Introduction to Machine Learning and Stochastic Optimization

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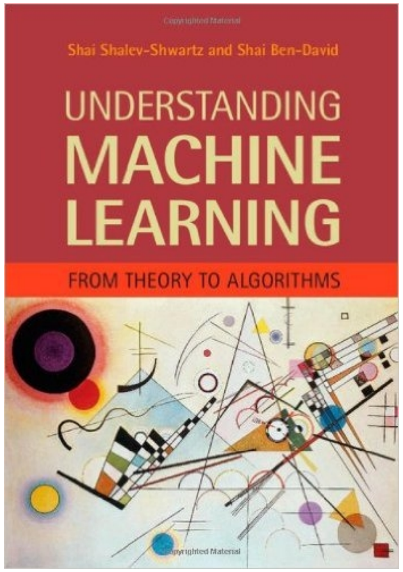
Spring School on Optimization and Data Science,
Novi Saad, March 2017

An Introduction to Supervised Learning

Some References

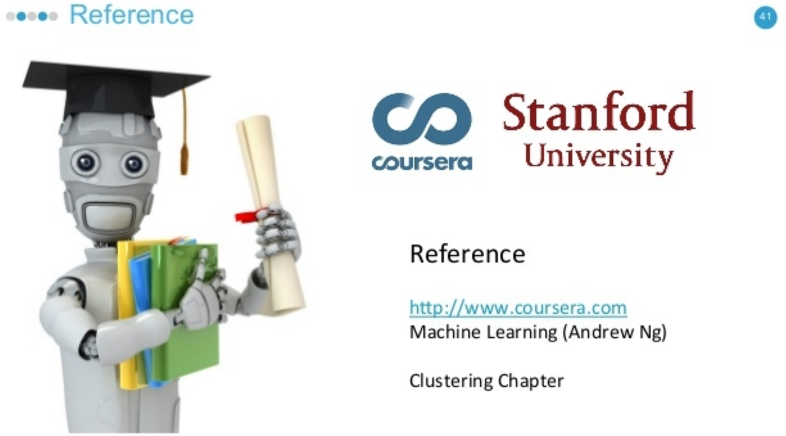
Graduate level

Understanding Machine Learning: From Theory to Algorithms



Undergraduate level

Stanford Machine Learning on Coursera by Andrew Ng



Is There a Cat in the Photo?

Yes

No

Is There a Cat in the Photo?

Yes

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Yes

Is There a Cat in the Photo?

No

Is There a Cat in the Photo?

Yes

Is There a Cat in the Photo?

Yes

No

x: Input/Feature

y: Output/Target

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

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

Labeled Data

x^1 

$y^1 = 1$

x^2 

$y^2 = 1$

x^3 

$y^3 = -1$

$\cdots$ x^n 

$y^n = 1$

Labeled Data

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

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

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y= -1 means no/false

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Learning Algorithm

Labeled Data

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y= *-1* means no/false

Learning Algorithm

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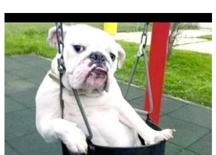
Learning Algorithm

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

$h\Big($  $\Big) \longrightarrow$ **-1**

Example: Linear Regression for Height

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

x_1^1	Sex	Male
x_2^1	Age	30
y^1	Height	1,72 cm

$\cdots$

x_1^n	Sex	Female
x_2^n	Age	70
y^n	Height	1,52 cm

Example: Linear Regression for Height

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Example Hypothesis: Linear Model

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

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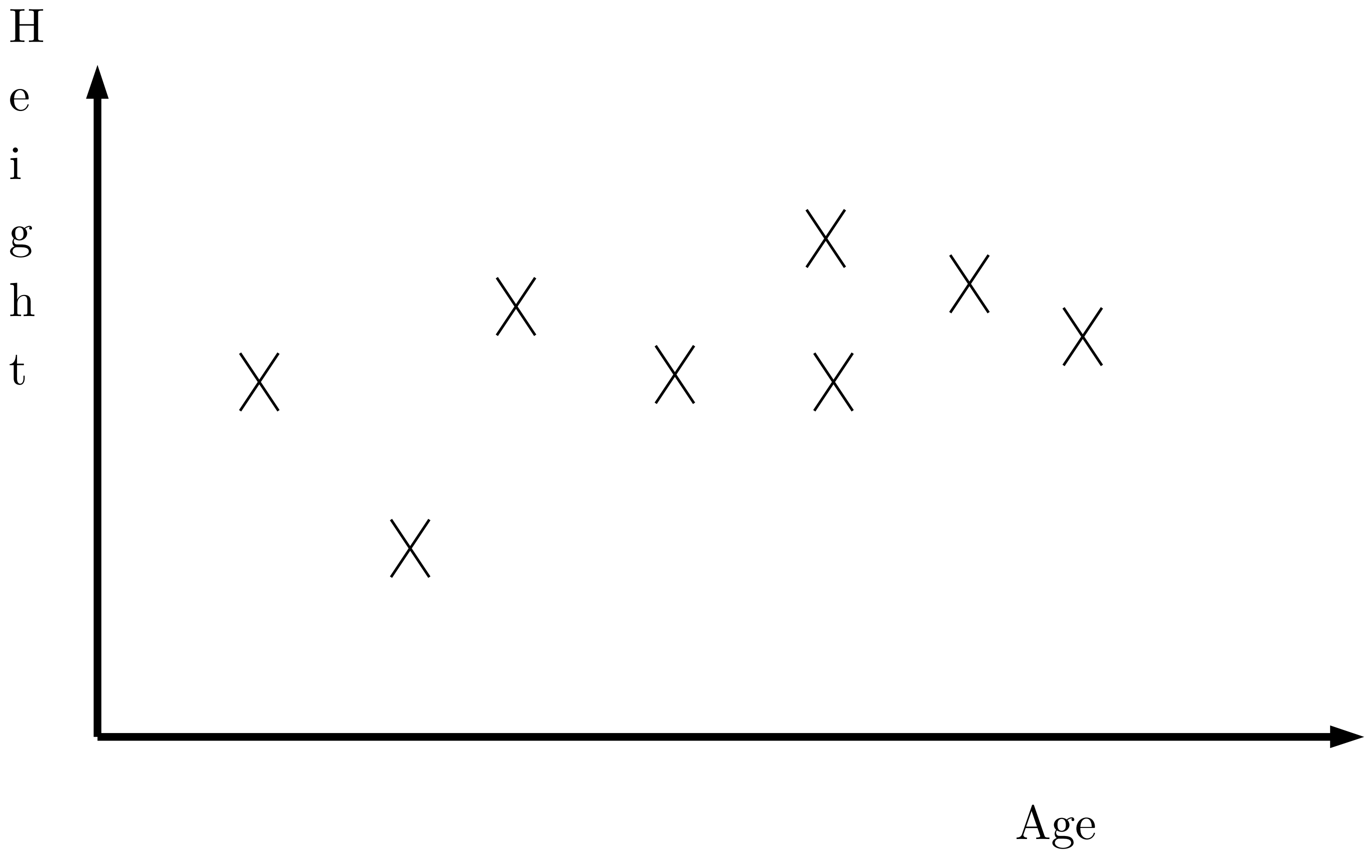
Example Hypothesis: Linear Model

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

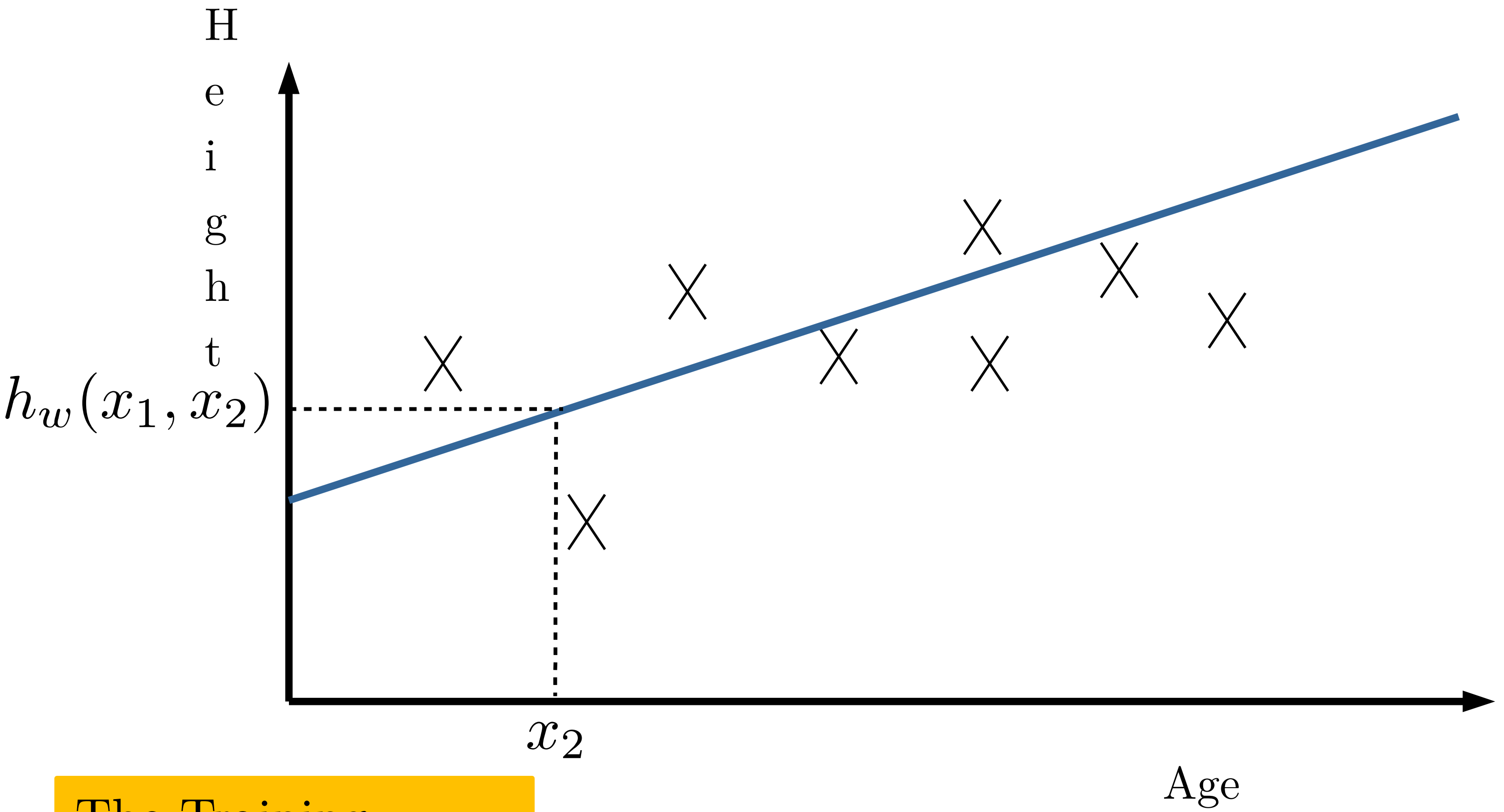
Example Training Problem:

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

Linear Regression for Height



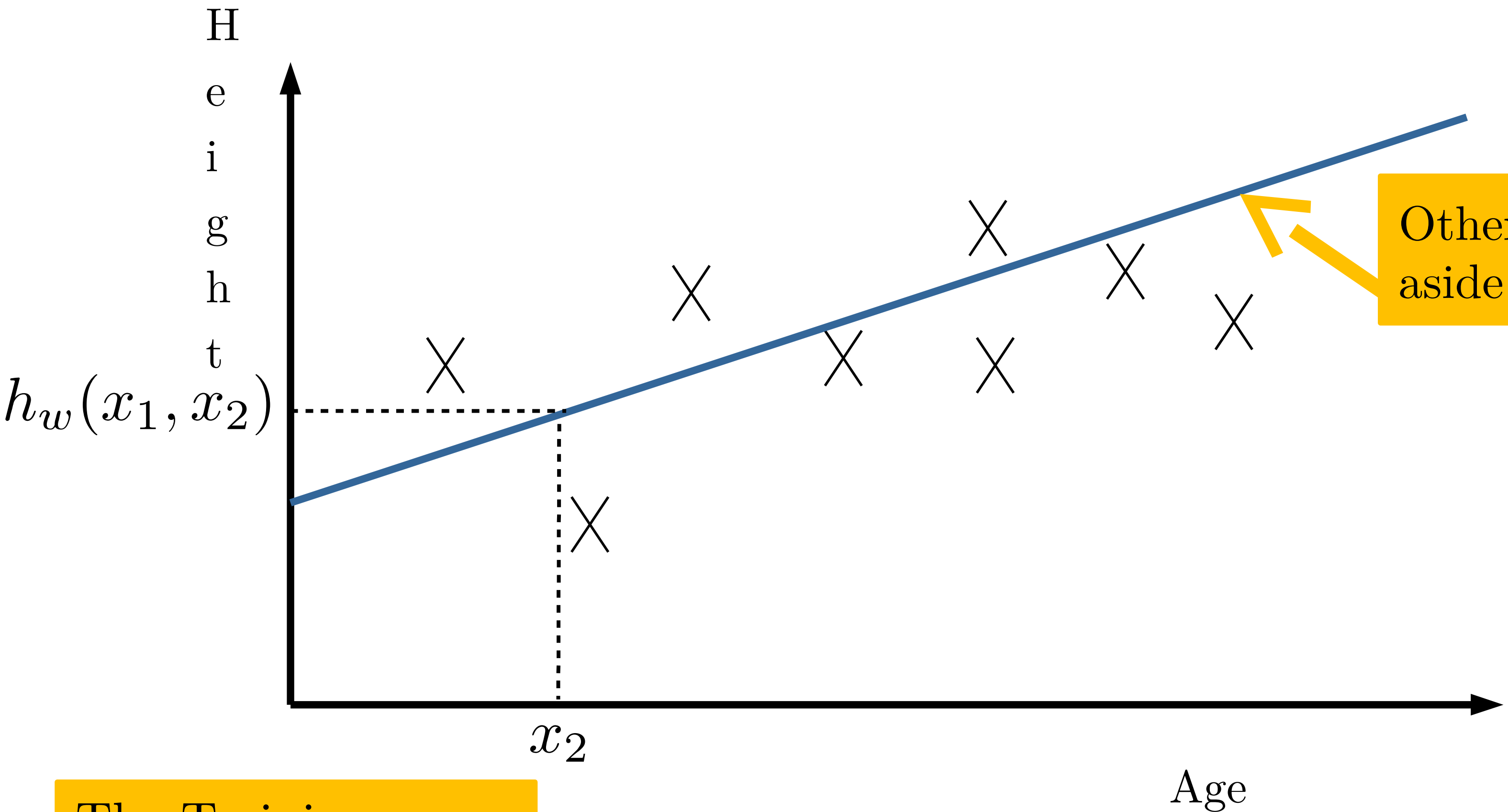
Linear Regression for Height



The Training Algorithm

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

Linear Regression for Height



Other options aside from linear?

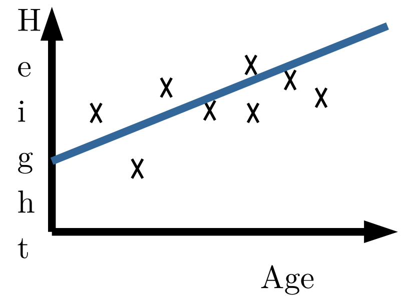
The Training Algorithm

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

Parametrizing the Hypothesis

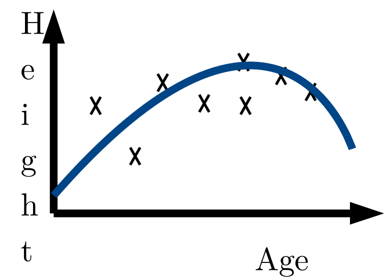
Linear:

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

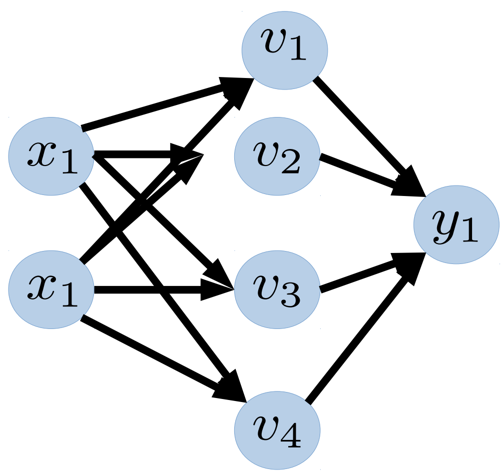


Polinomial:

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



Neural Net:



exe :

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

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

Loss Functions

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

Why a Squared Loss?

Loss Functions

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

Why a Squared Loss?

Let $y_h := h_w(x)$

Loss Functions

$$\begin{array}{rccc} \ell : & \mathbf{R} \times \mathbf{R} & \to & \mathbf{R}_+ \\ & (y_h, y) & \to & \ell(y_h, y) \end{array}$$

The Training Problem

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

Loss Functions

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

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Typically a convex function

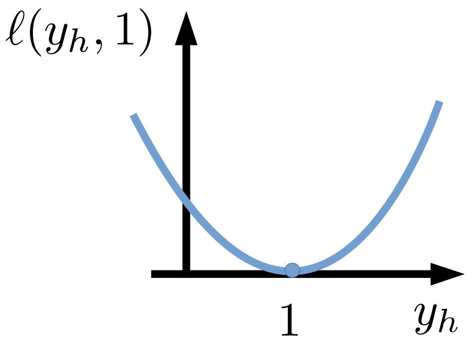
The Training Problem

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

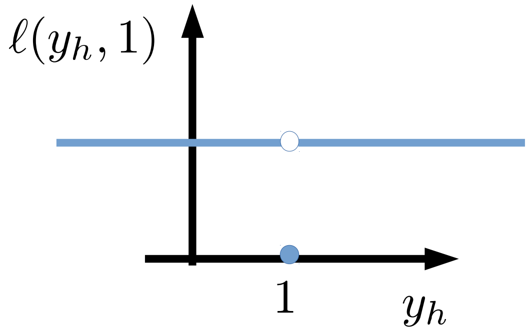
Choosing the Loss Function

Let $y_h := h_w(x)$

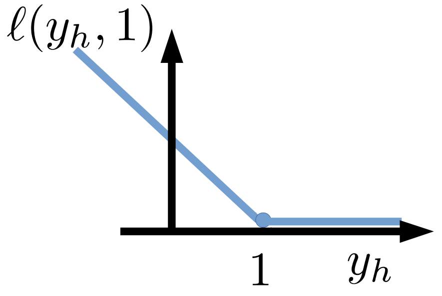
Quadratic Loss $\ell(y_h, y) = (y_h - y)^2$



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



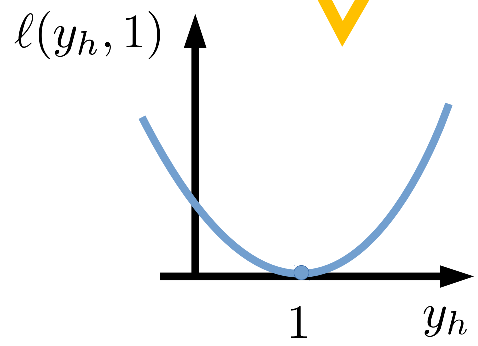
Hinge Loss $\ell(y_h, y) = \max\{0, 1 - y_h y\}$



Choosing the Loss Function

y=*1* in all figures

Let $y_h := h_w(x)$



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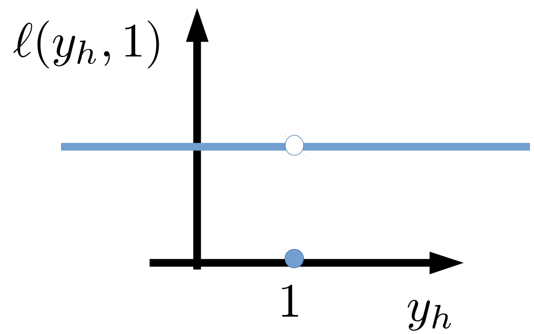

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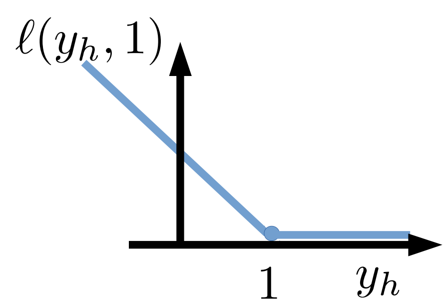

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Choosing the Loss Function

y=1 in all figures

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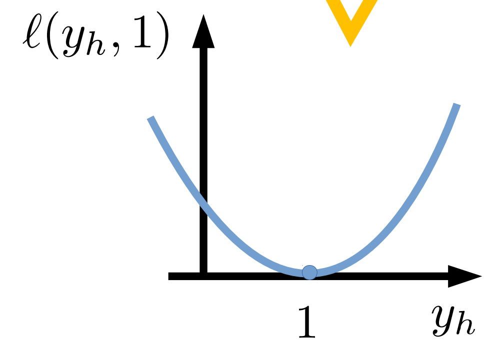

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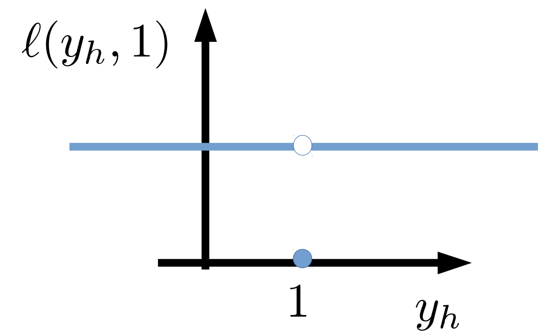

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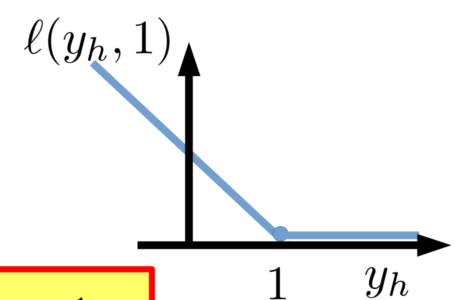


EXE: Plot the binary and hinge loss function in when $y = -1$

Loss Functions

Is a notion of Loss enough?

What happens when we do not have enough data?

Loss Functions

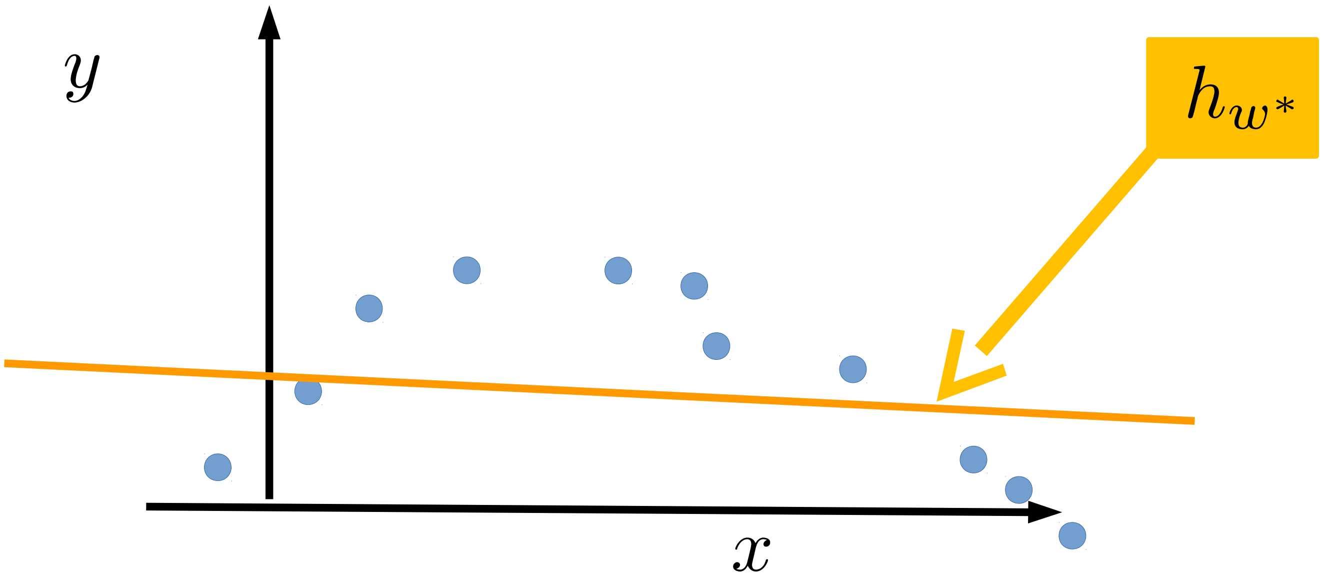
The Training Problem

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

Is a notion of Loss enough?

What happens when we do not have enough data?

Overfitting and Model Complexity

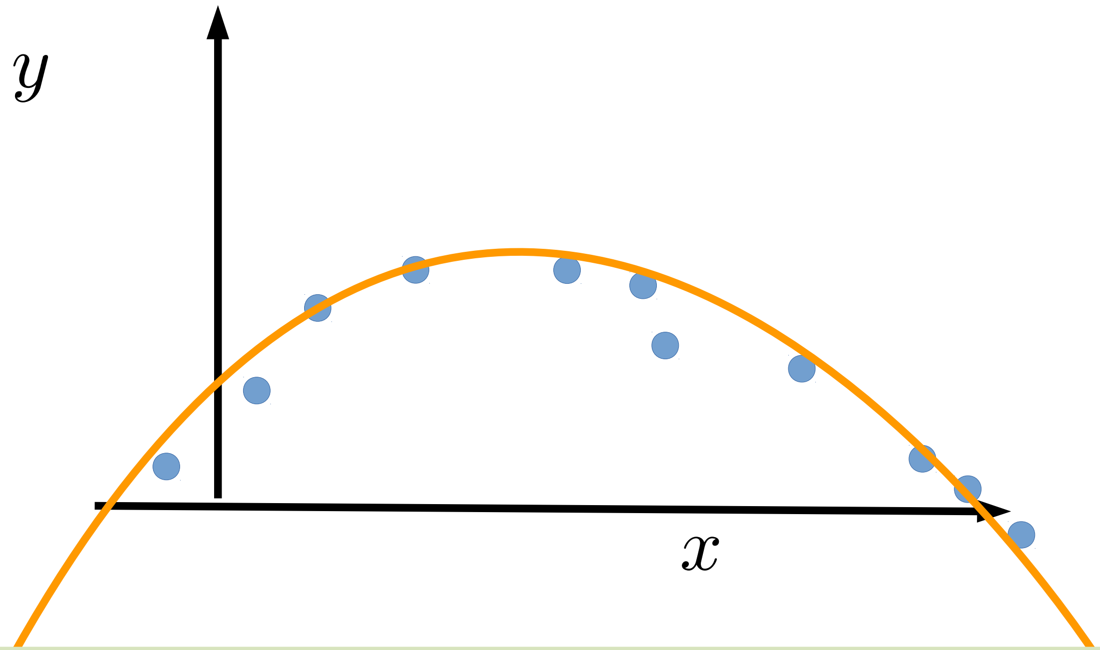


Fitting 1st order polynomial

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

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

Overfitting and Model Complexity



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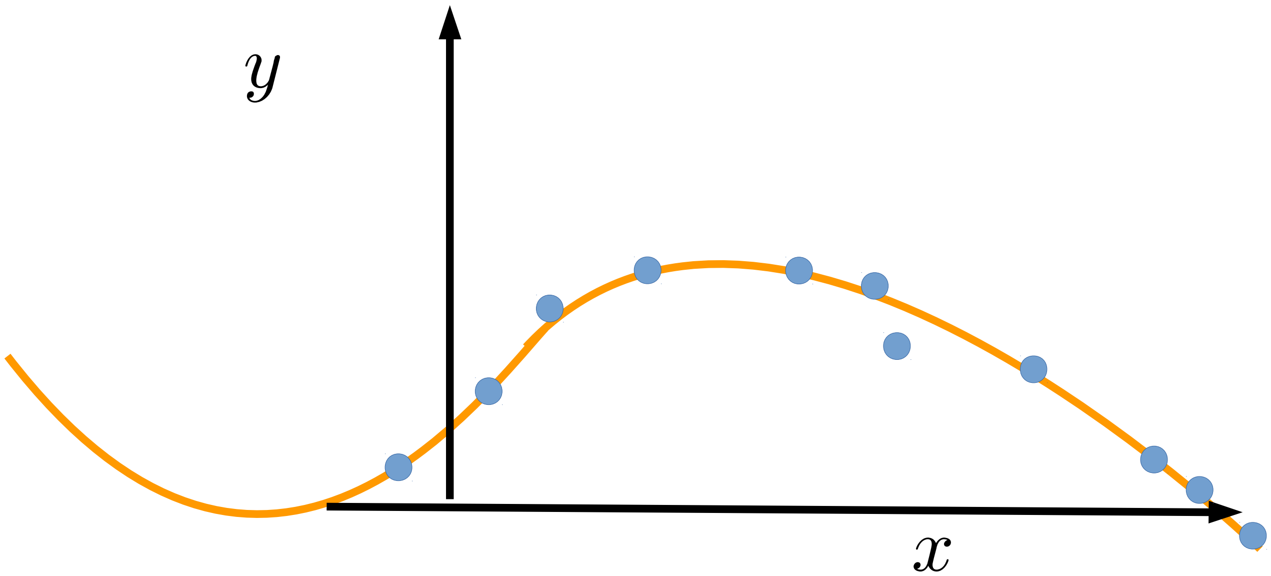
Overfitting and Model Complexity

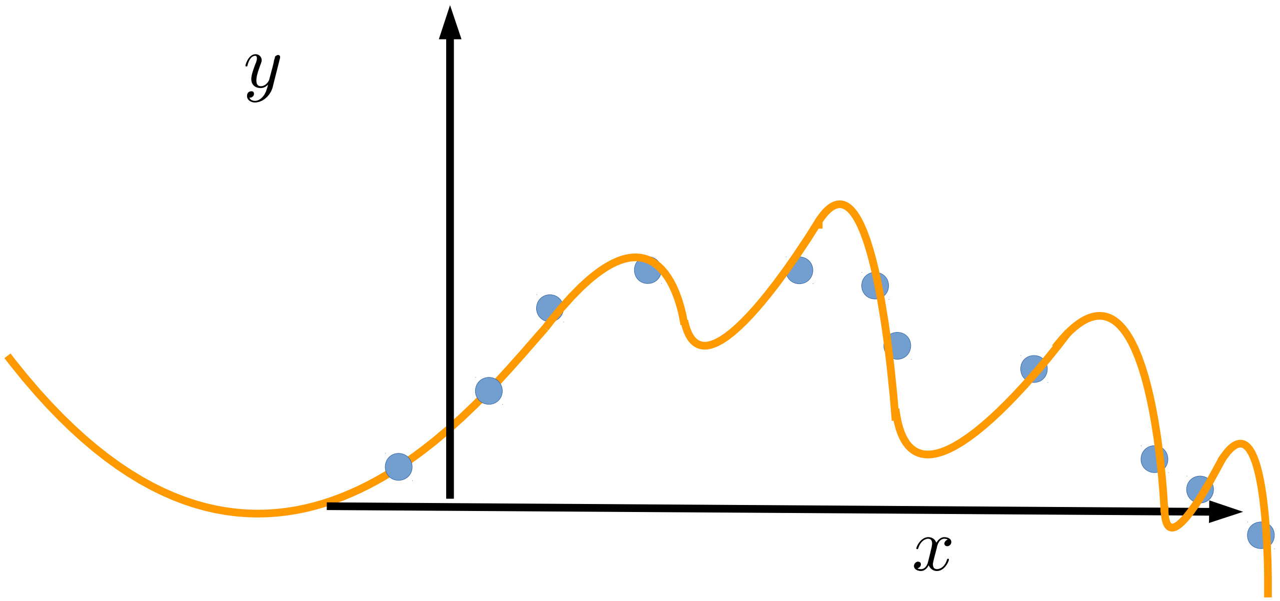


Fitting 3rd order polynomial

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

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

Overfitting and Model Complexity



Fitting 9th order polynomial

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

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

Regularization

Regularizor Functions

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

General Training Problem

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

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$$\min_{w \in \mathbf{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right)}_{\text{Goodness of fit, fidelity term ...etc}} + \lambda R(w)$$

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Regularization

Regularizor Functions

$$R : \mathbf{R}^d \rightarrow \mathbf{R}_+$$
$$w \rightarrow R(w)$$

Controls tradeoff between fit and complexity

General Training Problem

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Goodness of fit, fidelity term ...etc

Penlizes complexity

Regularization

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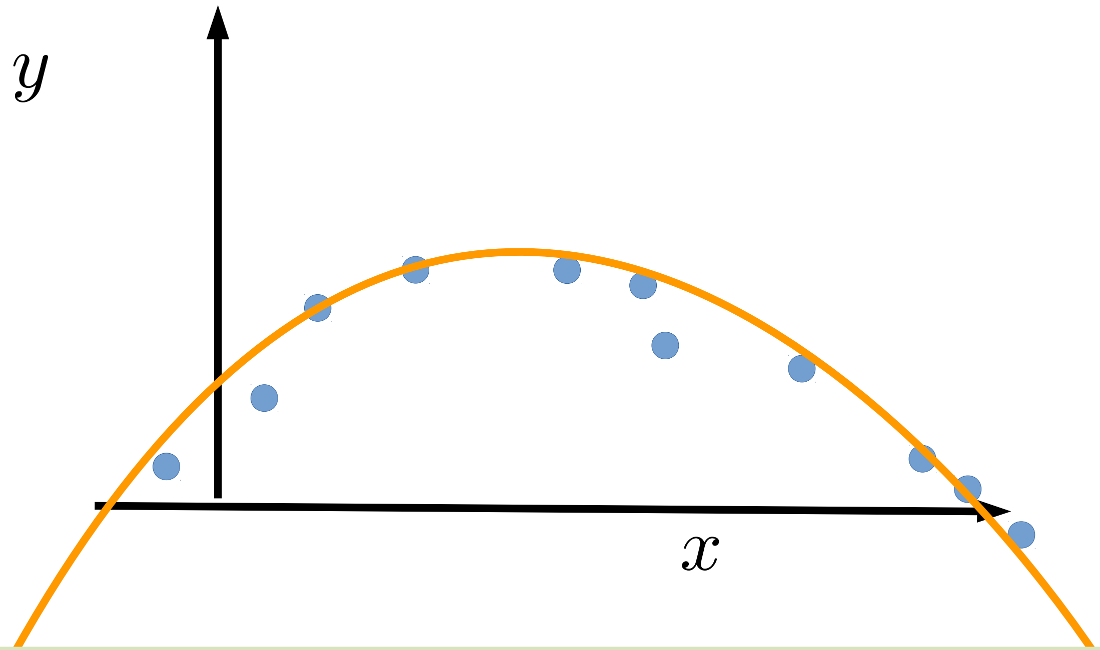
Exe:

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

Overfitting and Model Complexity

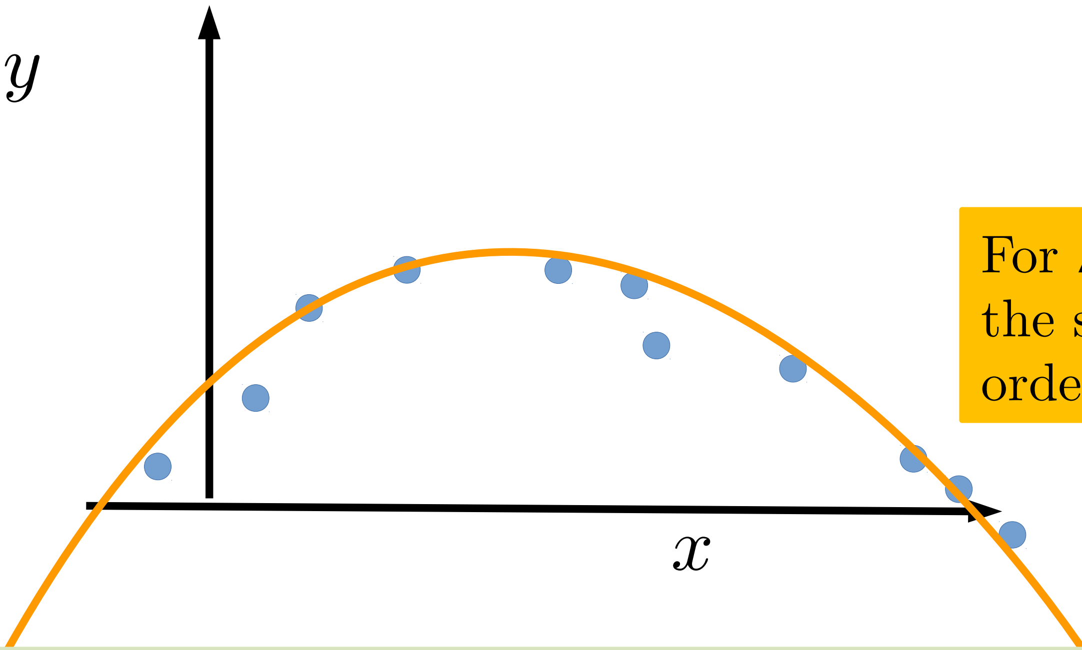


Fitting k^th order polynomial

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

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i\right)^2 + \lambda ||w||_2^2$$

Overfitting and Model Complexity



For λ big enough, the solution is a 2nd order polynomial

Fitting kth order polynomial

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

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i\right)^2 + \lambda ||w||_2^2$$

Exe: Ridge Regression

Linear hypothesis

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

L2 regularizor

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

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 regularizor

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

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 regularizor

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

Logistic loss

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

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: $(x^1, y^1), \ldots, (x^n, y^n)$

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(2) Choose a parametrization for hypothesis: $h_w(x)$

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(2) Choose a parametrization for hypothesis: $h_w(x)$

(3) Choose a loss function: $\ell(h_w(x), y) \geq 0$

(4) Solve the *training problem*:

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

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(5) Test and cross-validate. If fail, go back a few steps

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