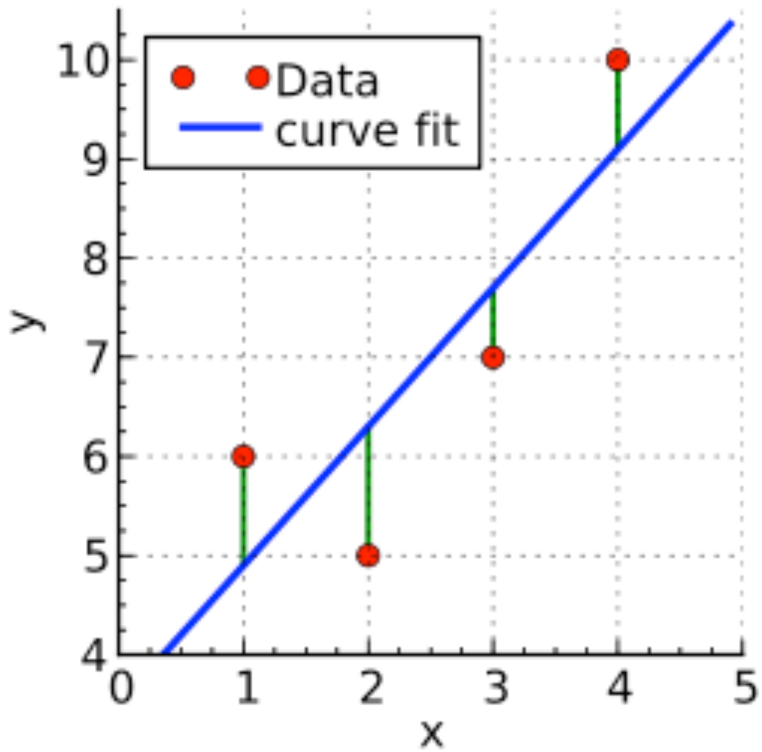
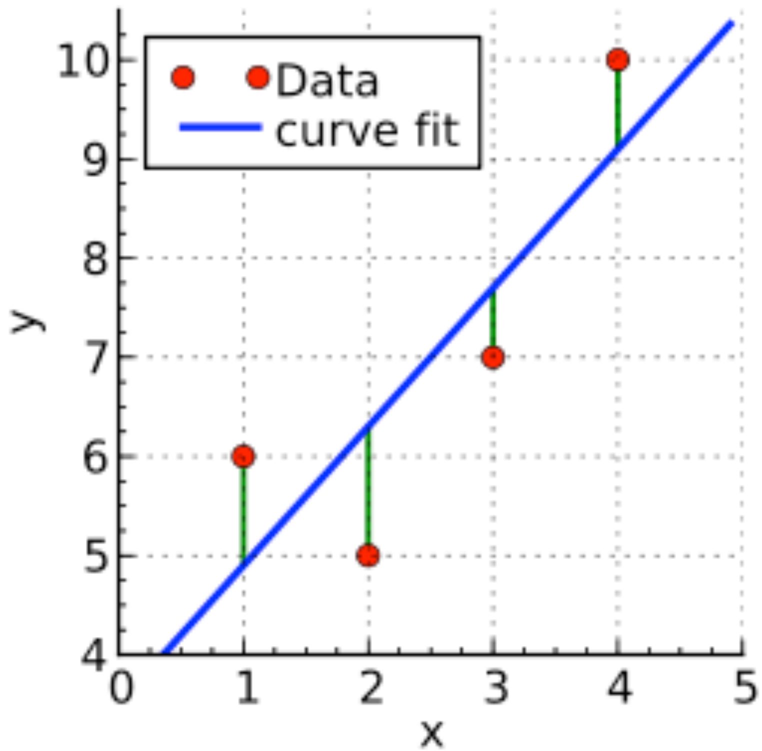
Linear regression in 1D



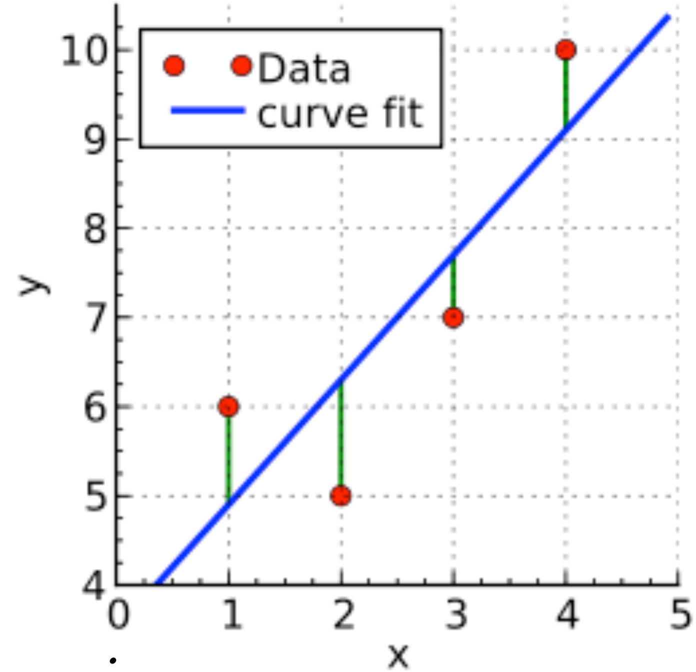
Linear regression in 1D



Training set: input–output pairs $\mathcal{S} = \{(x^i, y^i)\}, \quad i = 1 \ldots, N$

$$x^i \in \mathbb{R}, \quad y^i \in \mathbb{R}$$

Linear regression in 1D



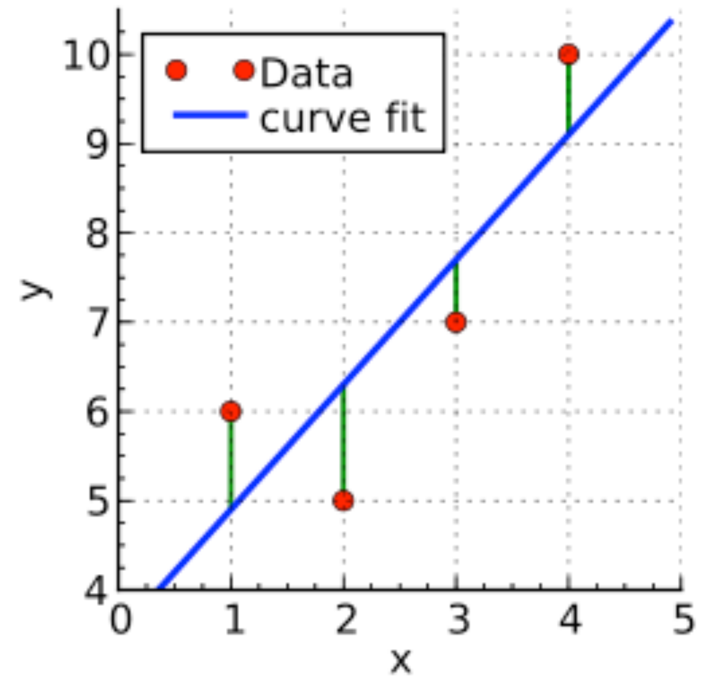
$$y^i = w_0 + w_1 x_1^i + \epsilon^i$$

$$= w_0 x_0^i + w_1 x_1^i + \epsilon^i, \quad x_0^i = 1, \quad \forall i$$

$$= \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$

Sum of squared errors criterion

$$y^i = \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$



Loss function: sum of squared errors

$$L(\mathbf{w}) = \sum_{i=1}^{N} (\epsilon^i)^2$$

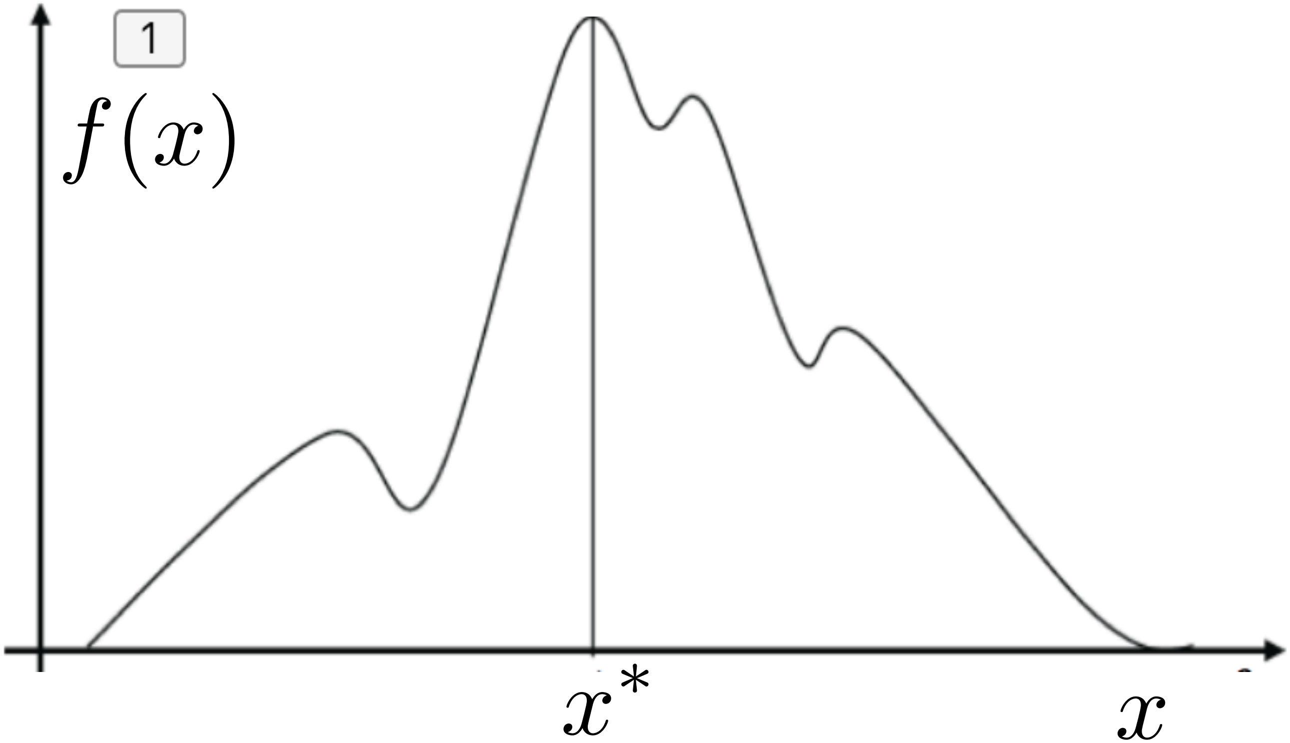
Expressed as a function of two variables:

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2$$

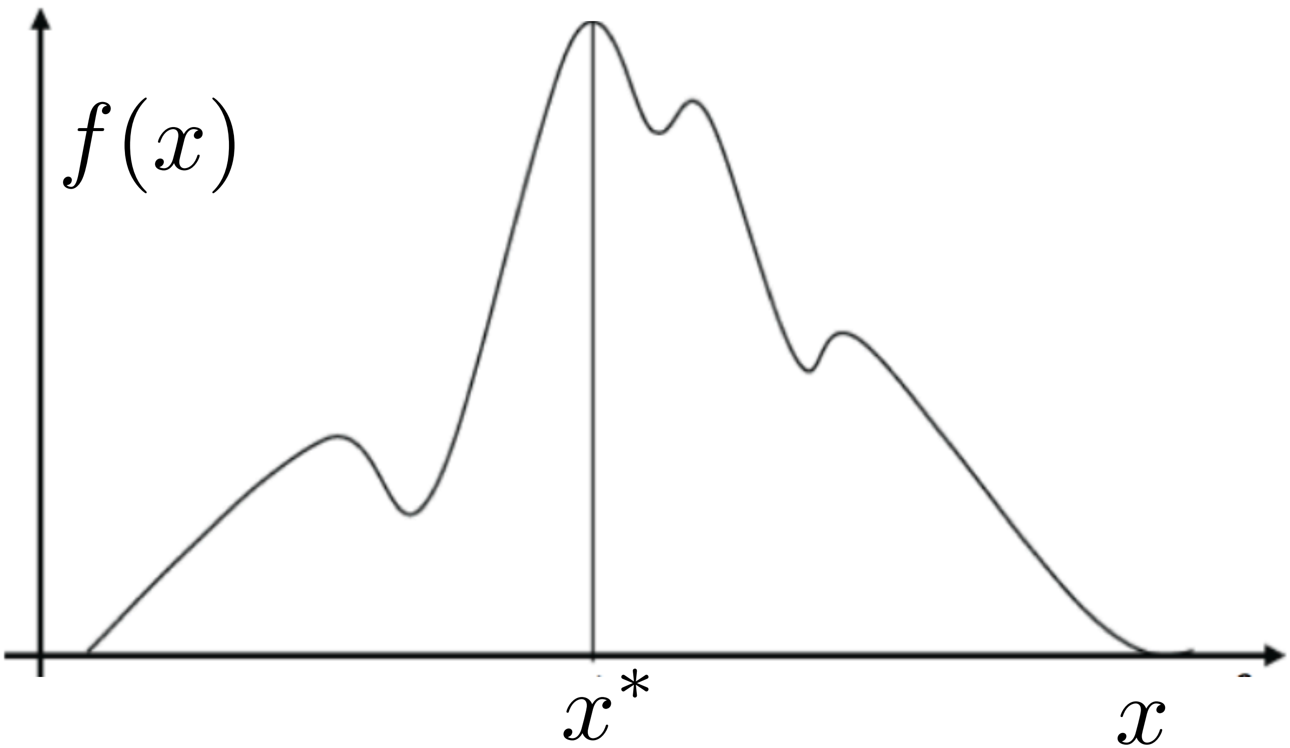
Question: what is the best (or least bad) value of w?

Answer: least squares

Calculus 101

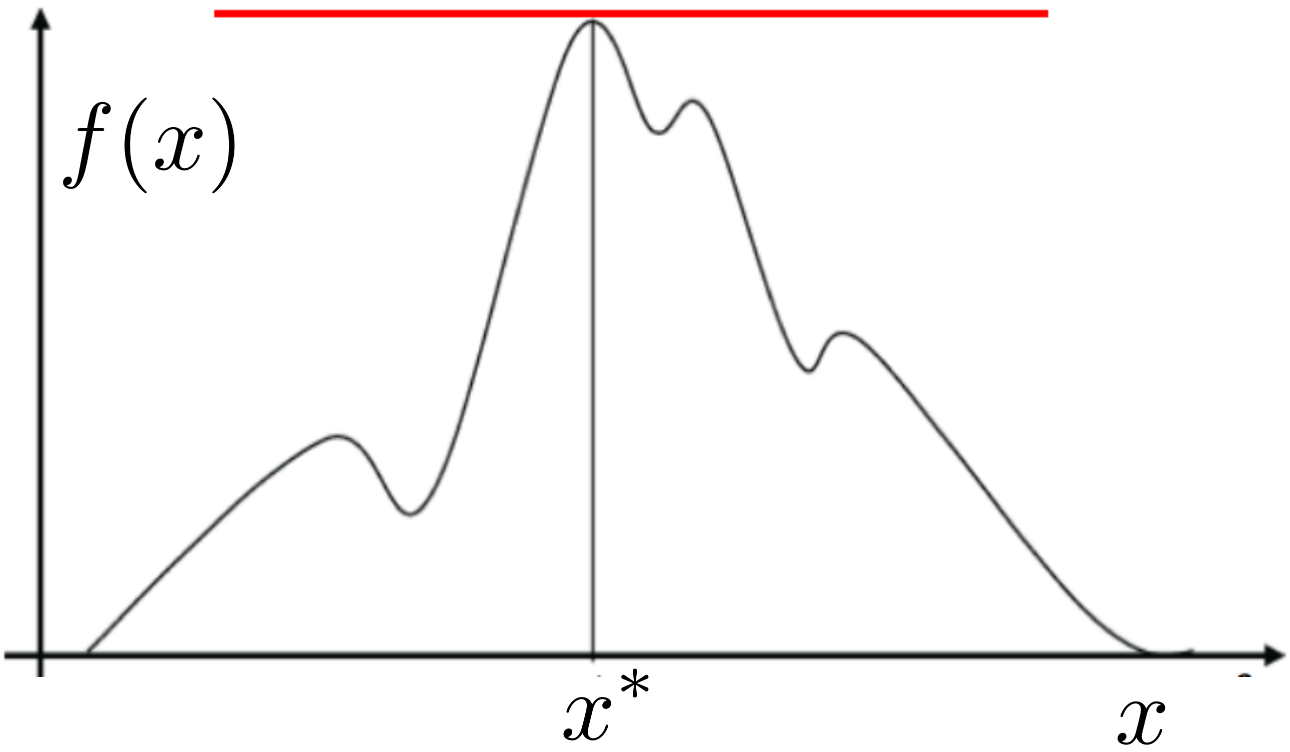


Calculus 101



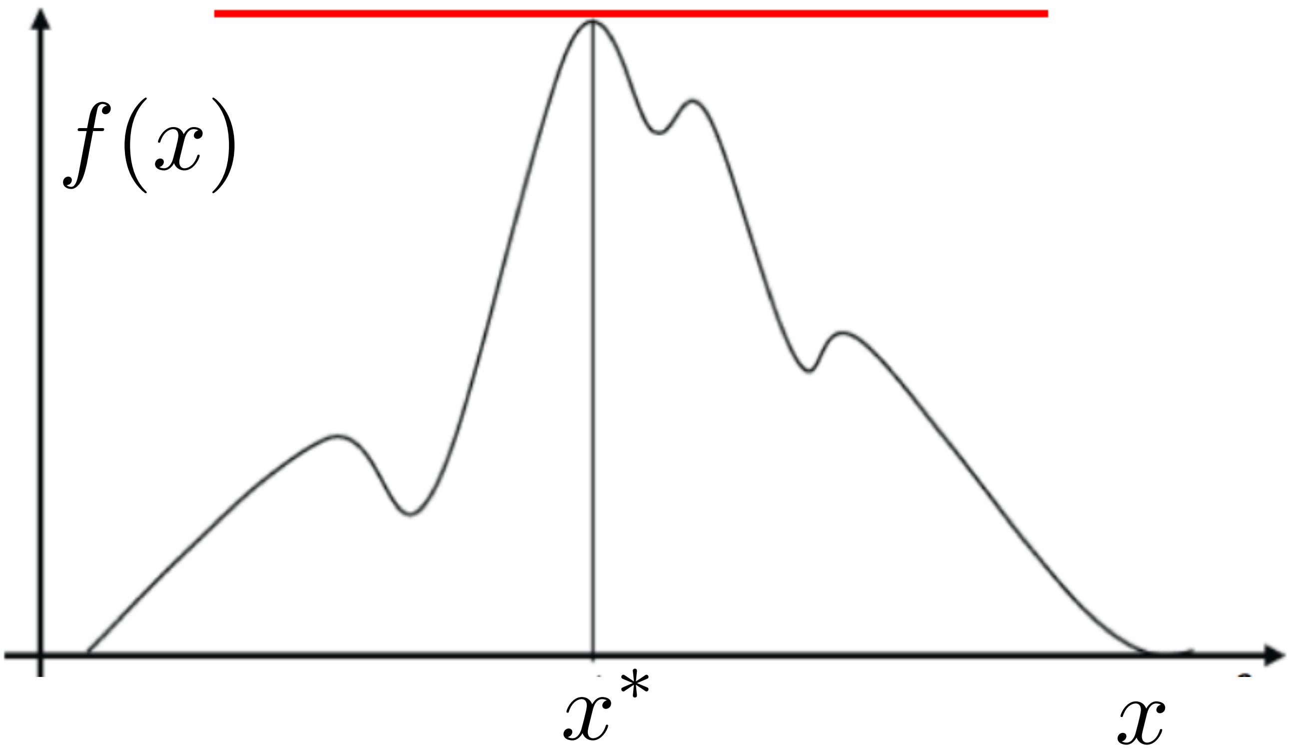
$$x^* = \mathrm{argmax}_x f(x)$$

Condition for maximum: derivative is zero



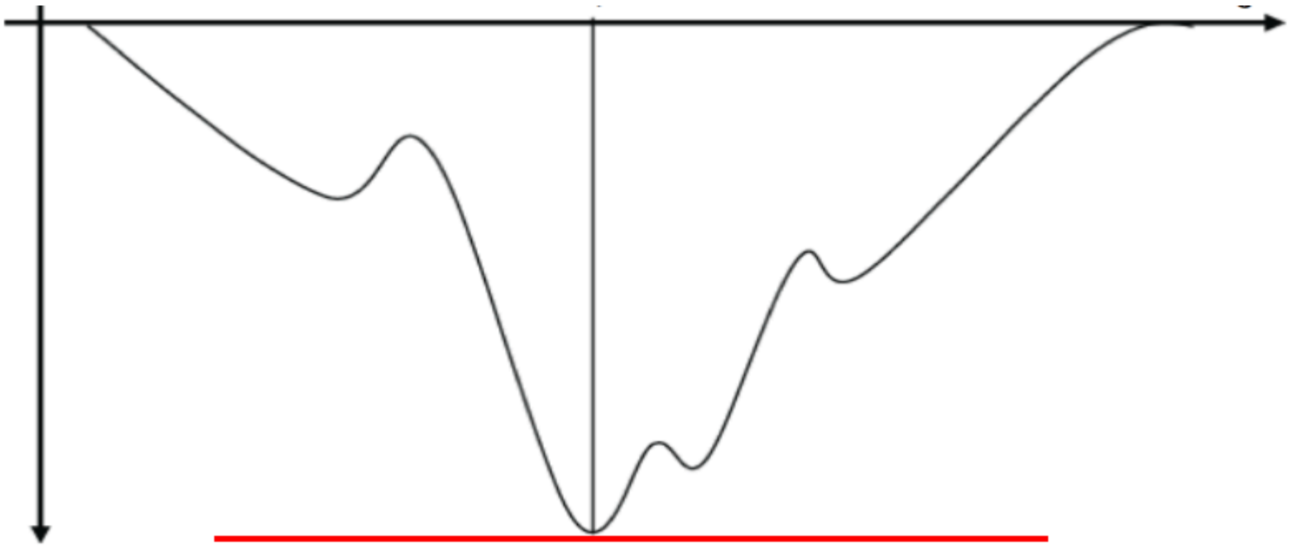
$$x^* = \mathrm{argmax}_x f(x)$$

Condition for maximum: derivative is zero



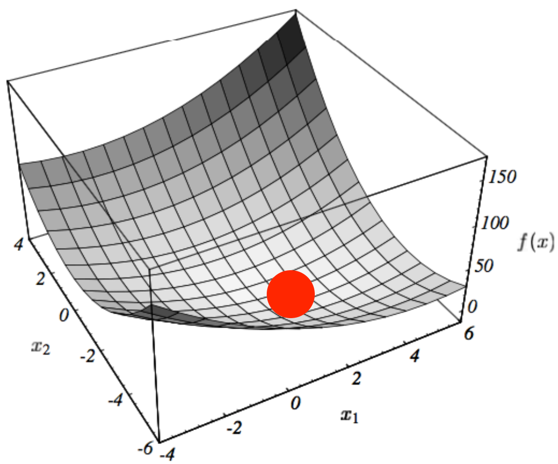
$$x^* = \mathrm{argmax}_x f(x) \quad \rightarrow \quad f'(x^*) = 0$$

Condition for minimum: derivative is zero



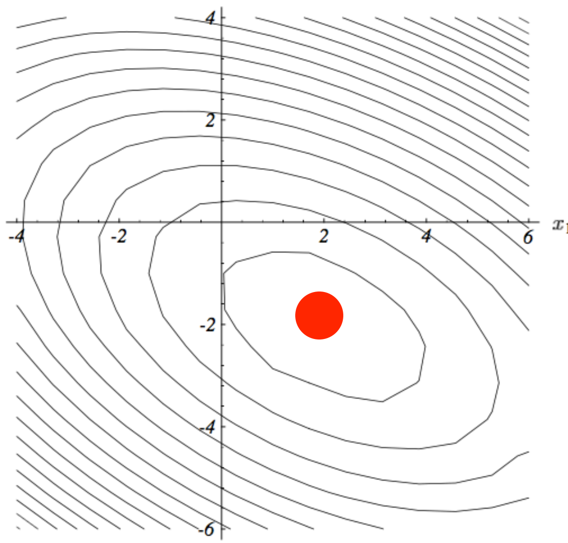
$$x^* = \text{argmin}_x f(x) \quad \rightarrow \quad f'(x^*) = 0$$

Vector calculus 101



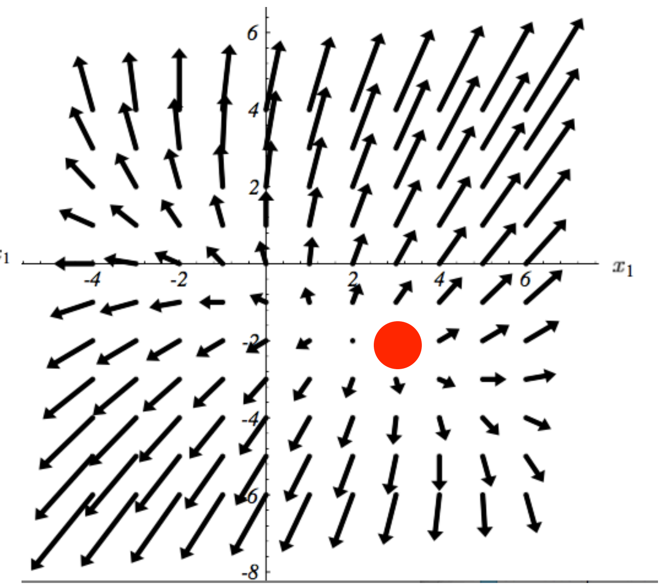
$$f(\mathbf{x})$$

2D function graph



$$f(\mathbf{x}) = c$$

isocontours



$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

gradient field

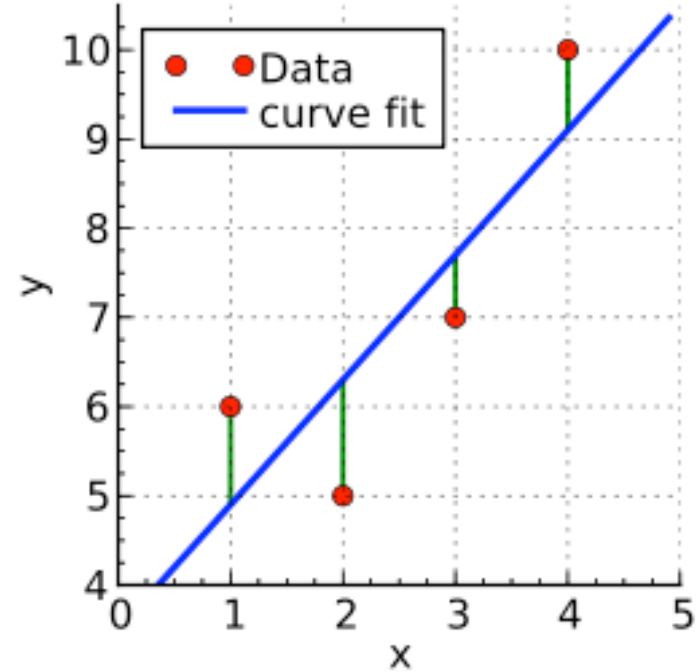
● **at minimum of function:** $\nabla f(\mathbf{x}) = \mathbf{0}$

Back to least squares..

$$y^i = \mathbf{w}^T \mathbf{x}^i + \epsilon^i$$

Loss function: sum of squared errors

$$L(\mathbf{w}) = \sum_{i=1}^{N} (\epsilon^i)^2$$



Expressed as a function of two variables:

training sample

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i \right) \right]^2$$

feature dimension

Question: what is the best (or least bad) value of w?

Answer: least squares

Fitting a line

$$L(w_0, w_1) = \sum_{i=1}^{N} \left[y^i - \left(w_0 x_0^i + w_1 x_1^i\right)\right]^2$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = \sum_{i=1}^{N} \frac{\partial \left[y^i - \left(w_0 x_0^i + w_1 x_1^i\right)\right]^2}{\partial w_0}$$

$$= \sum_{i=1}^{N} 2\left[y^i - \left(w_0 x_0^i + w_1 x_1^i\right)\right]\left(-x_0^i\right)$$

$$= -2 \sum_{i=1}^{N} \left(y^i x_0^i - w_0 x_0^i x_0^i - w_1 x_1^i x_0^i\right)$$

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = 0_N \quad \Leftrightarrow$$

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

Fitting a line, continued

$$\frac{\partial L(w_0, w_1)}{\partial w_0} = 0 \quad \Leftrightarrow$$

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

$$\frac{\partial L(w_0, w_1)}{\partial w_1} = 0 \quad \Leftrightarrow$$

$$\sum_{i=1}^{N} y^i x_1^i = w_0 \sum_{i=1}^{N} x_0^i x_1^i + w_1 \sum_{i=1}^{N} x_1^i x_1^i$$

2 linear equations, 2 unknowns

Fitting a line, continued

$$\sum_{i=1}^{N} y^i x_0^i = w_0 \sum_{i=1}^{N} x_0^i x_0^i + w_1 \sum_{i=1}^{N} x_1^i x_0^i$$

$$\sum_{i=1}^{N} y^i x_1^i = w_0 \sum_{i=1}^{N} x_0^i x_1^i + w_1 \sum_{i=1}^{N} x_1^i x_1^i$$

2x2 system of equations:

$$\left[\begin{array}{c} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{array} \right] = \left[\begin{array}{cc} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{array} \right] \left[\begin{array}{c} w_0 \\ w_1 \end{array} \right]$$

That's it!

Fitting a line, continued

2x2 system of equations:

$$\left[\begin{array}{c} \sum_{i=1}^{N} y^i x_0^i \\ \sum_{i=1}^{N} y^i x_1^i \end{array}\right] = \left[\begin{array}{cc} \sum_{i=1}^{N} x_0^i x_0^i & \sum_{i=1}^{N} x_0^i x_1^i \\ \sum_{i=1}^{N} x_0^i x_1^i & \sum_{i=1}^{N} x_1^i x_1^i \end{array}\right] \left[\begin{array}{c} w_0 \\ w_1 \end{array}\right]$$

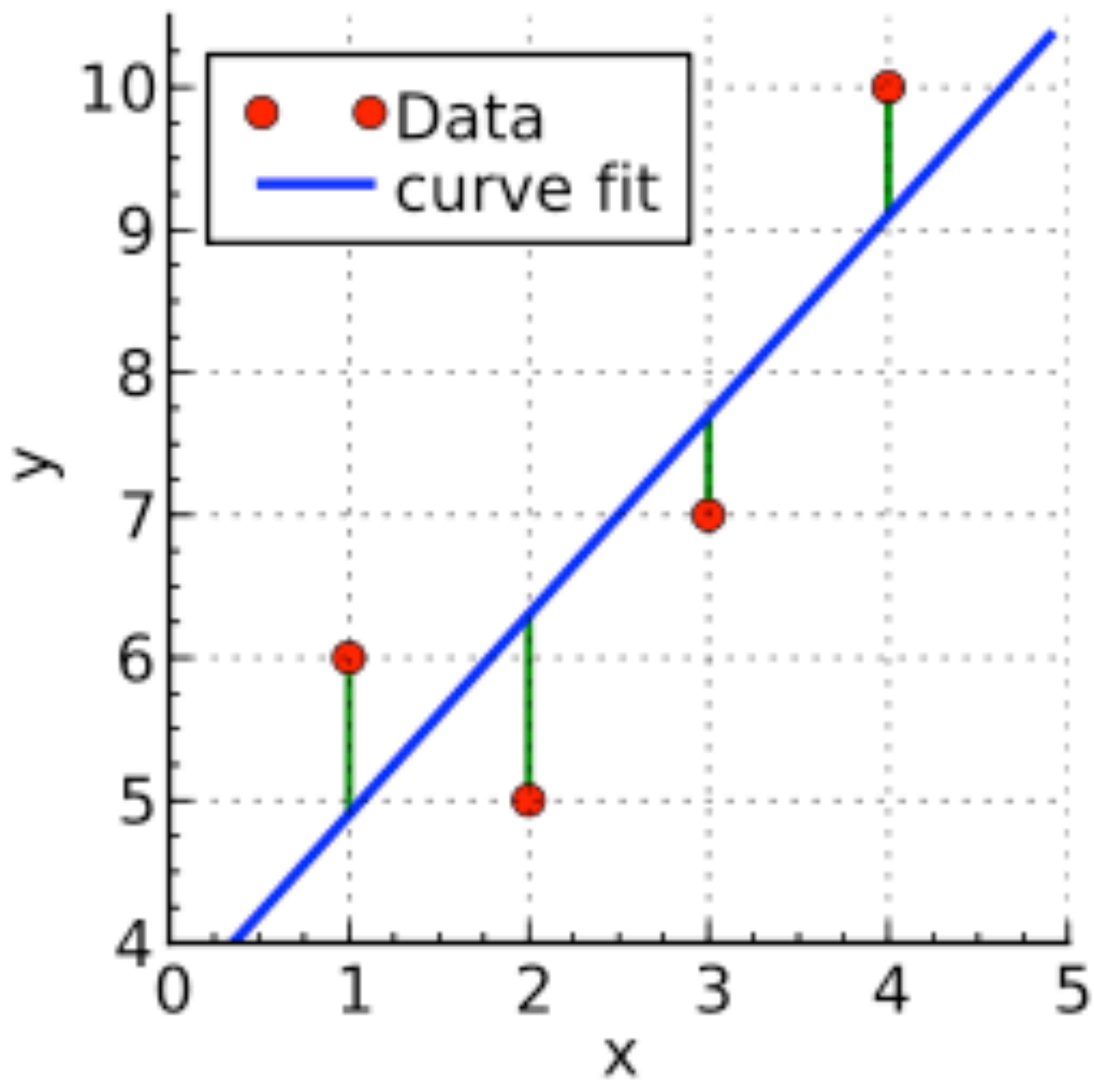
Or, without summations:

$$\mathbf{X}^T \mathbf{y} = \mathbf{X}^T \mathbf{X} \mathbf{w}$$

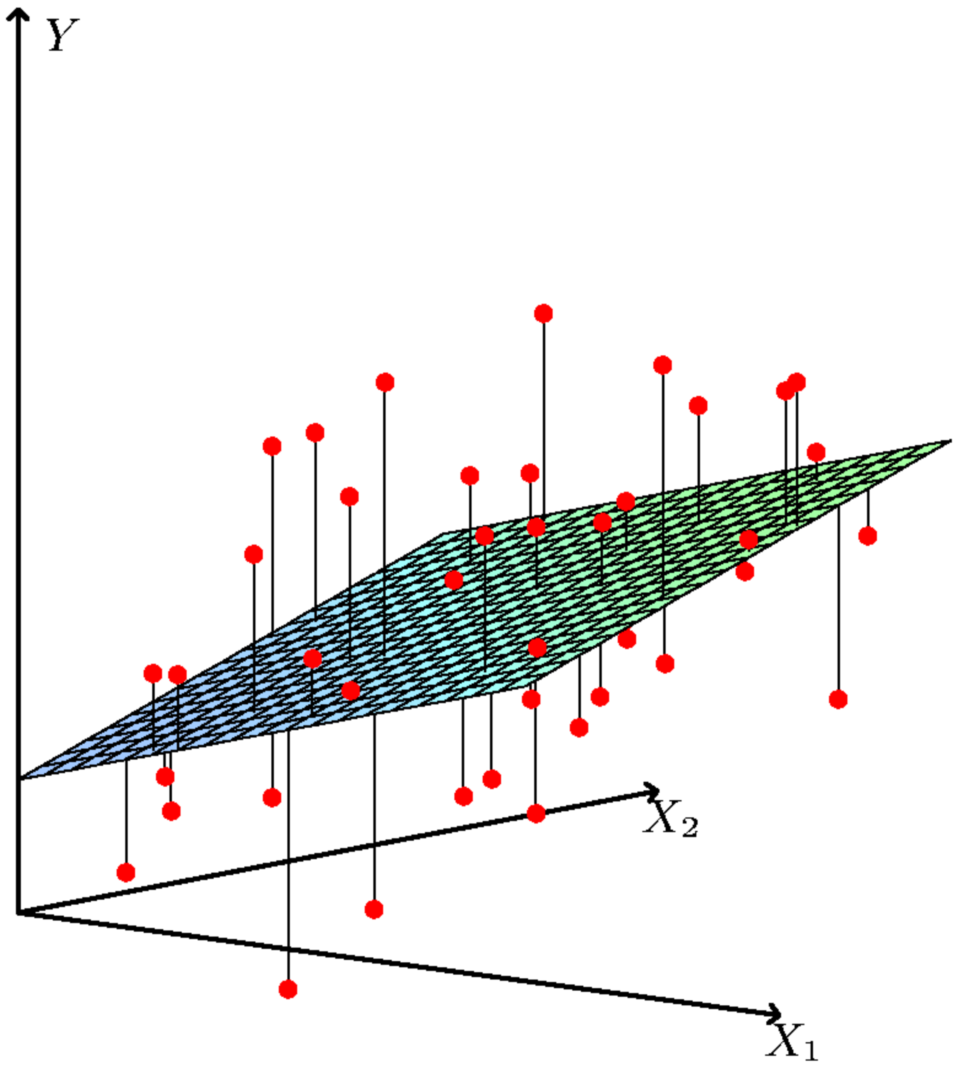
$$\mathbf{y} = \left[\begin{array}{c} y^1 \\ \vdots \\ y^N \end{array}\right] \quad \mathbf{X} = \left[\begin{array}{cc} x_0^1 & x_1^1 \\ \vdots & \vdots \\ x_0^N & x_2^N \end{array}\right]$$

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

Linear regression in 1D



Linear regression in 2D (or ND)



Least squares solution for linear regression

D: problem dimension

N: training set size

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} x_1^1 & \dots & x_D^1 \\ x_1^2 & \dots & x_D^2 \\ \vdots & & \\ x_1^N & \dots & x_D^N \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Nx1 **NxD** **Dx1** **Nx1**

Least squares solution for linear regression

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$

Least squares solution for linear regression

Loss function: $L(\mathbf{w}) = \sum_{i=1}^{N}(y^i - \mathbf{w}^T\mathbf{x}^i)^2 = \sum_{i=1}^{N}(\epsilon^i)^2$

$$L(\mathbf{w}) = \begin{bmatrix} \epsilon^1 & \epsilon^2 & \dots & \epsilon^N \end{bmatrix} \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

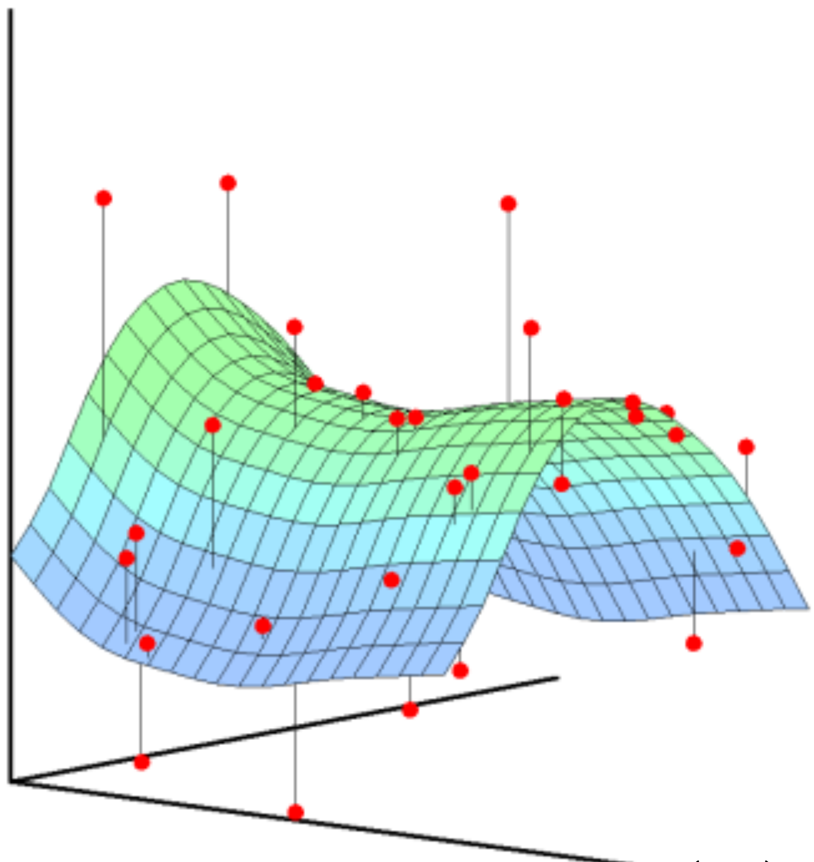
Least squares solution for linear regression

Loss function: $L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 = \sum_{i=1}^{N} (\epsilon^i)^2$

$$L(\mathbf{w}) = \left[\begin{array}{cccc} \epsilon^1 & \epsilon^2 & \dots & \epsilon^N \end{array} \right] \left[\begin{array}{c} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{array} \right]$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \qquad \mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$

Generalized linear regression



$$\mathbf{x} \to \boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \vdots \\ \phi_M(\mathbf{x}) \end{bmatrix}$$

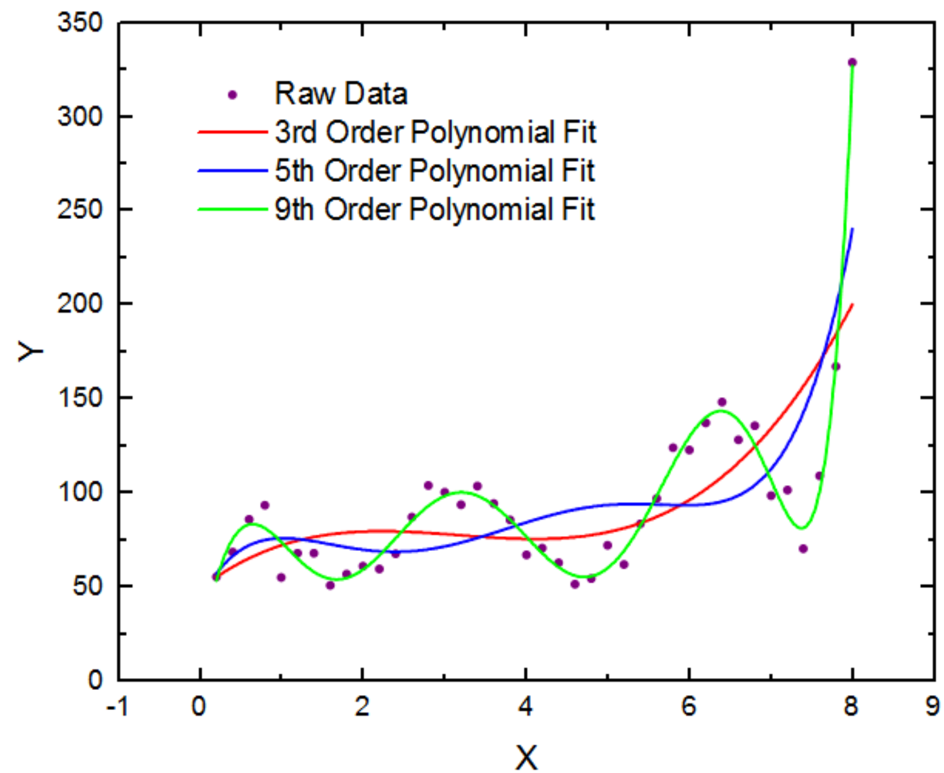
1D Example: 2nd degree polynomial fitting

$$\boldsymbol{\phi}(x) = \begin{bmatrix} 1 \\ x \\ (x)^2 \end{bmatrix}$$

$$\langle \mathbf{w}, \boldsymbol{\phi}(x) \rangle = w_0 + w_1 x + w_2 (x)^2$$

1D Example: k-th degree polynomial fitting

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x \\ \vdots \\ (x)^K \end{bmatrix}$$



$$\langle \mathbf{w}, \boldsymbol{\phi}(x) \rangle = w_0 + w_1 x + \ldots + w_k (x)^K$$

2D example: second-order polynomials

$$\mathbf{x} = (x_1, x_2)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ (x_1)^2 \\ (x_2)^2 \\ x_1 x_2 \end{bmatrix}$$

$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

Reminder: linear regression

Loss function: $$L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 = \sum_{i=1}^{N} (\epsilon^i)^2$$

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} x_1^1 & \dots & x_D^1 \\ x_1^2 & \dots & x_D^2 \\ \vdots & & \\ x_1^N & \dots & x_D^N \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Reminder: linear regression

Loss function: $L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \mathbf{x}^i)^2 = \sum_{i=1}^{N} (\epsilon^i)^2$

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} (\mathbf{x}^1)^T \\ \hline (\mathbf{x}^2)^T \\ \hline \vdots \\ \hline (\mathbf{x}^N)^T \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Generalized linear regression

Loss function: $L(\mathbf{w}) = \sum_{i=1}^{N} (y^i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}^i))^T = \sum_{i=1}^{N} (\epsilon^i)^2$

$$\begin{bmatrix} y^1 \\ y^2 \\ \vdots \\ y^N \end{bmatrix} = \begin{bmatrix} \boldsymbol{\phi}(\mathbf{x}^1)^T \\ \hline \boldsymbol{\phi}(\mathbf{x}^2)^T \\ \hline \vdots \\ \hline \boldsymbol{\phi}(\mathbf{x}^N)^T \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_M \end{bmatrix} + \begin{bmatrix} \epsilon^1 \\ \epsilon^2 \\ \vdots \\ \epsilon^N \end{bmatrix}$$

Nx1 **NxM** **Mx1** **Nx1**

$$\boldsymbol{\phi}(\mathbf{x}) : \mathbb{R}^D \rightarrow \mathbb{R}^M$$

Least squares solution for linear regression

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$

$$\mathbf{X} = \begin{bmatrix} (\mathbf{x}^1)^T \\ \hline (\mathbf{x}^2)^T \\ \hline \vdots \\ \hline (\mathbf{x}^N)^T \end{bmatrix}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon}$$

Minimize:

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

Least squares solution for generalized linear regression

$$\mathbf{y} = \mathbf{\Phi}\mathbf{w} + \boldsymbol{\epsilon}$$

$$\mathbf{\Phi} = \begin{bmatrix} \phi(\mathbf{x}^1)^T \\ \hline \phi(\mathbf{x}^2)^T \\ \hline \vdots \\ \hline \phi(\mathbf{x}^N)^T \end{bmatrix}$$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon}$$

Minimize:

$$\mathbf{w}^* = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}\mathbf{y}$$

2D example: second-order polynomials

$$\mathbf{x} = (x_1, x_2)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ (x_1)^2 \\ (x_2)^2 \\ x_1 x_2 \end{bmatrix}$$

$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

5D Example: fourth-order polynomials in 5D

$$\mathbf{x} = (x_1, \ldots, x_5)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_5 \\ \vdots \\ (x_1 x_2 x_3 x_4 x_5)^4 \end{bmatrix}$$

15625 Dimensions =>15625 parameters

What was happening before: approximations

Training: $S = \{(\mathbf{x}^i, y^i)\}, i =, 1, \ldots, N$

$$y^1 \simeq w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 \simeq w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

$$\vdots$$

$$y^N \simeq w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

If N>D (e.g. 30 points, 2 dimensions) we have more equations than unknowns: **overdetermined** system!

Input-output relations can only hold approximately!

What is happening now: overfitting

Training: $S = \{(\mathbf{x}^i, y^i)\}, i =, 1, \ldots, N$

$$y^1 = w_0 x_0^1 + w_1 x_1^1 + \ldots + w_D x_D^1$$

$$y^2 = w_0 x_0^2 + w_1 x_1^2 + \ldots + w_D x_D^2$$

$$\vdots$$

$$y^N = w_0 x_0^N + w_1 x_1^N + \ldots + w_D x_D^N$$

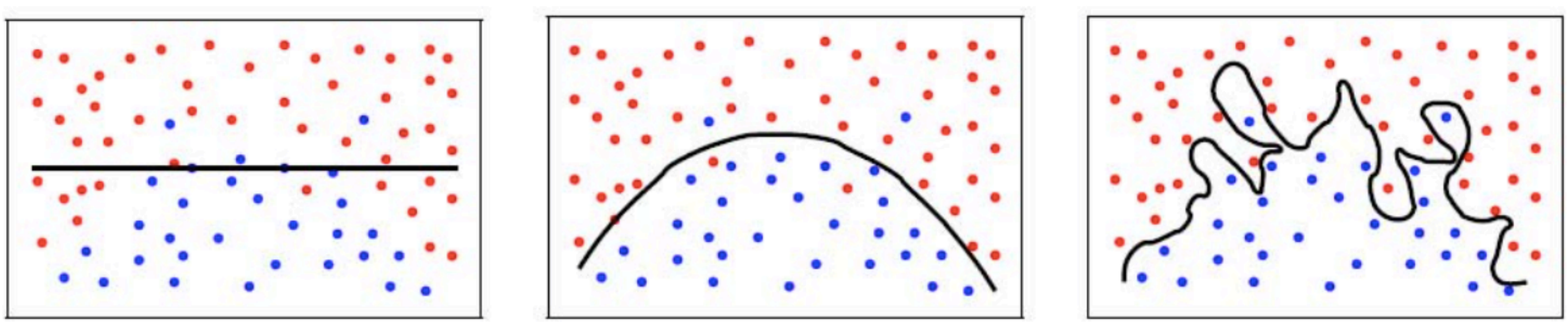
If N<D (e.g. 30 points, 15265 dimensions) we have more unknowns than equations: **underdetermined** system!

Input-output equations hold exactly, but we are simply memorizing data

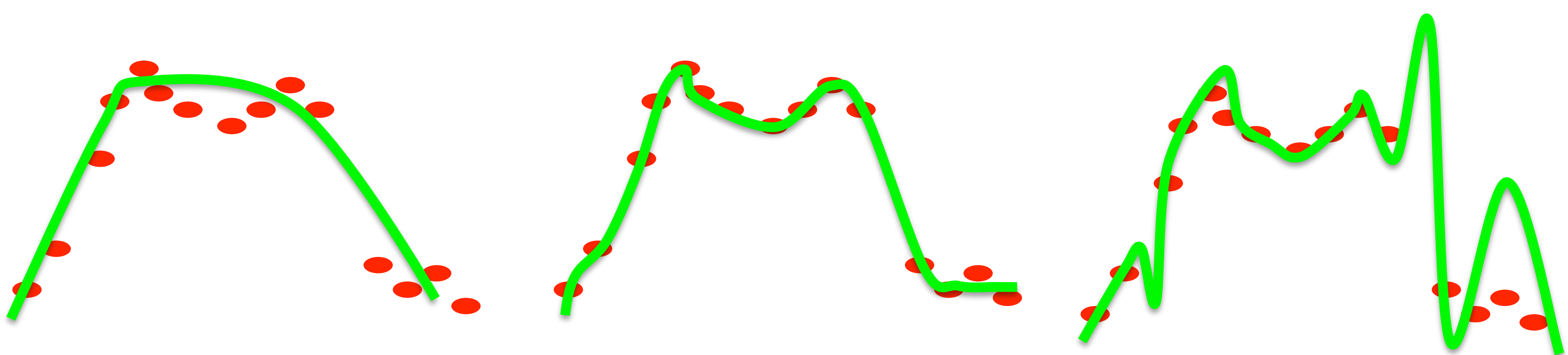
Overfitting, in images

Classification

Underfitting | just right | Overfitting



Regression



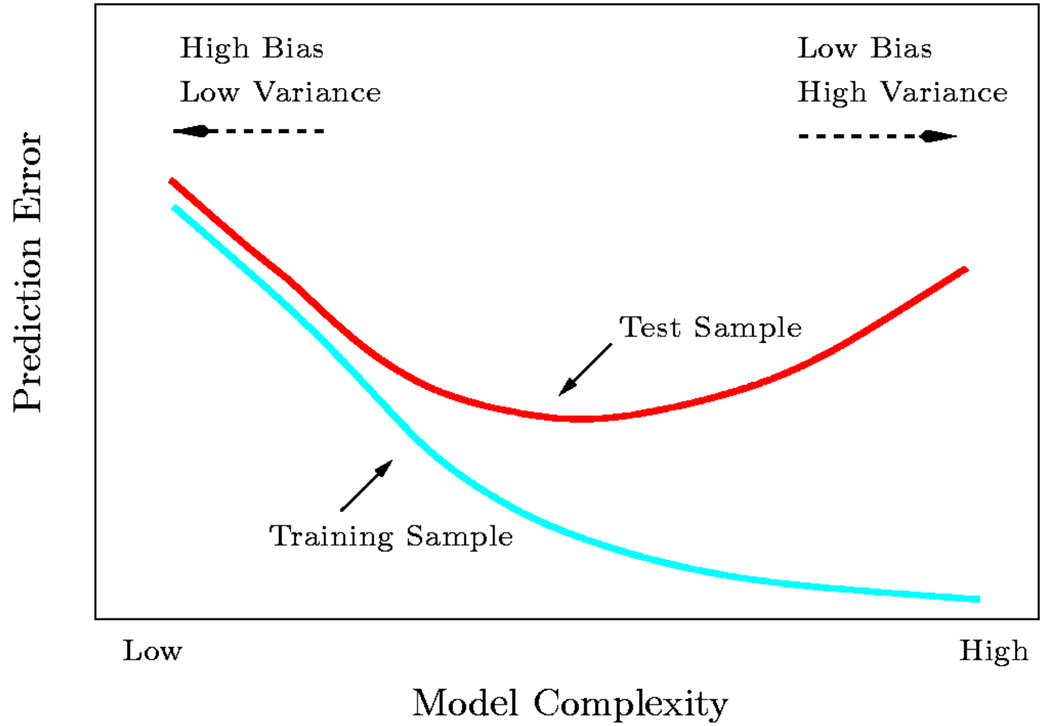
Tuning the model's complexity

A flexible model approximates the target function well in the training set

but can "overtrain" and have poor performance on the test set ("variance")

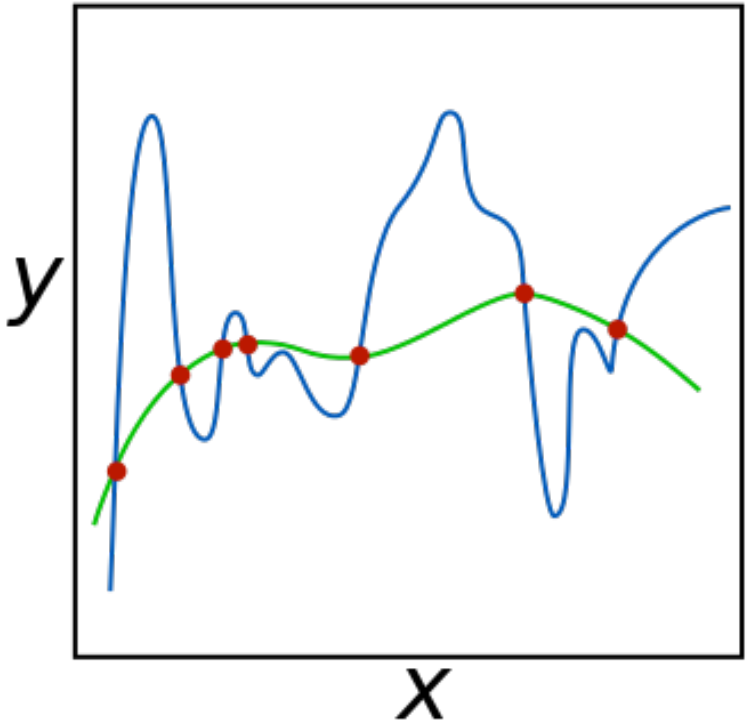
A rigid model's performance is more predictable in the test set

but the model may not be good even on the training set ("bias")



Regularization: keeping it simple

In high dimensions: too many solutions for the same problem



Regularization: prefer the least complex among them

How? Penalize complexity

How to control complexity?

Observation: problem started with high-dimensional embeddings

Guess: Number of dimensions relates to “complexity”

(Week 4: we will guess again!)

Intuition: with many parameters, we can fit anything

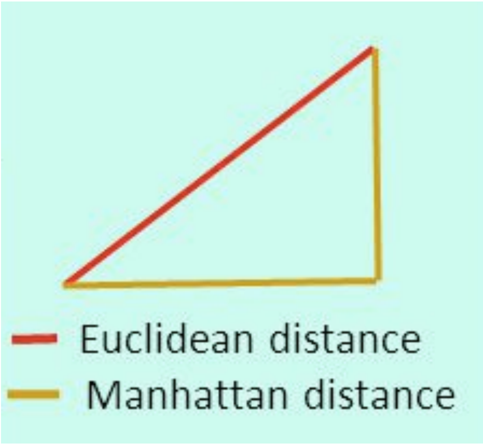
But what if we force the classifier not to use all of the parameters?

Idea: penalize the use of large parameter values

How do we measure “large”?

How do we enforce small values?

How do we measure “large”?



Method parameters: D-dimensional vector

$$\mathbf{w} = [w_1, w_2, \ldots, w_D]$$

“Large” vector: vector **norm**

L2, (“euclidean”) norm:

$$\|\mathbf{w}\|_2 \doteq \sqrt{\sum_{d=1}^{D} w_d^2} = \sqrt{\langle \mathbf{w}, \mathbf{w} \rangle}$$

L1, (“manhattan”) norm:

$$\|\mathbf{w}\|_1 \doteq \sum_{d=1}^{D} |w_d|$$

Lp norm, p>1:

$$\|\mathbf{w}\|_p \doteq \left(\sum_{d=1}^{D} w_d^p \right)^{1/p}$$

Regularized linear regression

$$\boldsymbol{\epsilon} = \mathbf{y} - \boldsymbol{\Phi}\mathbf{w}$$ residual vector

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon}$$ linear regression: minimize model error

Complexity term: (regularizer) $R(\mathbf{w}) \doteq \|\mathbf{w}\|_2^2 = \mathbf{w}^T \mathbf{w}$

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} + \lambda \mathbf{w}^T \mathbf{w}$$

"data fidelity"

complexity

minimum remains to be determined

scalar, remains to be determined

Least squares solution

$$
\begin{aligned}
L(\mathbf{w}) &= \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} \\
&= (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X}\mathbf{w}
\end{aligned}
$$

Condition for minimum:

$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

$$-2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\mathbf{w}^* = \mathbf{0}$$

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

Ridge regression: L2-regularized linear regression

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T \boldsymbol{\epsilon} + \lambda \mathbf{w}^T \mathbf{w}$$

$$= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X} \mathbf{w} + \mathbf{w}^T \mathbf{X}^T \mathbf{X} \mathbf{w} + \lambda \mathbf{w}^T \mathbf{I} \mathbf{w}$$

as before, for linear regression

identity matrix

$$= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X} \mathbf{w} + \mathbf{w}^T \left(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I} \right) \mathbf{w}$$

Condition for minimum:

$$\nabla L(\mathbf{w}^*) = \mathbf{0}$$

$$-2\mathbf{X}^T \mathbf{y} + 2(\mathbf{X}^T \mathbf{X} + \lambda I)\mathbf{w}^* = \mathbf{0}$$

$$\mathbf{w}^* = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Ridge regression, continued

Regularizer: $$R(\mathbf{w}) \doteq \|\mathbf{w}\|_2^2 = \mathbf{w}^T\mathbf{w}$$

New objective:

$$L(\mathbf{w}) = \boldsymbol{\epsilon}^T\boldsymbol{\epsilon} + \lambda\mathbf{w}^T\mathbf{w}$$

"data fidelity"

complexity

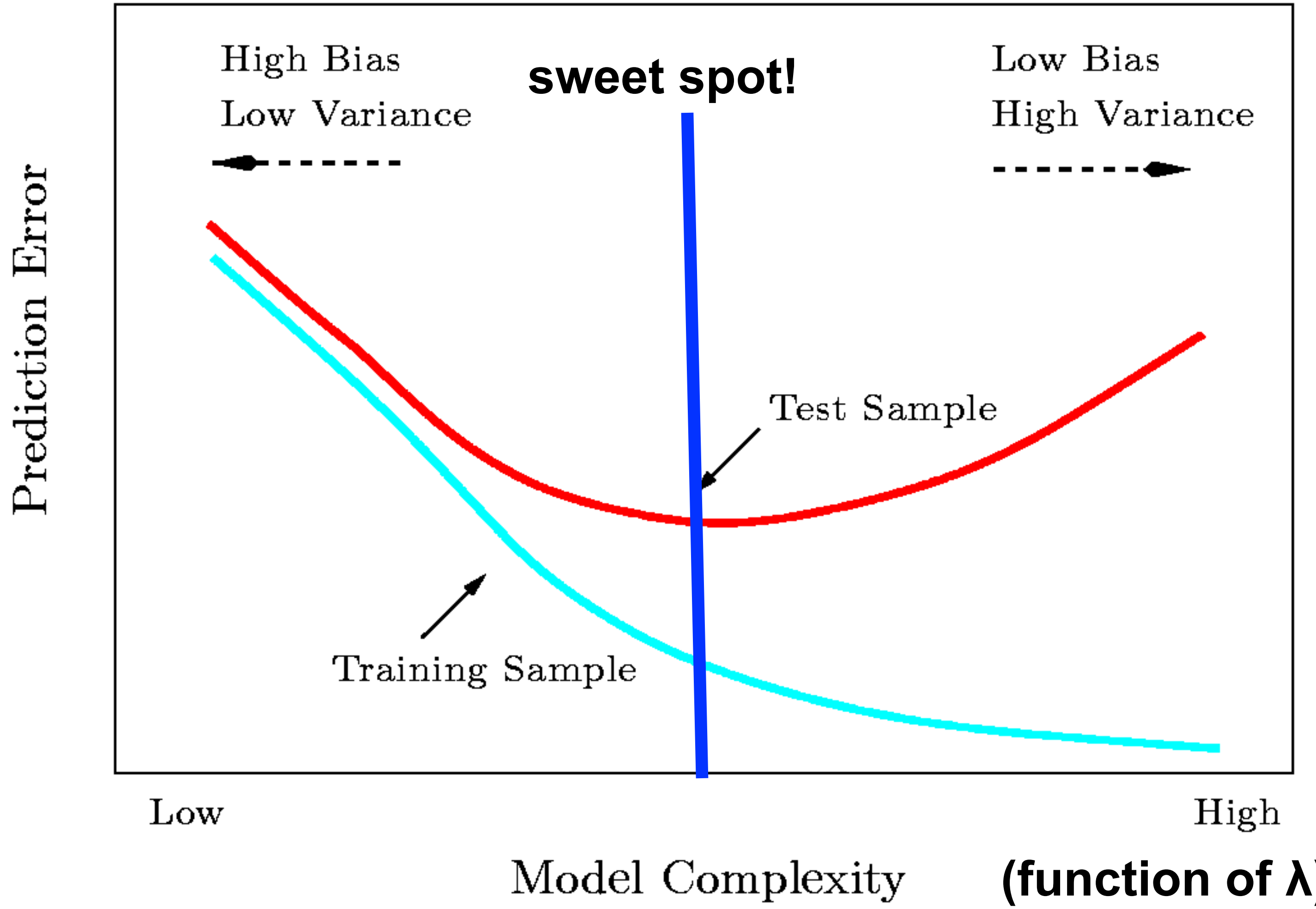
We just determined minimum

scalar, remains to be determined

λ: "hyperparameter"

Nᴏᴛᴇ: direct minimization w.r.t. it would lead to λ=0

Bias-Variance tradeoff as a function of λ



(function of λ)

Selecting λ with cross-validation

- Cross validation technique
  - Exclude part of the training data from parameter estimation
  - Use them only to predict the test error
- K-fold cross validation:
  - K splits, average K errors
- Use cross-validation for different values of λ parameter
  - pick value that minimizes cross-validation error

Least glorious, most effective of all methods