Machine Learning
CS342

Lecture 2: Linear Regression with Ordinary Least Squares (OLS)

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Department of COMPUTER SCIENCE

Recap: ML subfields

Machine Learning

Supervised Learning
- Regression ← **We are here**
- Classification
- Ranking
- Structured Prediction

$\mathcal{D} = \{\mathbf{X}, \mathbf{t}\}, \quad e.g. \quad \mathbf{X} \in \Re^{N \times D}, \mathbf{t} \in \Re^{N}$

Unsupervised Learning
- Clustering
- Dimensionality Reduction $\quad \mathcal{D} = \{\mathbf{X}\}, \quad \mathbf{X} \in \Re^{N \times D}$
- Manifold Learning

Reinforcement Learning
- Markov Decision Process (e.g. Robotics)
- Multi-Agent Systems $\quad \mathcal{D} = \{\mathbf{S}, \mathbf{A}, \mathbf{R}, \pi^*, \mathbf{V}\}$
- TD/Q-Learning (State-Action-Reward)

Recap: Definition of "learning from data"

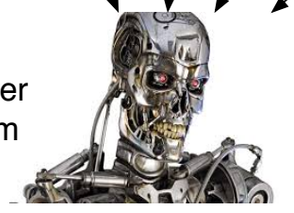
- Study of systems and algorithms that "**learn from data**"

- *A computer program is said to learn from experience **E* (data)** with respect to some class of tasks **T** and performance measure **P**, if its performance at tasks in **T**, as measured by **P**, improves with experience **E**.* [Tom Mitchell, 1998]

E: Data on Sarah

Learning Process

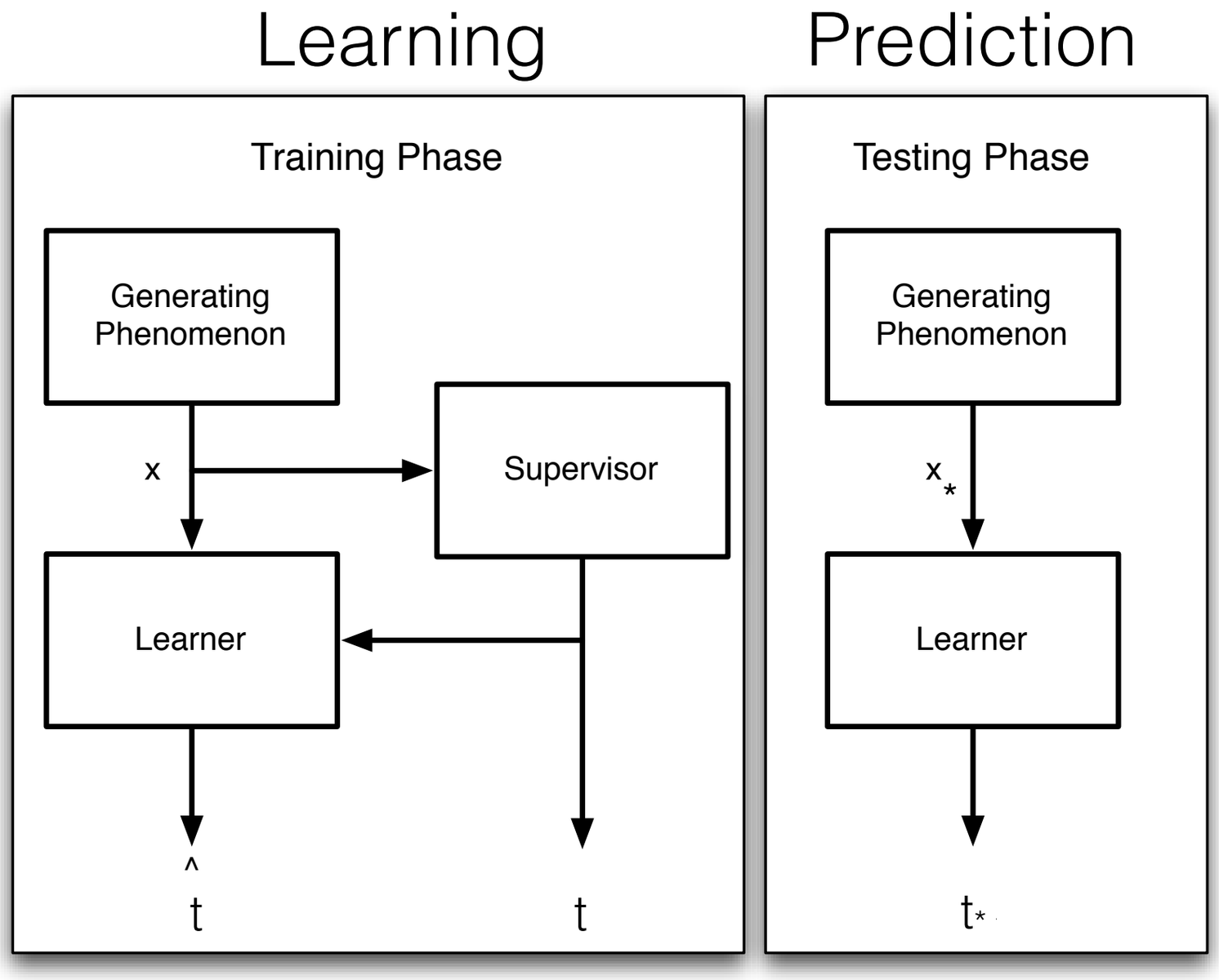
Computer Program



T: Find Sarah

P: % Correct recognitions

Recap: Schematic of Learning (Training) and Prediction phase



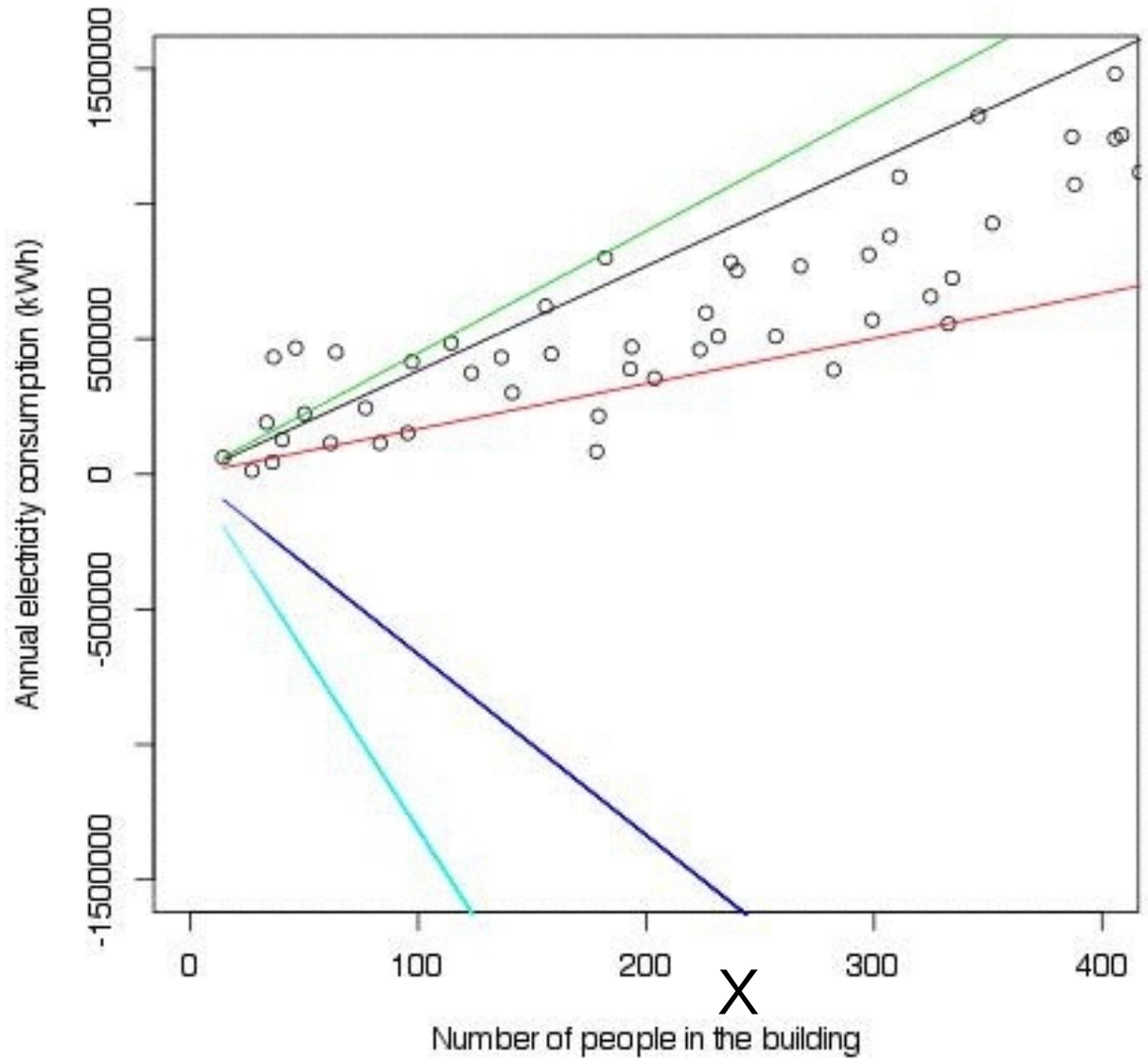
$$D_{\text{training}} = \{\mathbf{X}, \mathbf{t}\} = \{\mathbf{x}_n, t_n\}_{n=1}^{N} \qquad D_{\text{testing}} = \{\mathbf{X}_*\}$$

Recap: Linear Regression

Regression:

t is continuous

t



Hypothesis: The relationship between x and t is **linear**

$$\hat{t} = f(x; w_0, w_1) = w_0 + w_1 x$$

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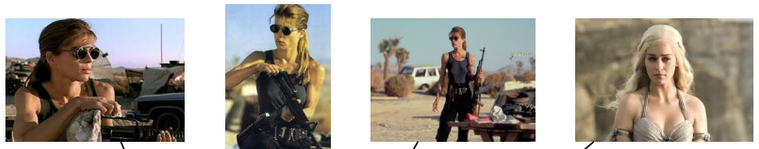
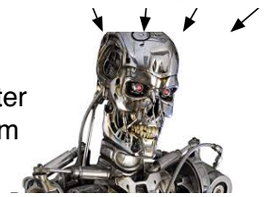
Recap: Supervised Learning components

E: Data on Sarah



Learning Process

Computer Program



T: Find Sarah

P: % Correct recognitions

Supervised Learning Process

Data
(inputs **X** / outputs **t**)

Hypothesis Space
(e.g. all lines in 2D)
Functions that map inputs to outputs

$$f(\mathbf{x};\mathbf{w}) : \mathbf{x} \rightarrow t$$

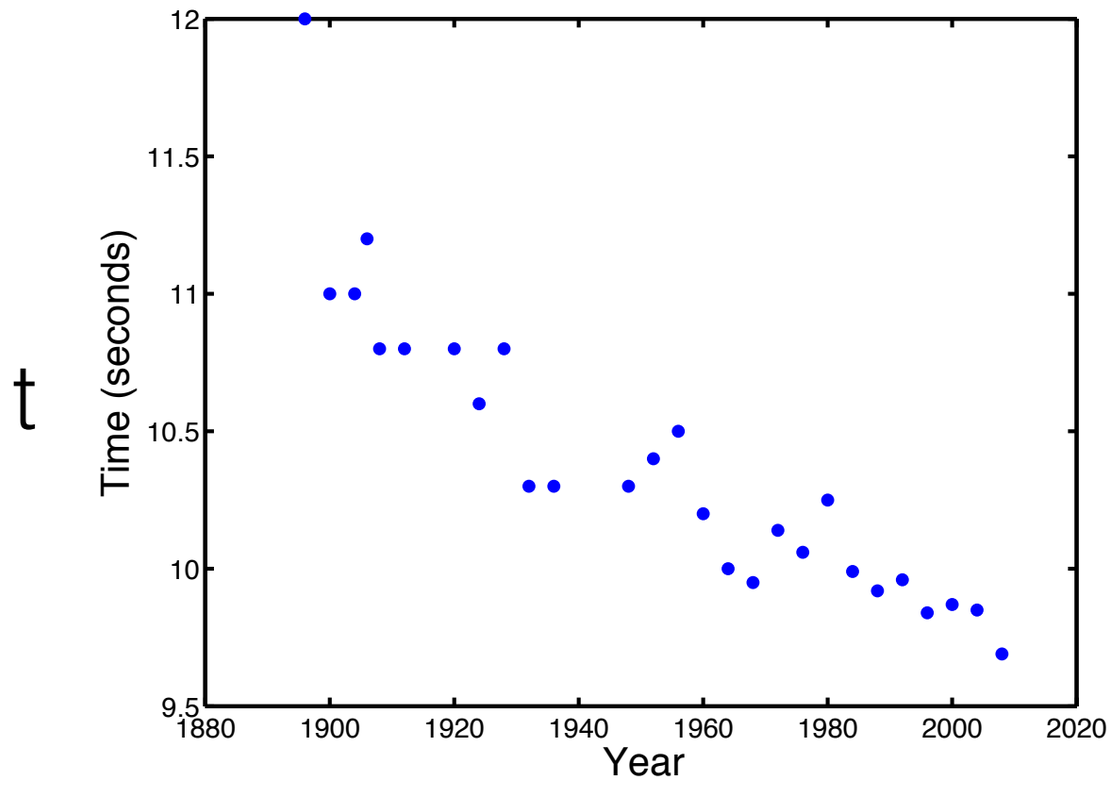
"Goodness" Metric
(e.g. a distance of f(x;w) to t)

Learning Program

Parameters $\mathbf{w}$ (choose a specific hypothesis/mapping)

Learning as parameter (hypothesis) inference

Revisit Olympics example: Univariate regression



Rogers & Girolami Ch. 1

t

X

Learn a mapping (function) of inputs x to outputs t

$$f(x; \mathbf{w}) : x \rightarrow t$$

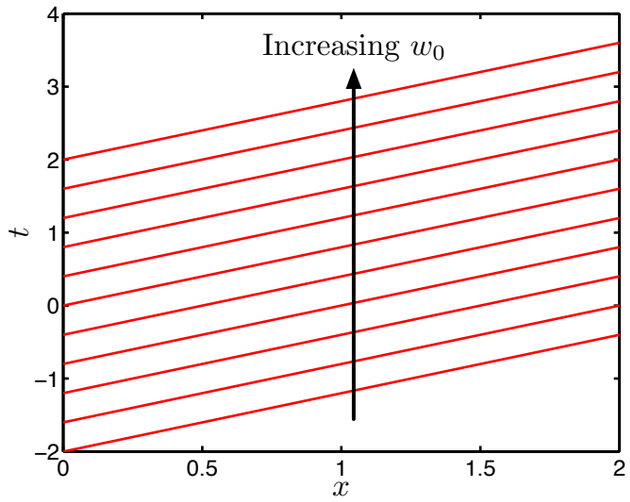
Hypothesis: linear relationship. So our hypothesis space is all lines in this space:

$$\hat{t} = f(x; \mathbf{w}) = w_0 + w_1 x$$

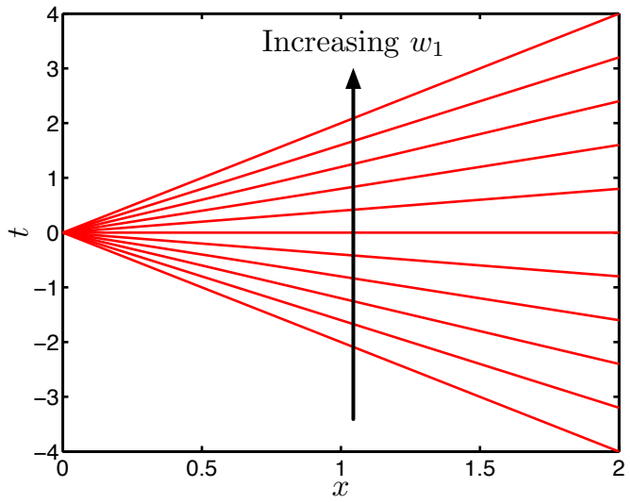
What is a good model?

$$\hat{t} = f(x; \mathbf{w}) = w_0 + w_1 x$$

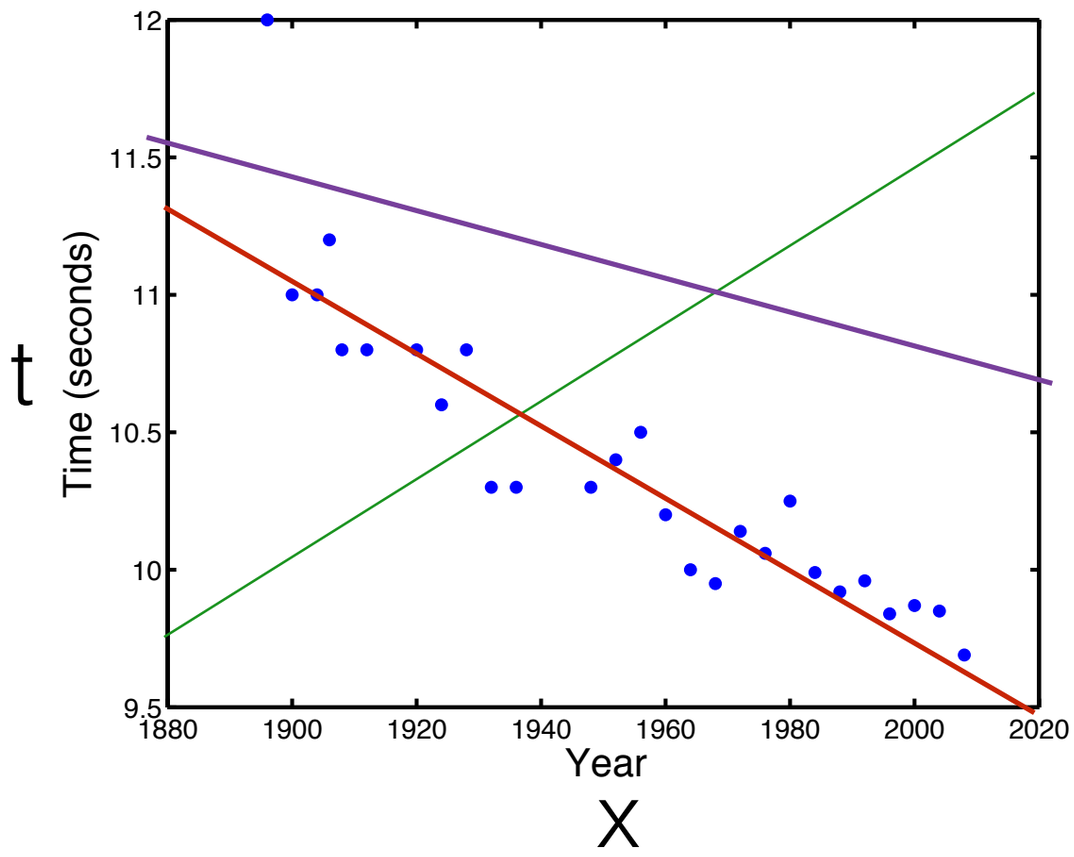
Different parameters
give us different lines/hypothesis



(a) Increasing w_0 changes the point at which the line crosses the t axis.



(b) Increasing w_1 changes the gradient of the line.



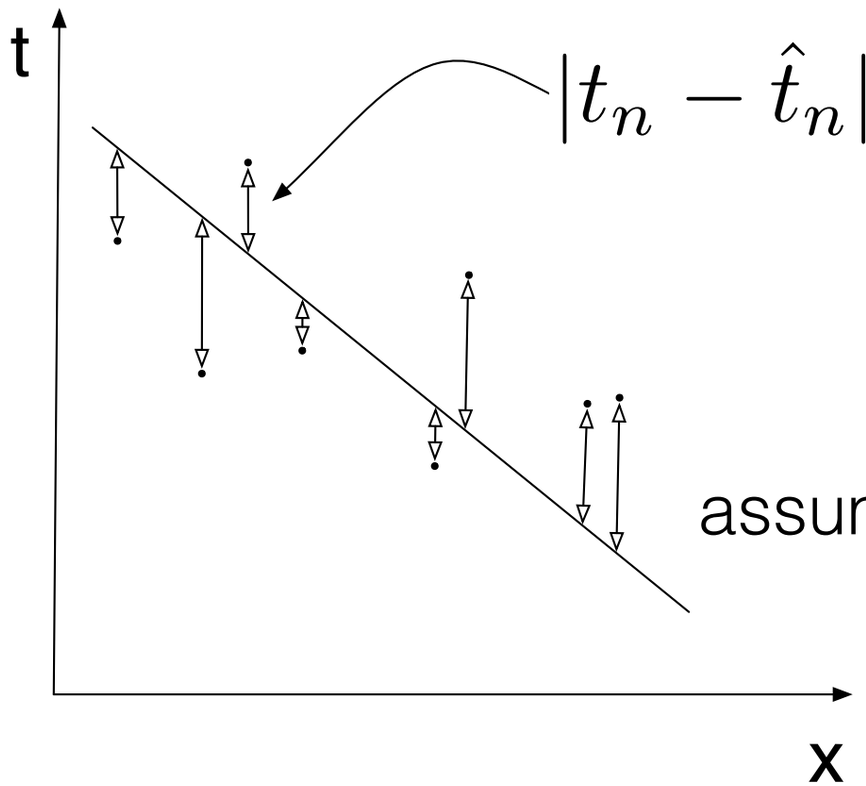
Ok so how do we find the right parameters?
What is one possible measure of “goodness”?

Loss functions

$$\hat{t} = f(x; \mathbf{w}) = w_0 + w_1 x$$

Line that passes as **close** as possible to all the points

n^{th} observation has $\{x_n, t_n\}$



$$|t_n - \hat{t}_n| = |t_n - f(x_n; \mathbf{w})|$$

assume "error" is in t direction

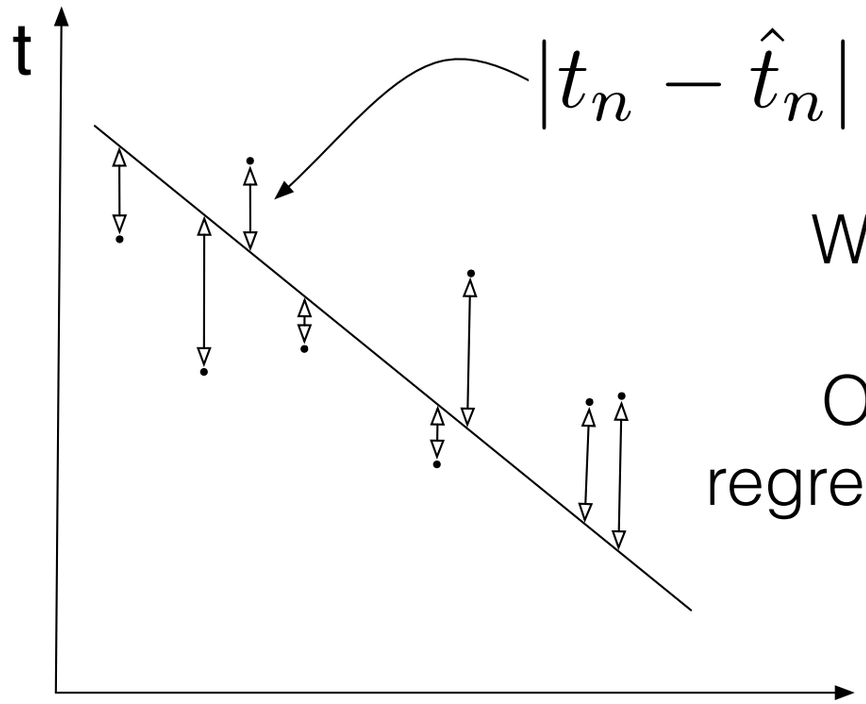
A natural choice is the ***squared loss*** function

$$\mathcal{L}_n(t_n, \hat{t}_n) = \mathcal{L}_n(t_n, f(x_n; \mathbf{w})) = (t_n - f(x_n; w_0, w_1))^2$$

Squared loss

Just square
the arrow length

a.k.a quadratic loss



$$|t_n - \hat{t}_n| = |t_n - f(x_n; \mathbf{w})|$$

Why vertical distance?

Orthogonal/Euclidean regression if we assume error is in both x and t

$$\mathcal{L}_n(t_n, \hat{t}_n) = \mathcal{L}_n(t_n, f(x_n; \mathbf{w})) = (t_n - f(x_n; w_0, w_1))^2$$

And the total loss for all inputs/observations?

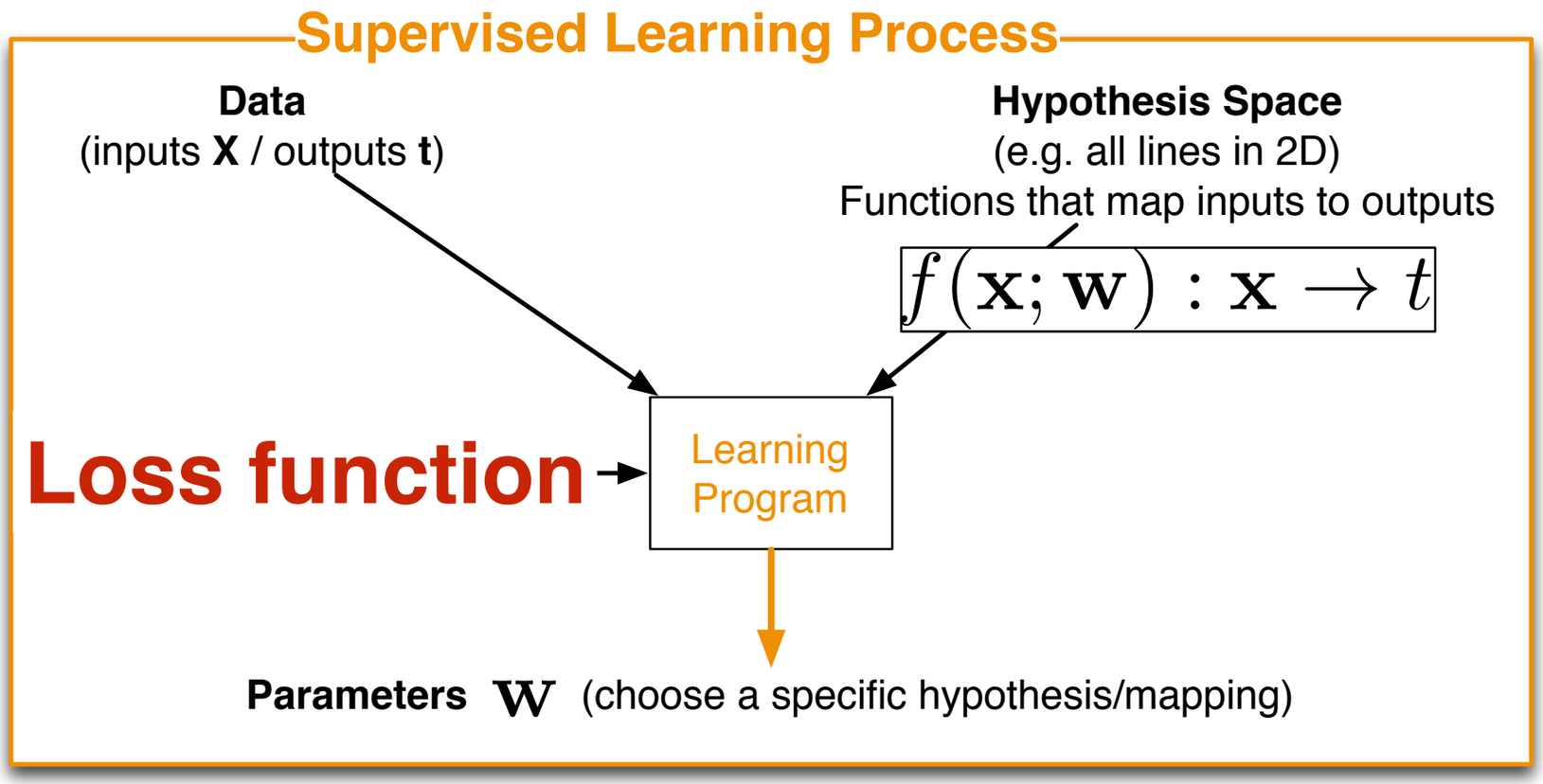
$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}_n$$

Any other Loss function you can think of?

$$\hat{\mathbf{t}} = \mathbf{X}\mathbf{w}$$

vector-matrix notation
see R&G p15-20!

Recap



Why do we use the squared error Loss?

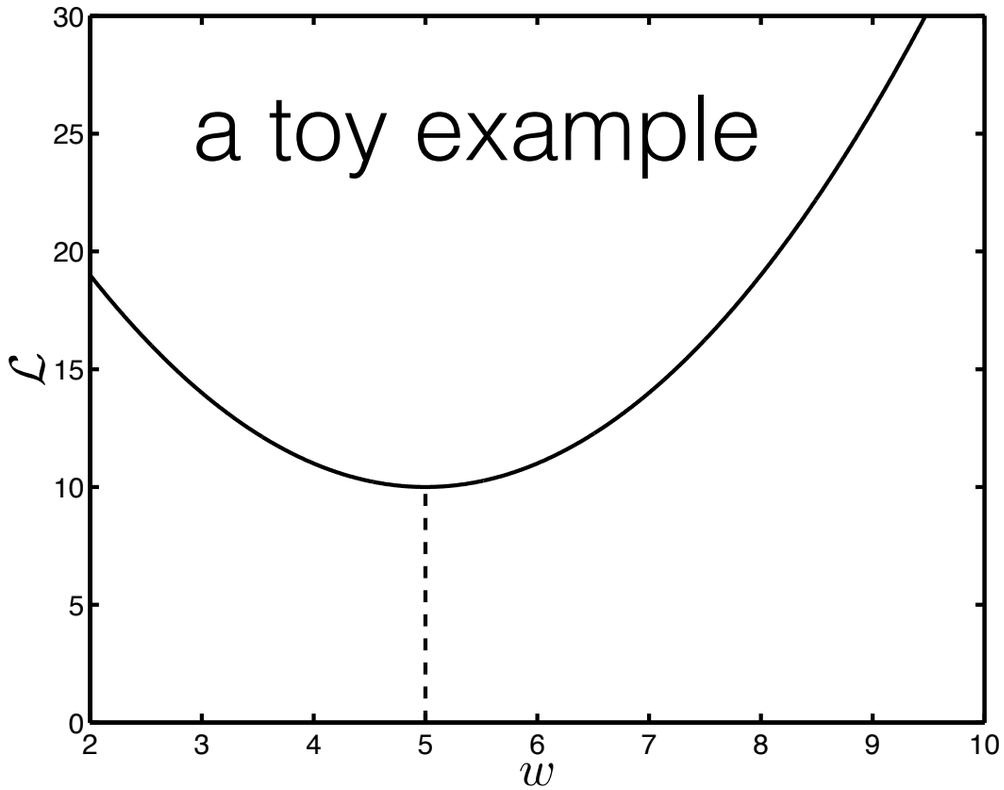
Because we can **analytically** derive (by simple math get a final expression by hand) the best* parameters/hypothesis.

Different lines (parameters) different Loss. Do you like loosing?

Final step: Minimise the Loss

$$\mathcal{L} = \frac{1}{N}\sum_{n=1}^{N}(t_n - f(x_n; w_0, w_1))^2$$

Find the parameters that minimise the Loss



What do we want? from words to math..

$$\widehat{w_0}, \widehat{w_1} \leftarrow \underset{w_0, w_1}{\operatorname{argmin}} \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(t_n, f(x_n; w_0, w_1))$$

Optimisation problem

Some necessary math

$$\widehat{w_0}, \widehat{w_1} \leftarrow \underset{w_0, w_1}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}_n(t_n, f(x_n; w_0, w_1))$$

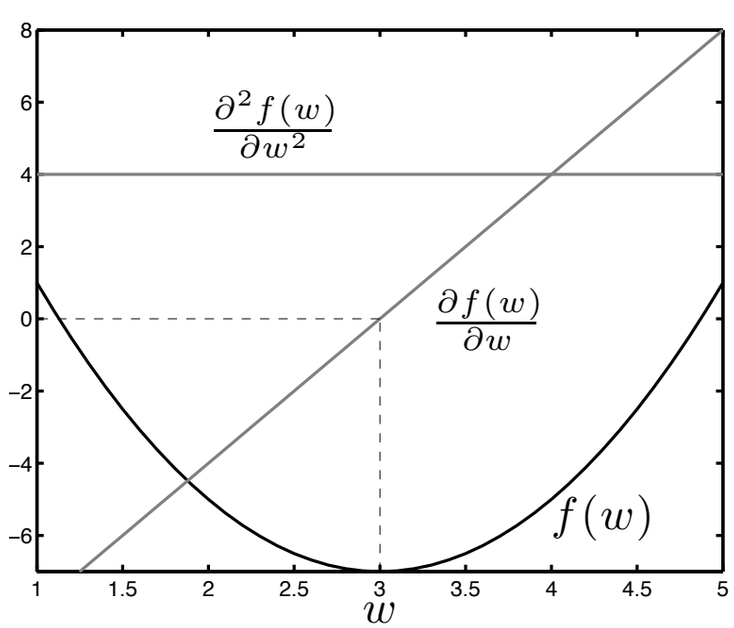
1. Replace with the expression for the specific Loss
2. Equate first derivative of Loss to zero to get **w** (find potential minima)
3. Examine second derivative of Loss at **w** to determine if unique minima

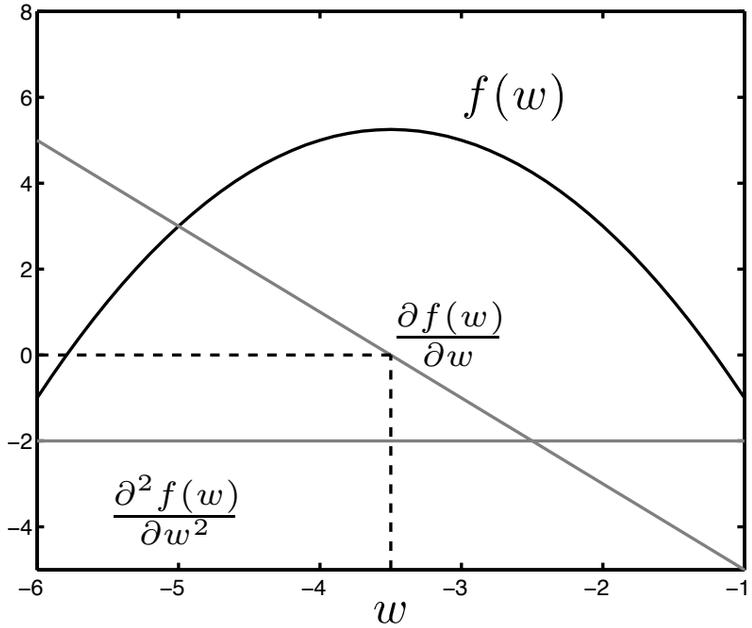
Find OLS parameters by $\frac{\partial \mathcal{L}}{\partial \mathbf{w}} \rightarrow 0$

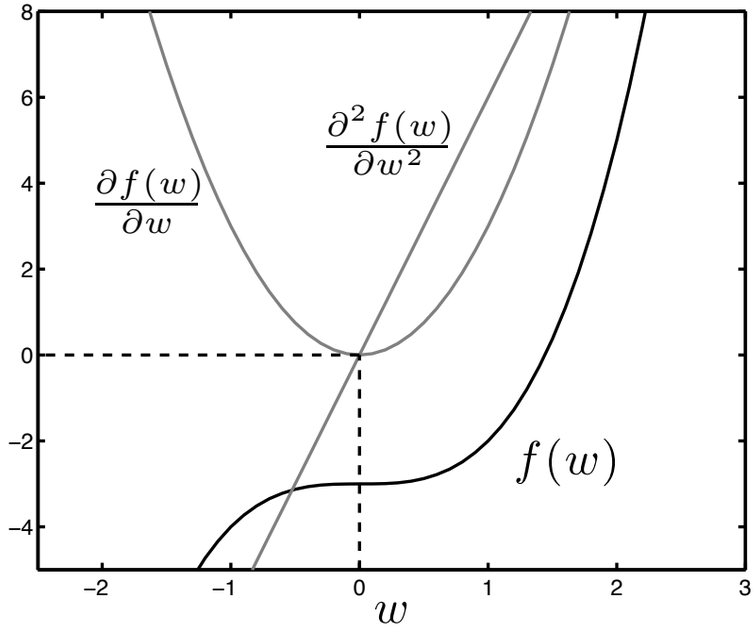
$$\text{if} \quad \frac{\partial^2 \mathcal{L}}{\partial^2 \mathbf{w}} > 0 \quad \text{we are at a minima}$$

The squared error Loss is **convex and smooth** so single global minima

Minima of a function







Derive OLS solutions (board/lab)

$$\widehat{w_0} = \bar{t} - w_1 \overline{x} = \frac{1}{N} \sum_{n=1}^{N} t_n - w_1 \sum_{n=1}^{N} x_n$$

Final form is:

$$\widehat{w_1} = \frac{\overline{xt} - \overline{x}\,\overline{t}}{\overline{x^2} - (\overline{x})^2}$$

Thats it!
Learning from data

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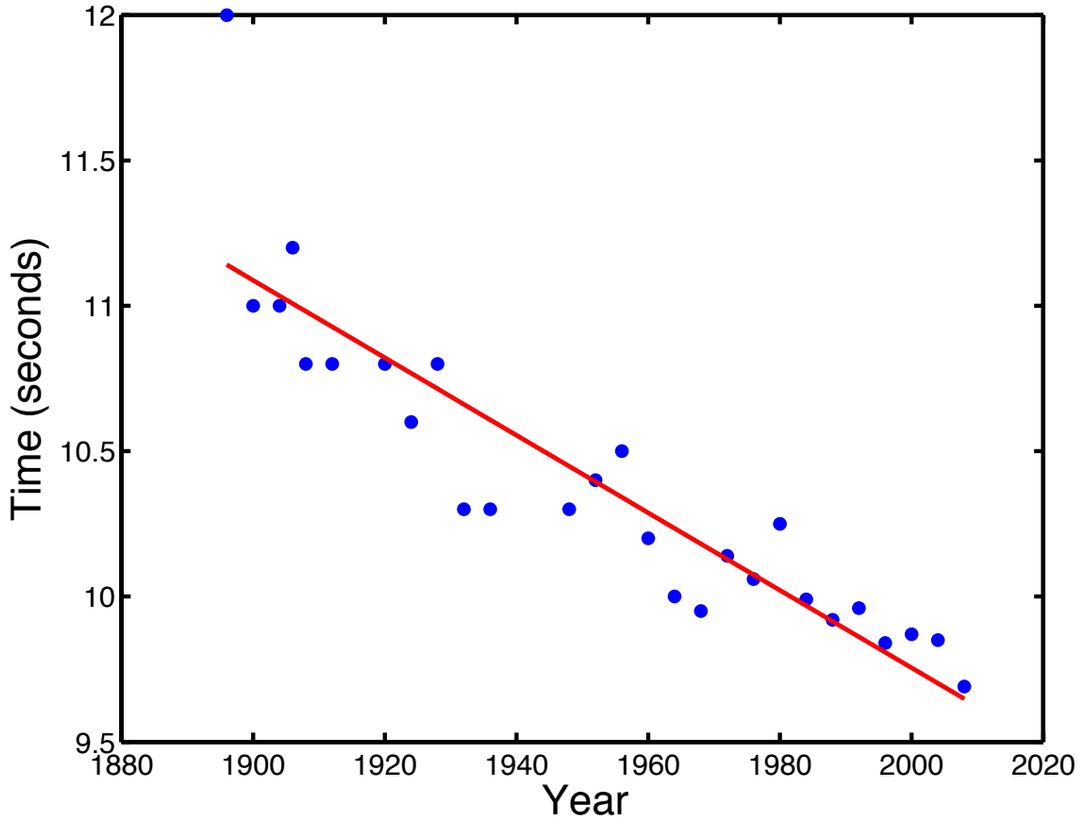
Breath!

You have just looked inside the box of your first ML model!

Making Predictions

The Ordinary Least Squares (OLS) fit to our training data

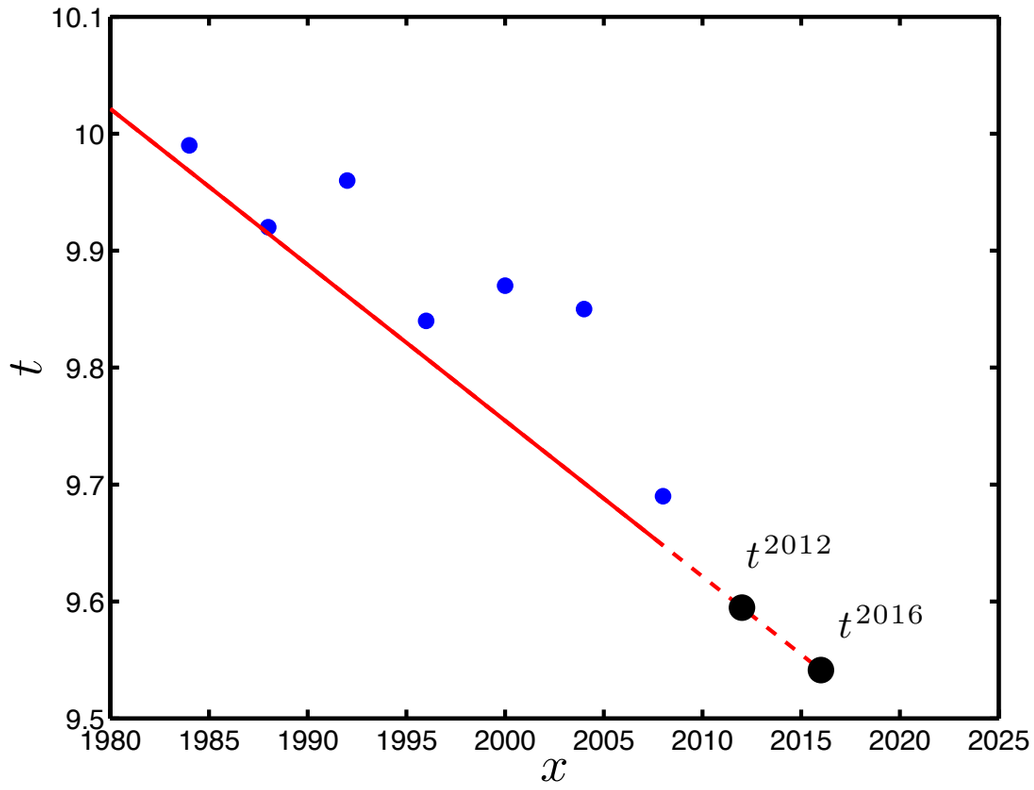


$$\hat{t} = f(x; \mathbf{w}) = w_0 + w_1 x$$

but we now have learned values for w so write:

$$\hat{t} = f(x; \mathbf{w}) = \widehat{w_0} + \widehat{w_1} x$$

What would our model predict for future?

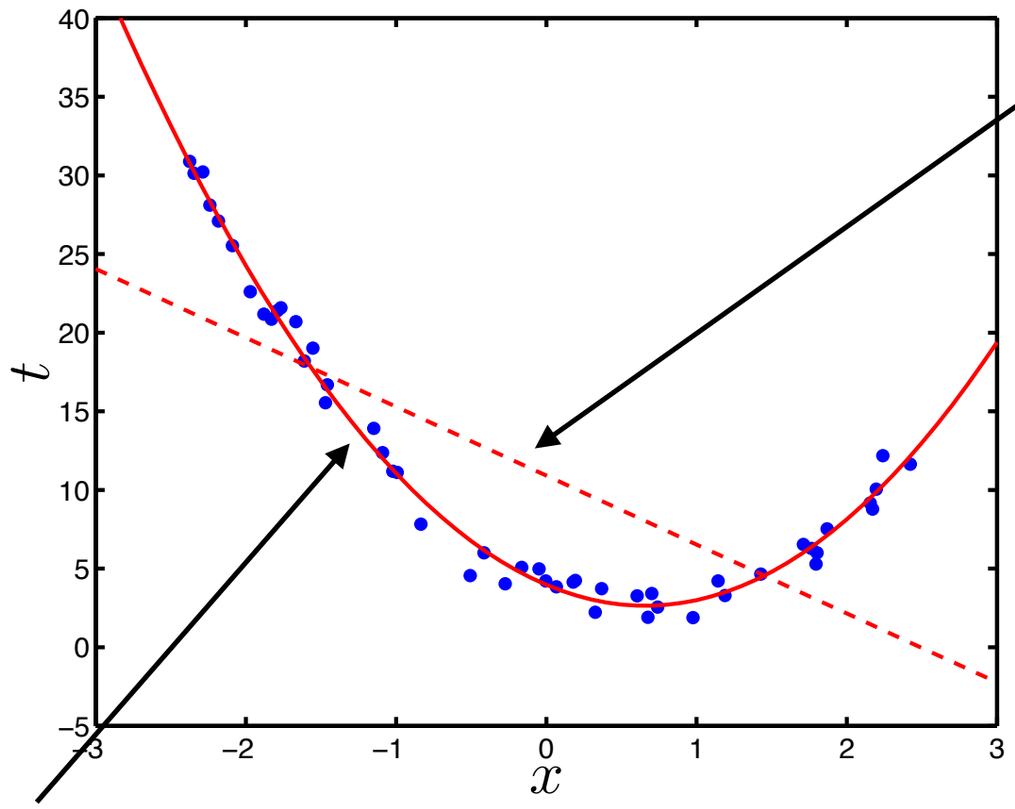


our prediction is $t^* = \widehat{w_0} + \widehat{w_1} x^*$

Can we create non-linear responses from a linear model?

linear regression (OLS): **linear in w**, linear in data x

$$f(x; \mathbf{w}) = w_0 + w_1 x$$



Pretty restrictive hypothesis space?

Demo

linear regression (OLS): **linear in w**, non-linear in data x

$$f(x; \mathbf{w}) = w_0 + w_1 x + w_2 x^2 = w_0 + w_1 \mathrm{x}_1 + w_2 \mathrm{x}_2$$

Still a linear structure (hyper-plane) but in a higher dimensional space

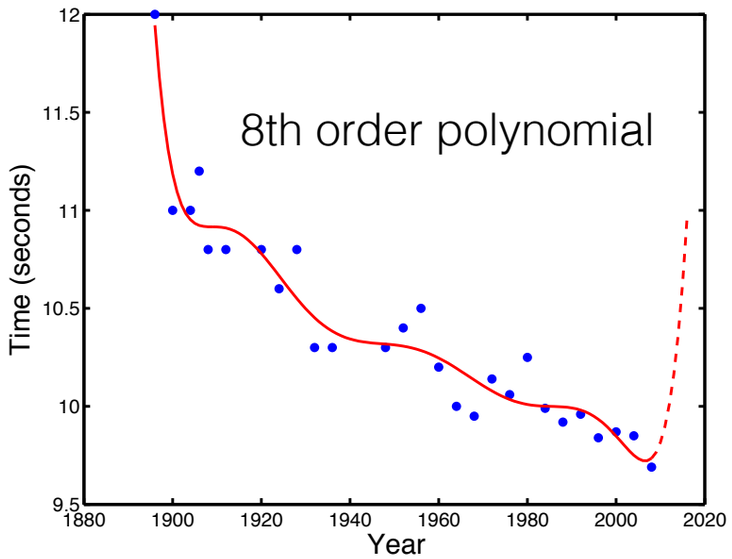
Feature engineering! A black art

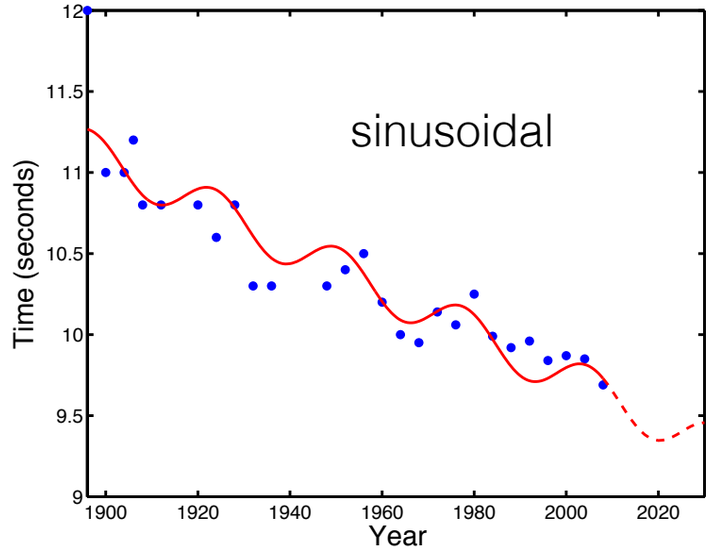
we map input space into new space called feature space

$$\mathbf{X} \rightarrow \Phi(\mathbf{X}) \quad \text{where} \quad \mathbf{X} \in \Re^{N \times D} \quad \Phi(\mathbf{X}) \in \Re^{N \times D*} \quad D* \gg D$$

From simple polynomial expansions to other functions

$$\mathbf{X} = \begin{bmatrix} x_1^0 & x_1^1 & x_1^2 & \cdots & x_1^K \\ x_2^0 & x_2^1 & x_2^2 & \cdots & x_2^K \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ x_N^0 & x_N^1 & x_N^2 & \cdots & x_N^K \end{bmatrix}$$





Whole fields of AI that deal with this problem for specific data types:
Computer Vision: Images, Video
NLP: Documents, Text
Acoustics: Sound

Matrix Derivation of OLS solution (see Ch1. R&G book p15)

We have input data **X** with N observations (rows) and D attributes (columns), and also have N outputs/targets **t**, one for every input.
e.g. If N=3 and D=2 our data would look like:

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix} \quad \text{and} \quad \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix}$$

We will fit a linear model: line or (hyper-)plane in higher dimensions:

$$f(\mathbf{x}_n; \mathbf{w}) = w_0 + w_1 x_{n1} + \cdots + w_d x_{nd} + \cdots + w_D x_{nD}$$

for the example above this becomes:

$$f(\mathbf{x}_n; \mathbf{w}) = w_0 + w_1 x_{n1} + w_2 x_{n2}$$

And we decided to use the squared error or quadratic loss:

$$\mathcal{L}_n(t_n, \hat{t}_n) = (t_n - f(\mathbf{x}_n; \mathbf{w}))^2$$

Matrix Derivation of OLS solution (see Ch1. R&G book p15)

we can transform our **X** to include a column of 1s in the left and hence re-write our function in a compact vector-matrix format

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} \\ 1 & x_{21} & x_{22} \\ 1 & x_{31} & x_{32} \end{bmatrix} \quad \text{and} \quad \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix}$$

we could use another symbol instead of X to denote this but we are "overloading" notation and still call it **X**.

$$f(\mathbf{x}_n; \mathbf{w}) = w_0 + w_1 x_{n1} + w_2 x_{n2} = \mathbf{x}_n \mathbf{w}$$

where $\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$ So for all n our linear model is: $\mathbf{X}\mathbf{w}$

Matrix Derivation of OLS solution (see Ch1. R&G book p15)

So our squared error Loss function that we want to minimise can be written as:

$$\mathcal{L} = \frac{1}{N}(\mathbf{t} - \mathbf{X}\mathbf{w})^{\mathrm{T}}(\mathbf{t} - \mathbf{X}\mathbf{w})$$

We want to differentiate the loss wrt to the parameters and set it to zero:

expanding the brackets to re-write the loss

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \frac{\partial}{\partial \mathbf{w}}\left(\frac{1}{N}(\mathbf{t}^{\mathrm{T}}\mathbf{t} - \mathbf{t}^{\mathrm{T}}\mathbf{X}\mathbf{w} - \mathbf{w}^{\mathrm{T}}\mathbf{X}^{\mathrm{T}}\mathbf{t} + \mathbf{w}^{\mathrm{T}}\mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{w})\right) = 0$$

noting that second and third term inside parenthesis are equal
and following rules of differentiation (see p21, table 1.4):

$$-2\mathbf{X}^{\mathrm{T}}\mathbf{t} + 2\mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{w} = 0$$

we get the final solution: $\mathbf{w} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{t}$