

# Optimization for Machine Learning

## Introduction into supervised learning

Lecturer: Robert M. Gower



Master IASD: AI Systems and Data Science, 2019

# Core Info

- **Where:** ENS: 07/11 amphi Langevin, 03/12 U209, 05/12 amphi Langevin.
- **Online:** Teaching materials for these 3 classes:  
<https://gowerrobert.github.io/>
- **Google docs with course info:** Can also be found on  
<https://gowerrobert.github.io/>

# Outline of my three classes

- 07/11/19 Foundations and the empirical risk problem, revision probability, SGD (Stochastic Gradient Descent) for ridge regression
- 03/12/19 SGD for convex optimization. Theory and variants
- 05/12/19 Lab on SGD and variants

# Detailed Outline today

- 13:30 – 14:00: Introduction to empirical risk minimization and classification and SGD
- 14:00 – 15:00 Revision on probability
- 15:00 – 15:30: Tea Time! Break
- 15:30 – 17:00: Exercises and proof of convergence of SGD for ridge regression

# An Introduction to Supervised Learning

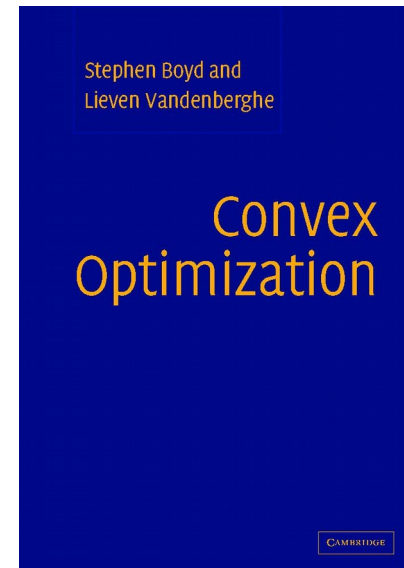
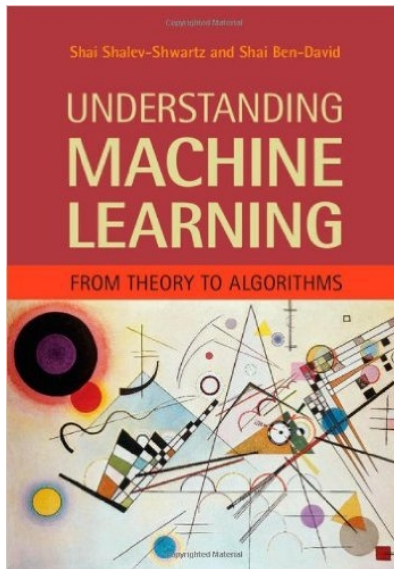
# References classes today

Chapter 2

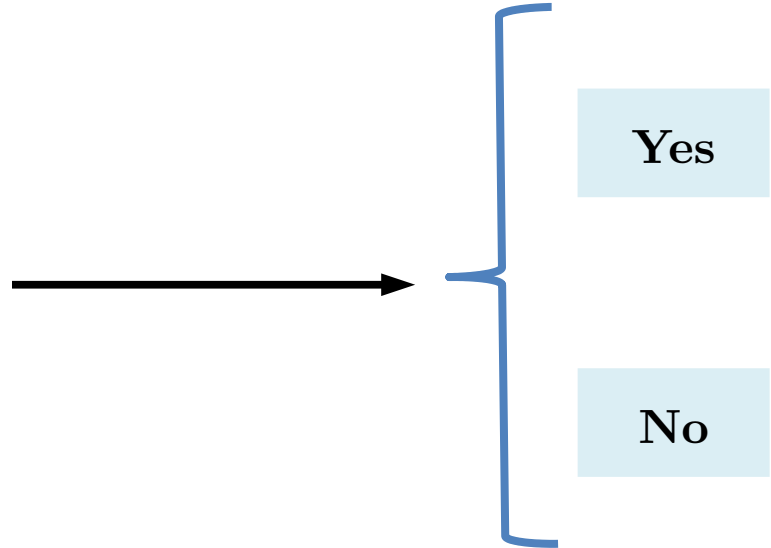
Pages 67 to 79

Understanding Machine Learning: From Theory to Algorithms

Convex Optimization,  
Stephen Boyd



# Is There a Cat in the Photo?



# Is There a Cat in the Photo?



Yes



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Yes

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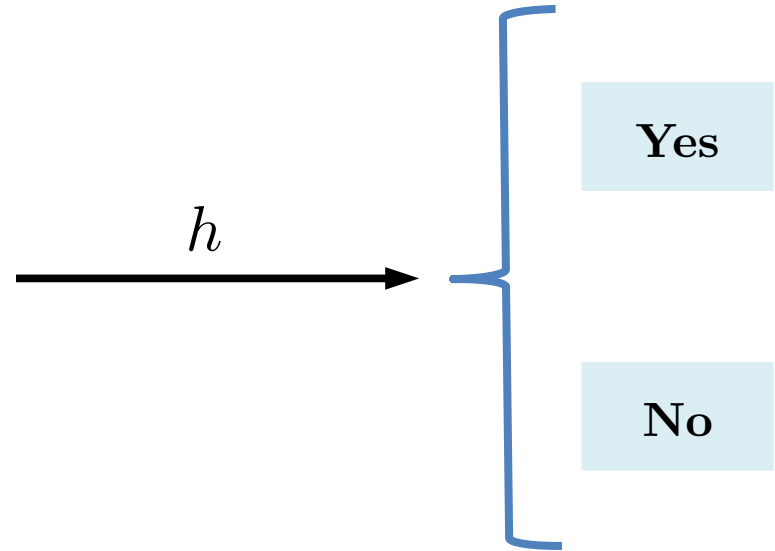
No

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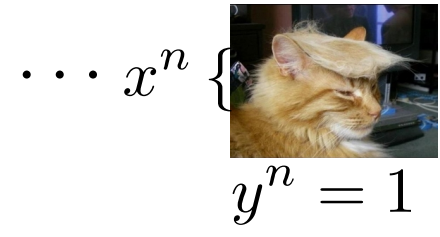
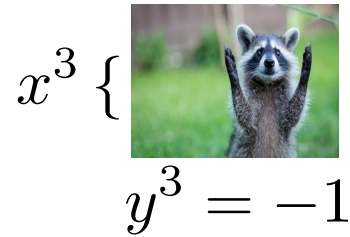
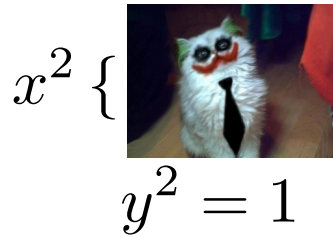
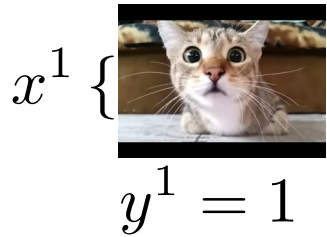
$x$ : Input/Feature

$y$ : Output/Target


Find mapping  $h$  that assigns the “correct” target to each input


$$h : x \in \mathbf{R}^d \longrightarrow y \in \mathbf{R}$$


# Labeled Data: The training set




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$x^1$  {   $y^1 = 1$

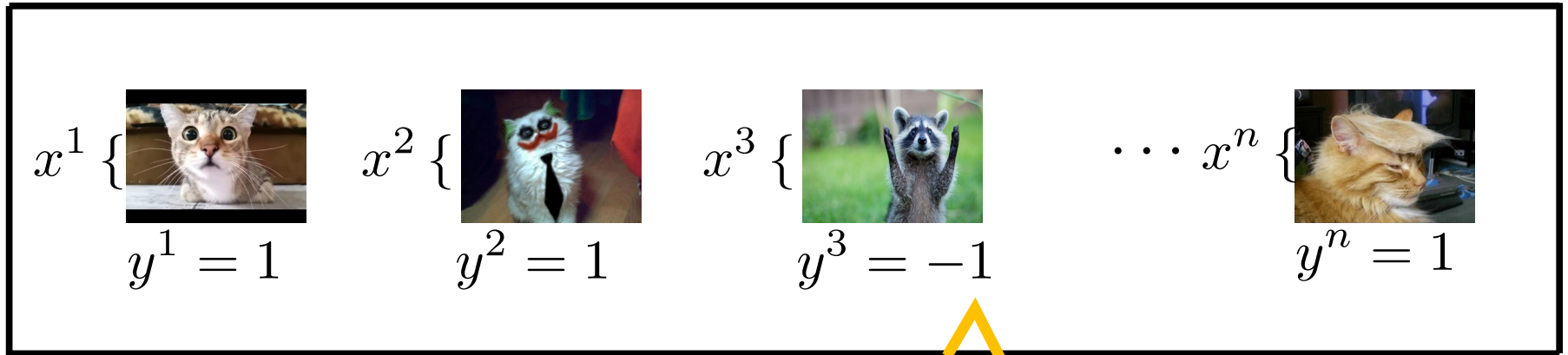
$x^2$  {   $y^2 = 1$

$x^3$  {   $y^3 = -1$

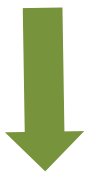
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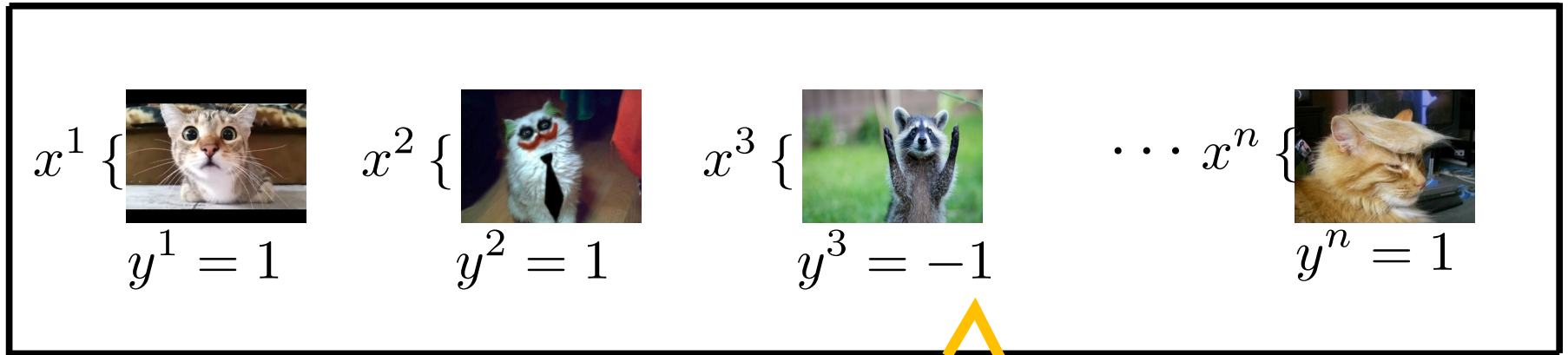


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Learning Algorithm

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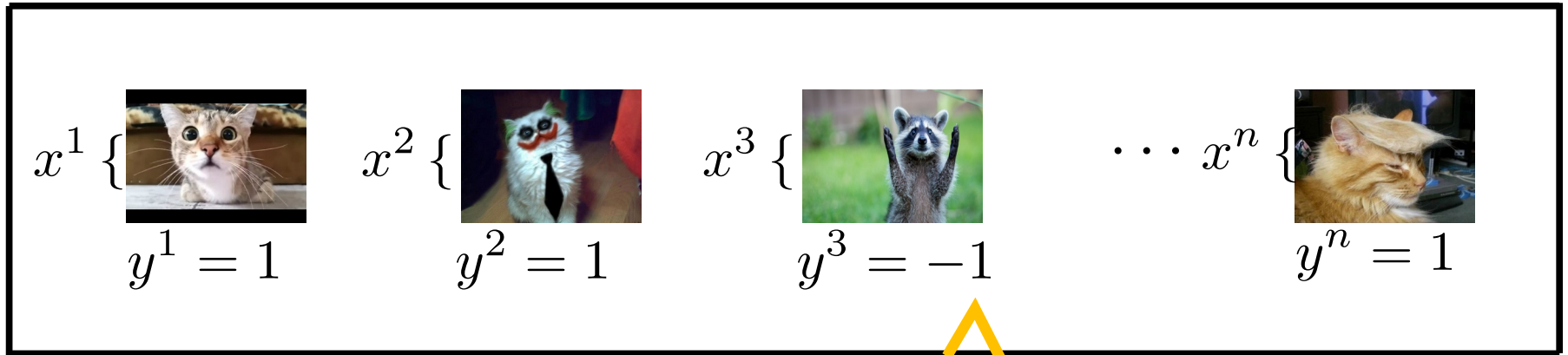
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$h : x \in X \rightarrow y \in \mathbf{R}$



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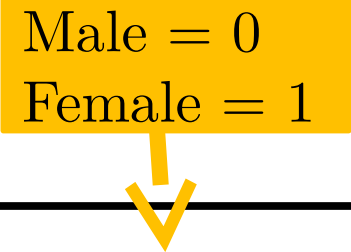
$h$  (  )



-1

# Example: Linear Regression for Height

Male = 0  
Female = 1



Labelled data  $x \in \mathbf{R}^2, y \in \mathbf{R}_+$

$x_1^1$	{	Sex	0
$x_2^1$	{	Age	30
$y^1$	{	Height	1,72 cm

...

$x_1^n$	{	Sex	1
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**Example Hypothesis: Linear Model**

$$h_w(x_1, x_2) = w_0 + x_1 w_1 + x_2 w_2 \stackrel{x_0=1}{=} \langle w, x \rangle$$

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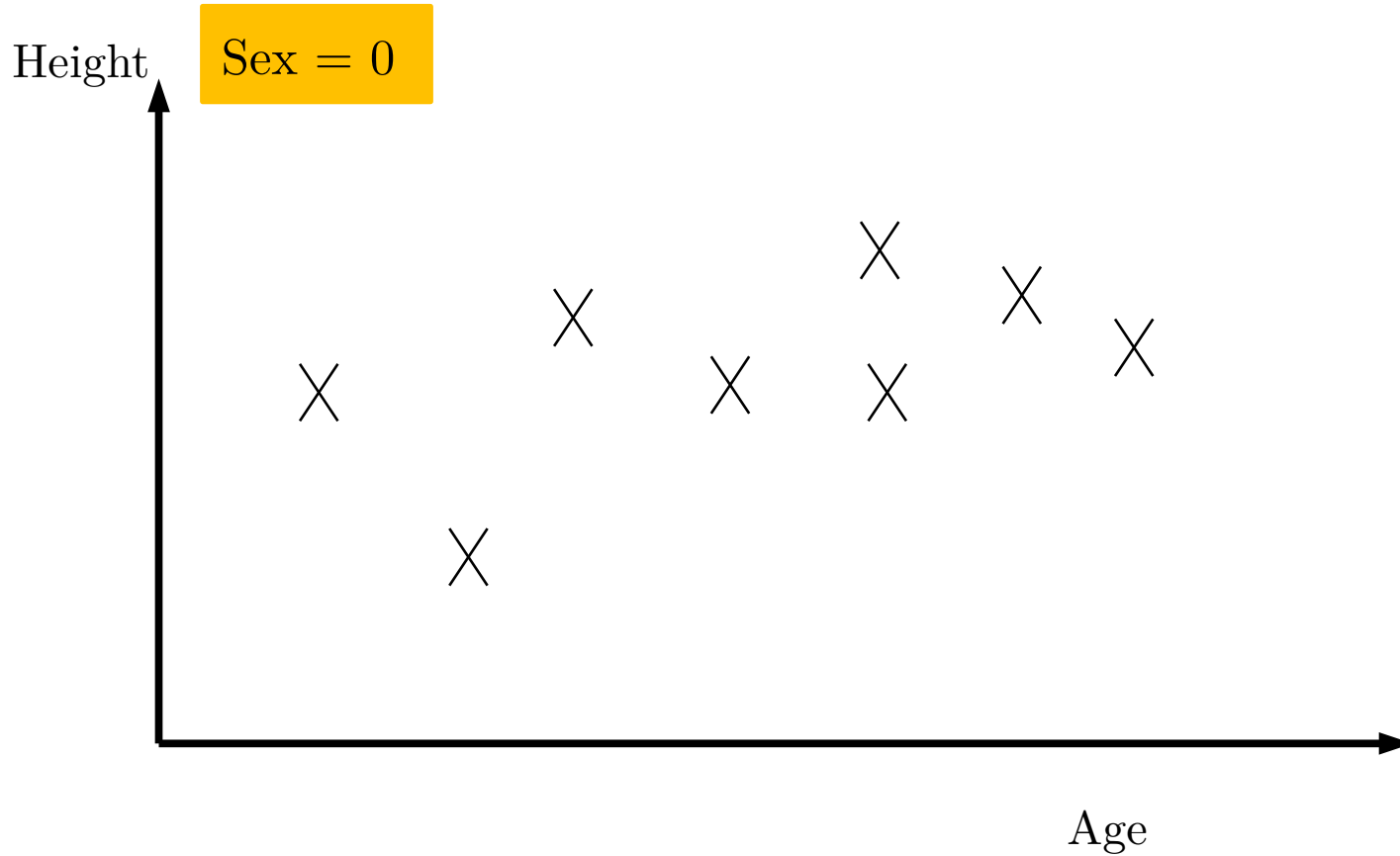
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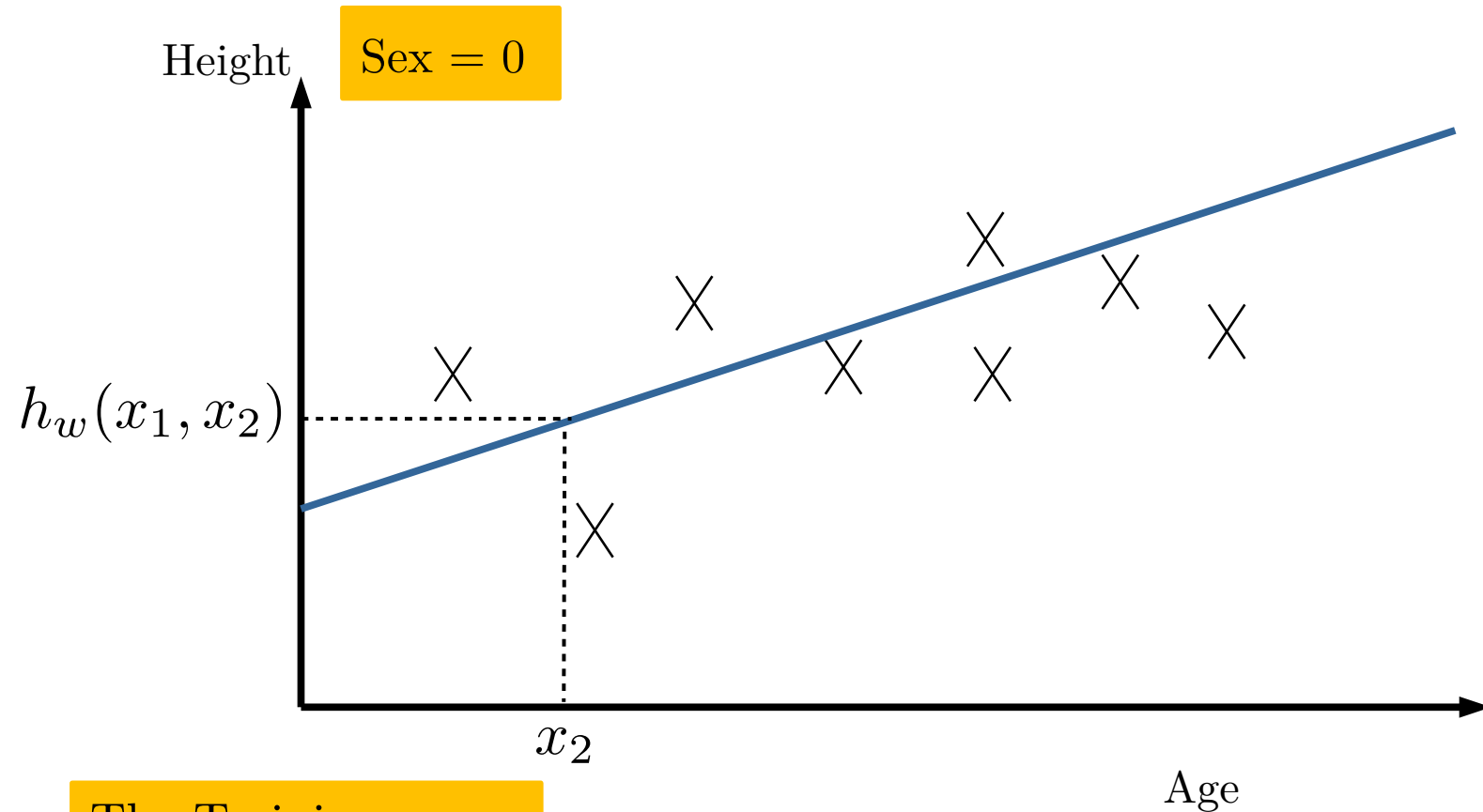
**Example Training Problem:**

$$\min_{w \in \mathbf{R}^3} \frac{1}{n} \sum_{i=1}^n (h_w(x_1^i, x_2^i) - y^i)^2$$

# Linear Regression for Height



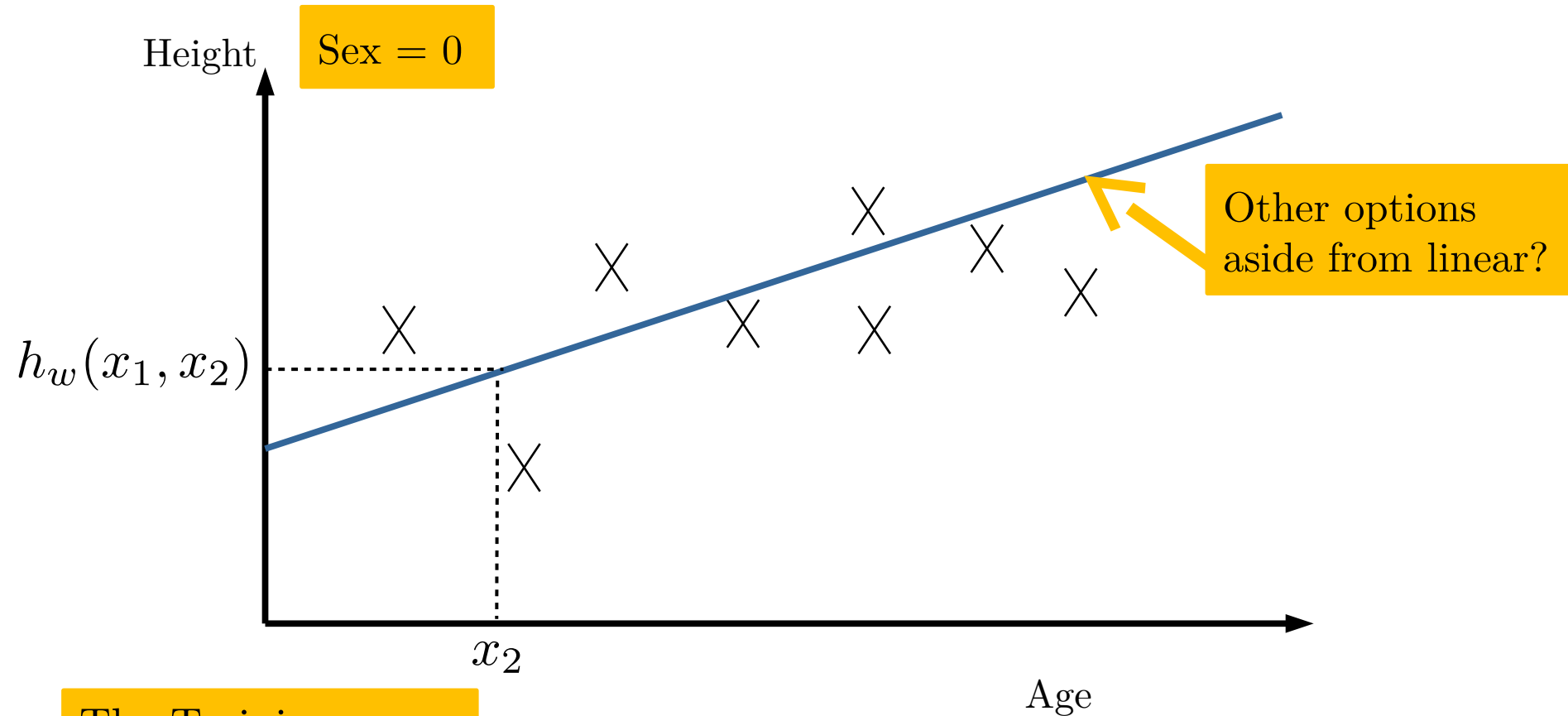
# Linear Regression for Height



The Training  
Algorithm

$$\min_{w \in \mathbf{R}^3} \frac{1}{n} \sum_{i=1}^n (h_w(x_1^i, x_2^i) - y^i)^2$$

# Linear Regression for Height



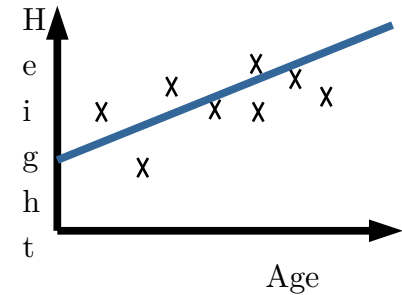
The Training  
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# Parametrizing the Hypothesis

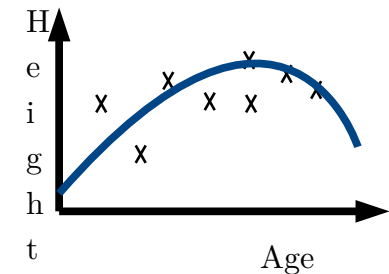
Linear:

$$h_w(x) = \sum_{i=0}^d w_i x_i$$

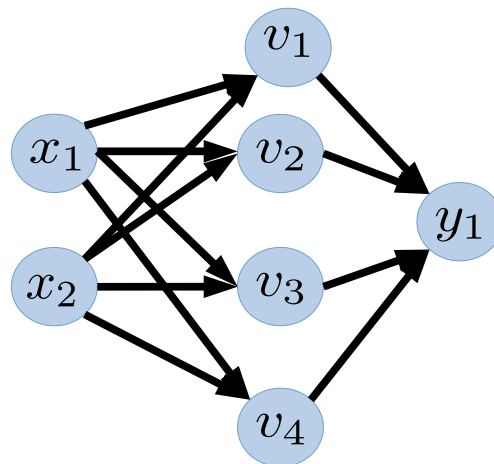


Polynomial:

$$h_w(x) = \sum_{i,j=0}^d w_{ij} x_i x_j$$



Neural Net:



exe :

$$v_1 = \text{sign}(w_{11}x_1 + w_{12}x_2)$$

$$v_4 = 1 / (1 + \exp(w_{41}x_1 + w_{42}x_2))$$



# Loss Functions

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n (h_w(x^i) - y^i)^2$$

Why a Squared Loss?

# Loss Functions

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Why a Squared Loss?

Let  $y_h := h_w(x)$

**Loss Functions**

$$\begin{aligned} \ell : \mathbf{R} \times \mathbf{R} &\rightarrow \mathbf{R}_+ \\ (y_h, y) &\rightarrow \ell(y_h, y) \end{aligned}$$

**The Training Problem**

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(h_w(x^i), y^i)$$

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Typically a convex function

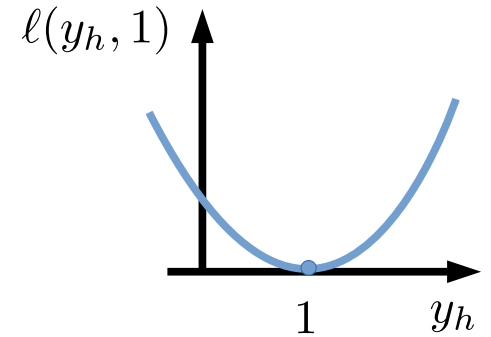
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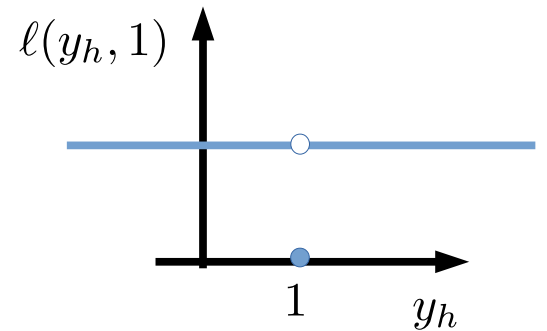
# Choosing the Loss Function

Let  $y_h := h_w(x)$

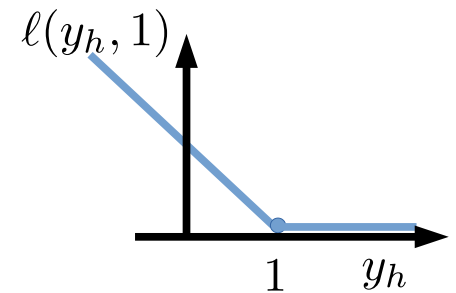
Quadratic Loss  $\ell(y_h, y) = (y_h - y)^2$



Binary Loss  $\ell(y_h, y) = \begin{cases} 0 & \text{if } y_h = y \\ 1 & \text{if } y_h \neq y \end{cases}$



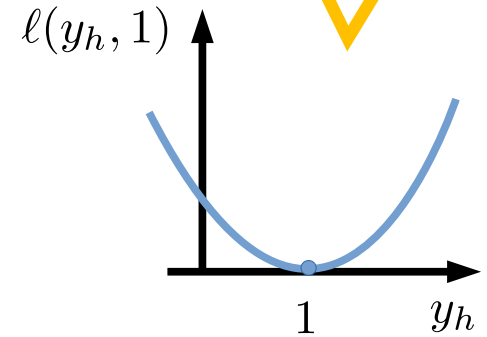
Hinge Loss  $\ell(y_h, y) = \max\{0, 1 - y_h y\}$



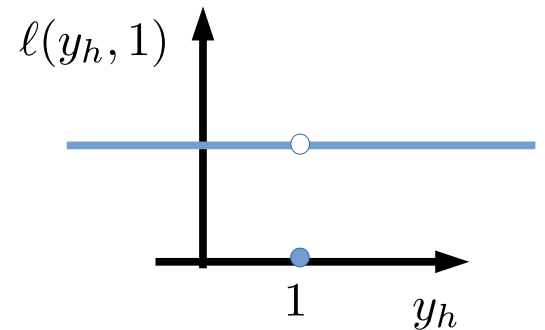
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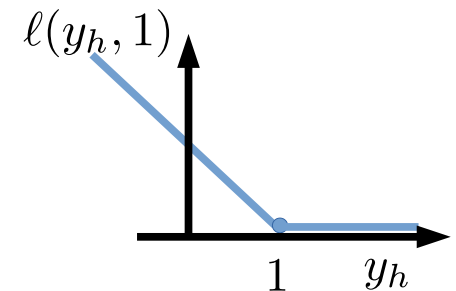
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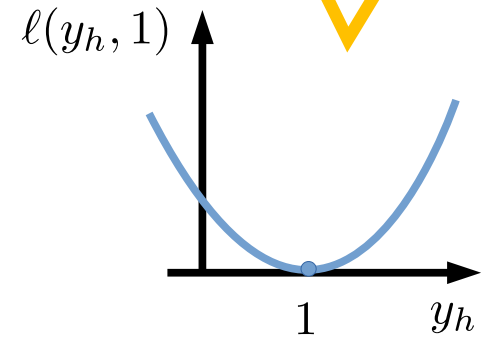
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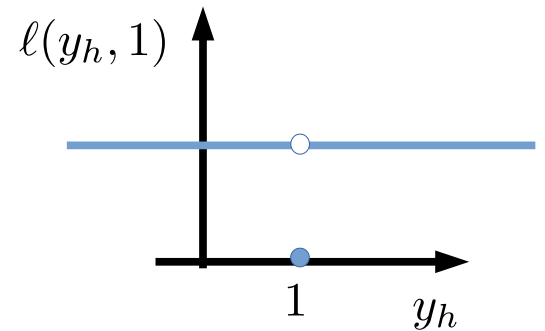
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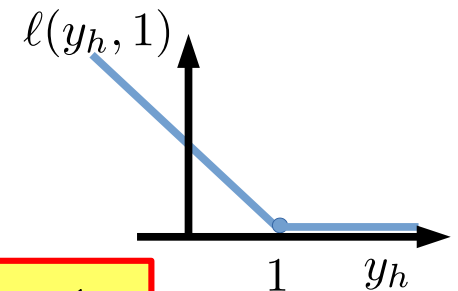
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**EXE:** Plot the binary and hinge loss function in when  $y = -1$

# Loss Functions

Is a notion of Loss enough?

What happens when we do not have enough data?

# Loss Functions

## The Training Problem

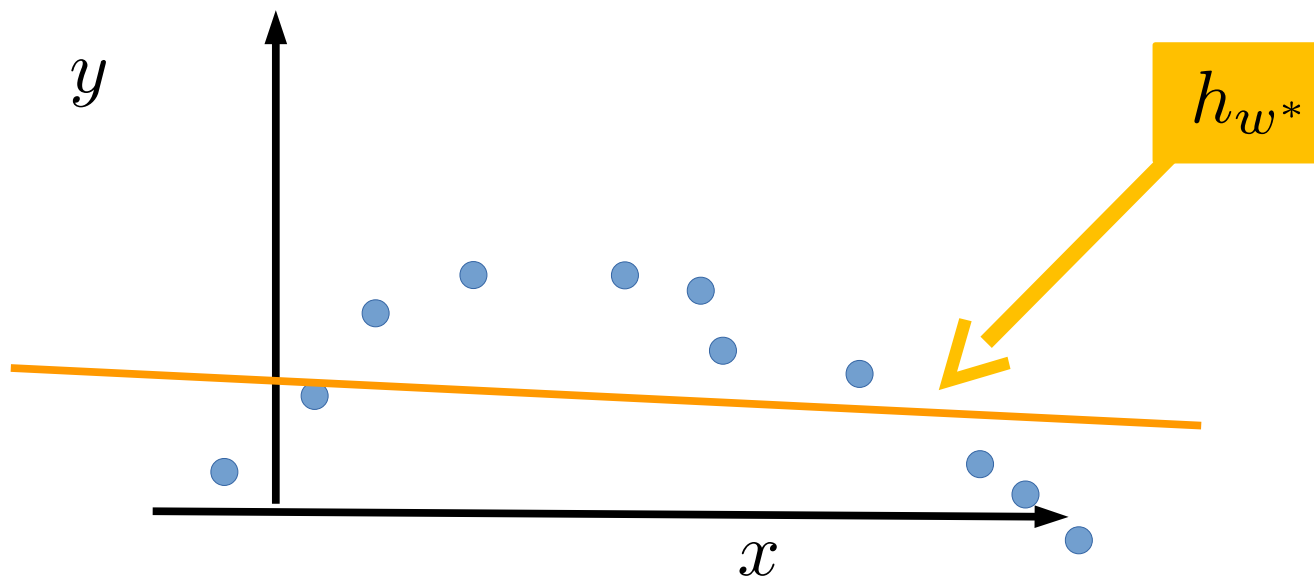
$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \ell (h_w(x^i), y^i)$$

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# Overfitting and Model Complexity

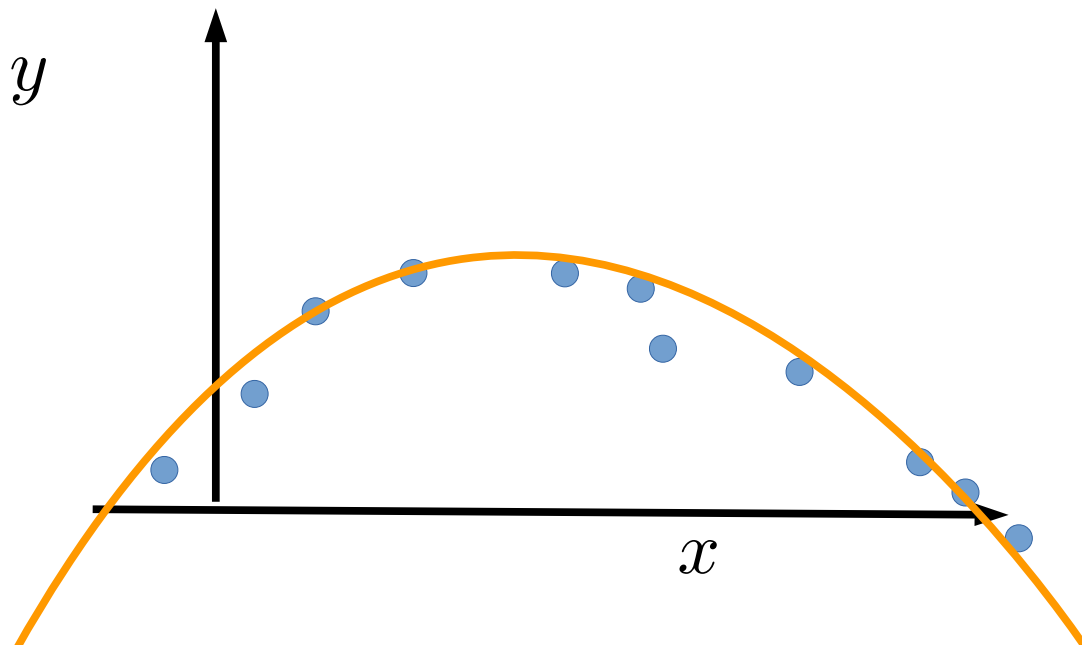


Fitting 1<sup>st</sup> order polynomial

$$h_w = \langle w, x \rangle$$

$$w^* = \arg \min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n (h_w(x^i) - y^i)^2$$

# Overfitting and Model Complexity

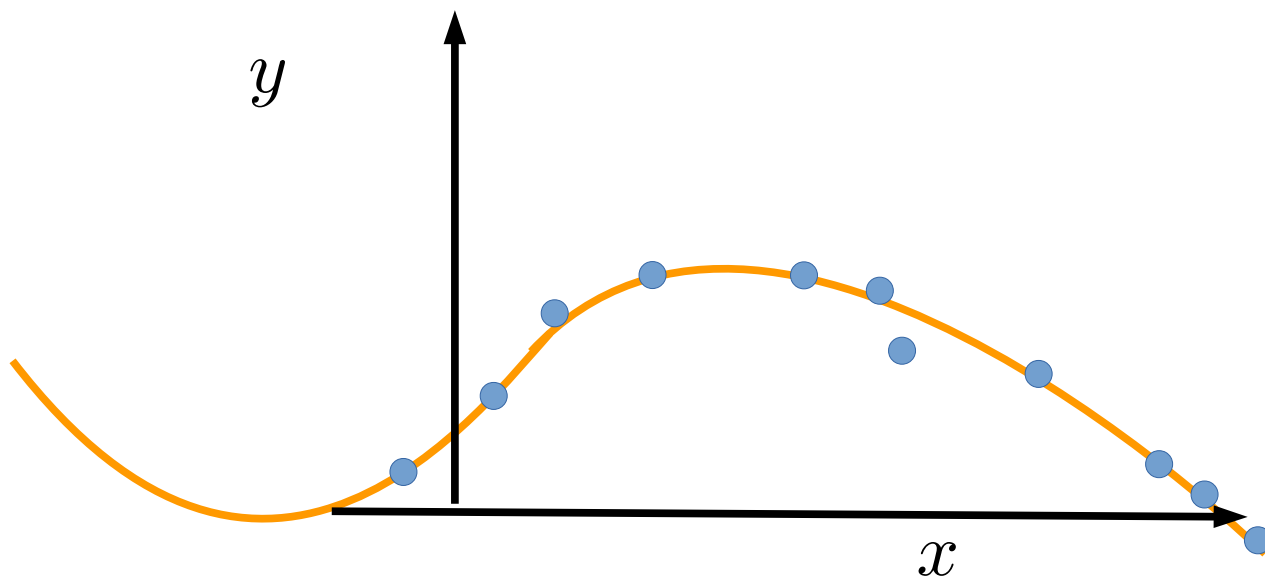


Fitting 2<sup>nd</sup> order polynomial

$$h_w = w_0 + w_1x + w_2x^2$$

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# Overfitting and Model Complexity

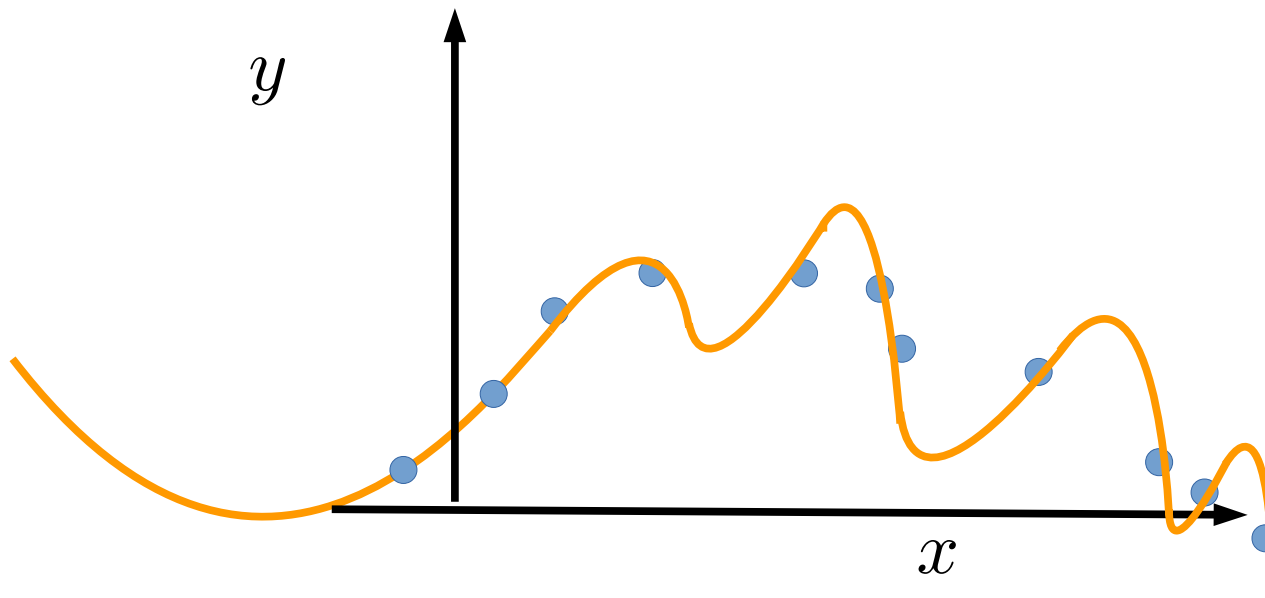


Fitting 3<sup>rd</sup> order polynomial

$$h_w = \sum_{i=0}^3 w_i x^i$$

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# Overfitting and Model Complexity



Fitting 9<sup>th</sup> order polynomial

$$h_w = \sum_{i=0}^9 w_i x^i$$

$$w^* = \arg \min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n (h_w(x^i) - y^i)^2$$

# Regularization

## Regularizer Functions

$$\begin{aligned} R : \mathbf{R}^d &\rightarrow \mathbf{R}_+ \\ w &\rightarrow R(w) \end{aligned}$$

## General Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(h_w(x^i), y^i) + \lambda R(w)$$

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Penalizes  
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Controls tradeoff  
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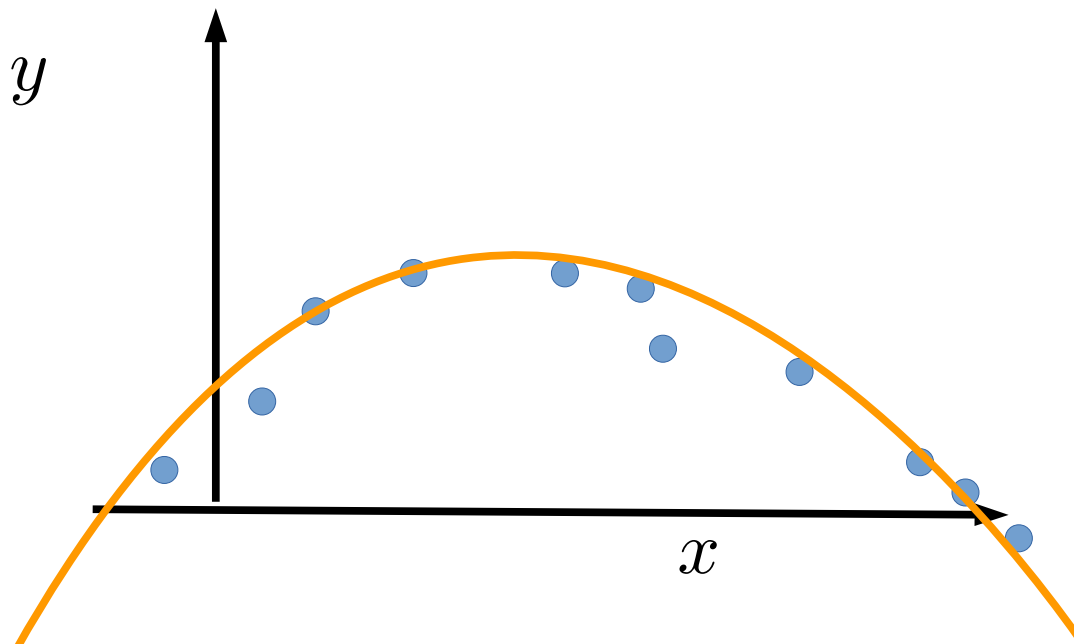
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Exe:

$$R(w) = \|w\|_2^2, \quad \|w\|_1, \quad \|w\|_p, \quad \text{other norms } \dots$$

# Overfitting and Model Complexity

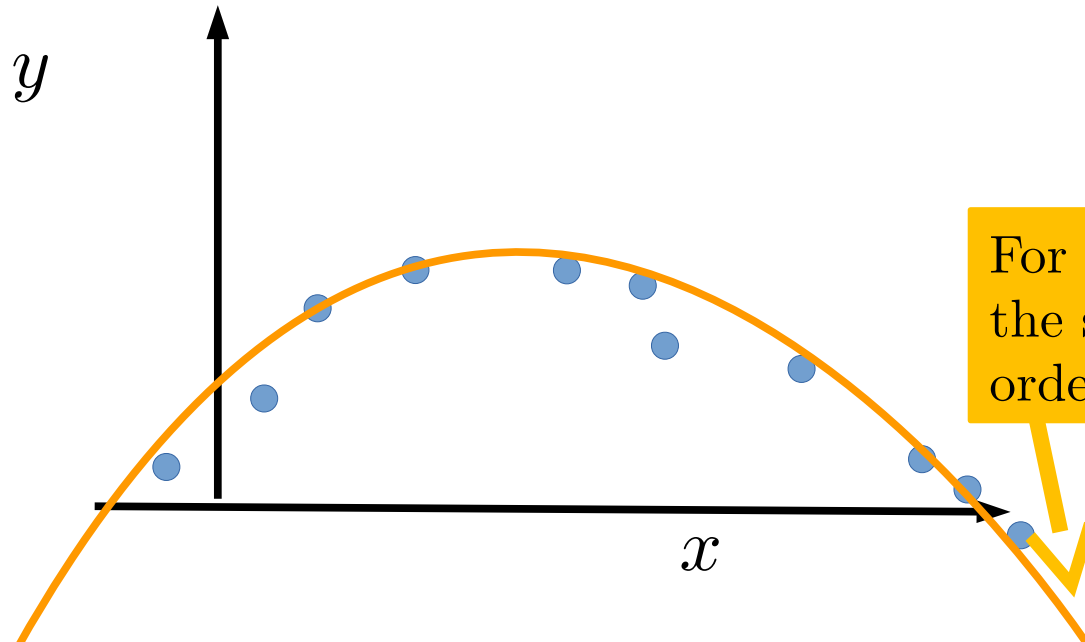


Fitting  $k^{\text{th}}$  order polynomial

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# Exe: Ridge Regression

**Linear hypothesis**

$$h_w(x) = \langle w, x \rangle$$



**L2 regularizer**

$$R(w) = ||w||_2^2$$

**L2 loss**

$$\ell(y_h, y) = (y_h - y)^2$$



**Ridge Regression**

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n (y^i - \langle w, x^i \rangle)^2 + \lambda ||w||_2^2$$

# Exe: Support Vector Machines

**Linear hypothesis**

$$h_w(x) = \langle w, x \rangle$$



**L2 regularizer**

$$R(w) = ||w||_2^2$$

**Hinge loss**

$$\ell(y_h, y) = \max\{0, 1 - y_h y\}$$



**SVM with soft margin**

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \max\{0, 1 - y^i \langle w, x^i \rangle\} + \lambda ||w||_2^2$$

# Exe: Logistic Regression

**Linear hypothesis**

$$h_w(x) = \langle w, x \rangle$$



**L2 regularizer**

$$R(w) = ||w||_2^2$$

**Logistic loss**

$$\ell(y_h, y) = \ln(1 + e^{-yy_h})$$



**Logistic Regression**

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-y^i \langle w, x^i \rangle}) + \lambda ||w||_2^2$$

# The Machine Learners Job

(1) Get the labeled data:  $(x^1, y^1), \dots, (x^n, y^n)$

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- (4) Solve the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(h_w(x^i), y^i) + \lambda R(w)$$

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# Re-writing as Sum of Terms

## A Datum Function

$$f_i(w) := \ell(h_w(x^i), y^i) + \lambda R(w)$$

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \ell(h_w(x^i), y^i) + \lambda R(w) &= \frac{1}{n} \sum_{i=1}^n (\ell(h_w(x^i), y^i) + \lambda R(w)) \\ &= \frac{1}{n} \sum_{i=1}^n f_i(w) \end{aligned}$$

## Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n f_i(w) =: f(w)$$

Can we use this  
sum structure?

# The Training Problem

Solving the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^n f_i(w)$$

Reference method: Gradient descent

$$\nabla \left( \frac{1}{n} \sum_{i=1}^n f_i(w) \right) = \frac{1}{n} \sum_{i=1}^n \nabla f_i(w)$$

## Gradient Descent Algorithm

Set  $w^0 = 0$ , choose  $\alpha > 0$ .

for  $t = 0, 1, 2, \dots, T - 1$

$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^n \nabla f_i(w^t)$$

Output  $w^T$

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## Problem with Gradient Descent:

Each iteration requires computing a gradient  $\nabla f_i(w)$  for each data point. One gradient for each cat on the internet!

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# Stochastic Gradient Descent

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## Unbiased Estimate

Let  $j$  be a random index sampled from  $\{1, \dots, n\}$  selected uniformly at random. Then

$$\mathbb{E}_j[\nabla f_j(w)] = \frac{1}{n} \sum_{i=1}^n \nabla f_i(w) = \nabla f(w)$$

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**EXE:** Let  $\sum_{i=1}^n p_i = 1$  and  $j \sim p_j$ . Show  $\mathbb{E}[\nabla f_j(w)/(np_j)] = \nabla f(w)$

# Stochastic Gradient Descent

## SGD 0.0 Constant stepsize

Set  $w^0 = 0$ , choose  $\alpha > 0$

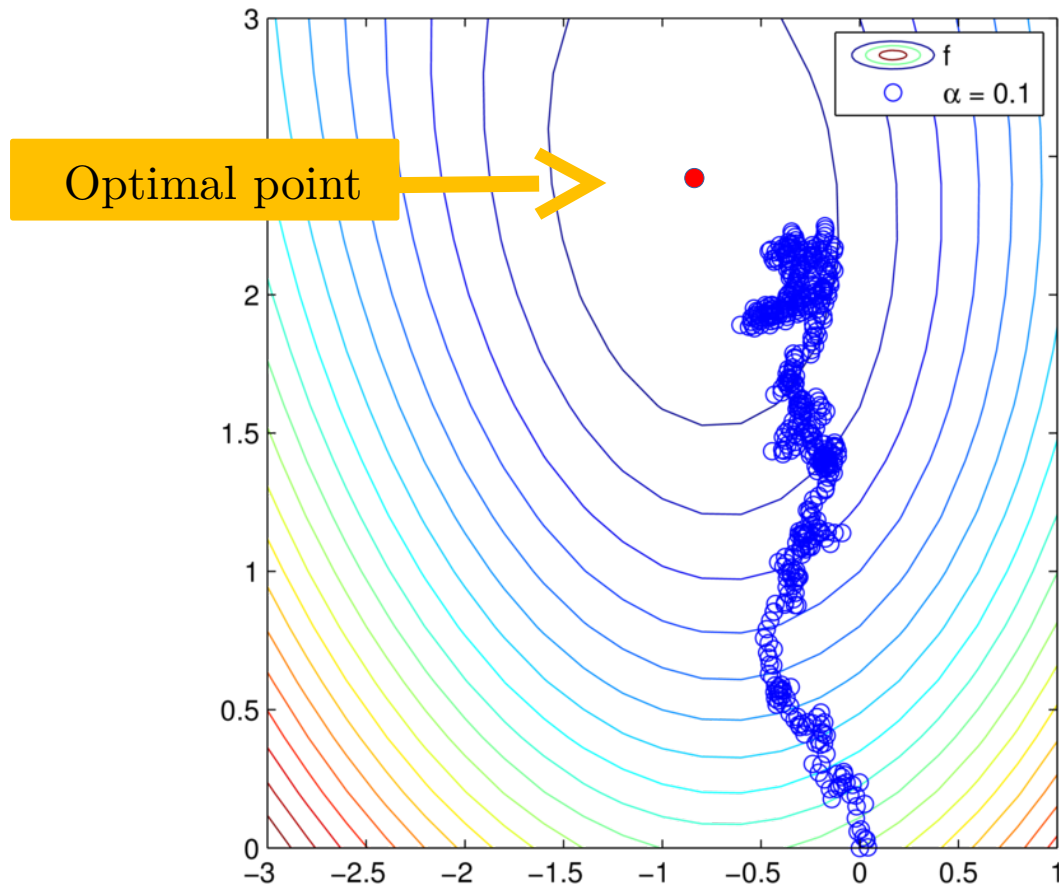
for  $t = 0, 1, 2, \dots, T - 1$

    sample  $j \in \{1, \dots, n\}$

$$w^{t+1} = w^t - \alpha \nabla f_j(w^t)$$

Output  $w^T$

# Stochastic Gradient Descent



# Detailed Outline today

- 13:30 – 14:00: Introduction to empirical risk minimization and classification and SGD
- 14:00 – 15:00 **Revision on probability**
- 15:00 – 15:30: **Tea Time! Break**
- 15:30 – 17:00: **Exercises and proof of convergence of SGD for ridge regression**

# Assumptions for Convergence

**Strong Convexity**

$$f(y) \geq f(w) + \langle \nabla f(w), y - w \rangle + \frac{\lambda}{2} \|y - w\|_2^2, \quad \forall w, y$$



$$y = w^*$$

$$2\langle \nabla f(w), w - w^* \rangle \geq \lambda \|w - w^*\|_2^2$$

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# Complexity / Convergence

## Theorem

If  $0 < \alpha \leq \frac{1}{\lambda}$  then the iterates of the SGD 0.0 method satisfy

$$\mathbb{E} [\|w^t - w^*\|_2^2] \leq (1 - \alpha\lambda)^t \|w^0 - w^*\|_2^2 + \frac{\alpha}{\lambda} B^2$$

**EXE:** Do exercises on convergence of random sequences.

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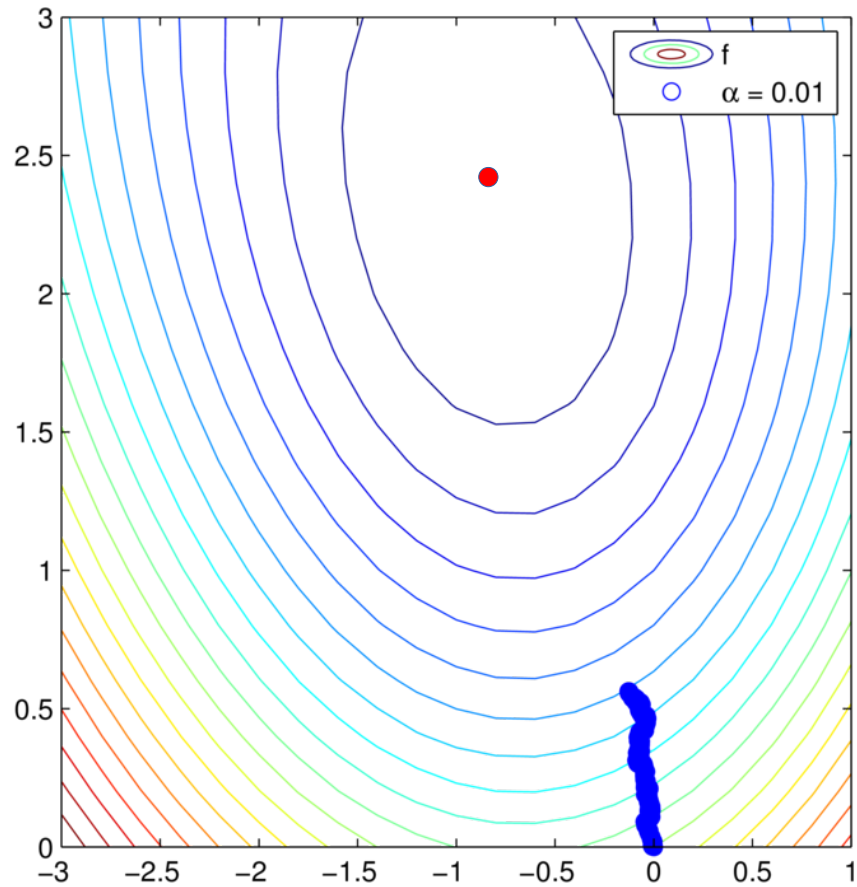
Shows that  $\alpha \approx \frac{1}{\lambda}$

Shows that  $\alpha \approx 0$

**EXE:** Do exercises on convergence of random sequences.

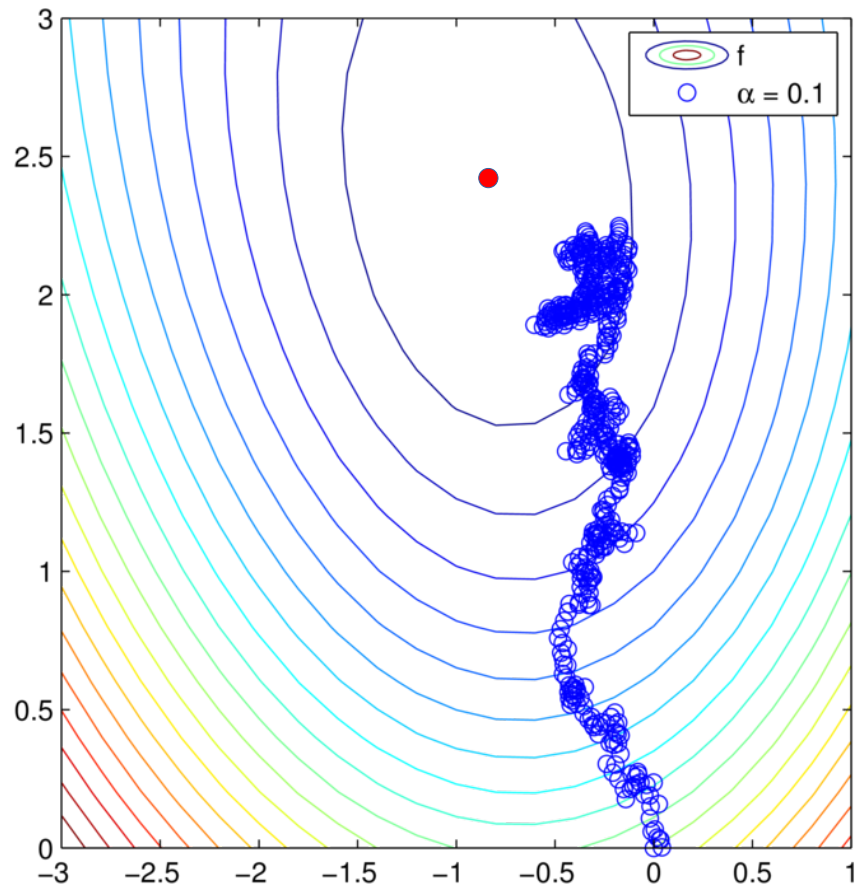
# Stochastic Gradient Descent

$\alpha = 0.01$



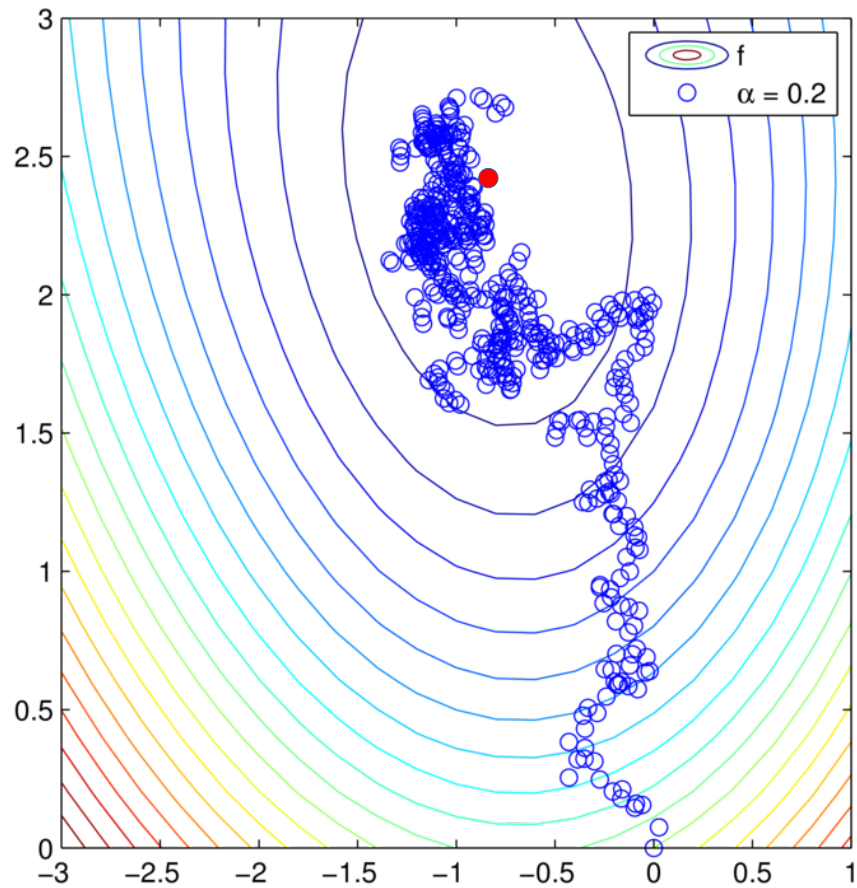
# Stochastic Gradient Descent

$\alpha = 0.1$



# Stochastic Gradient Descent

$\alpha = 0.2$





# Stochastic Gradient Descent

$\alpha = 0.5$

