COMS 4721: Machine Learning for Data Science

Lecture 2, 1/19/2017

Prof. John Paisley

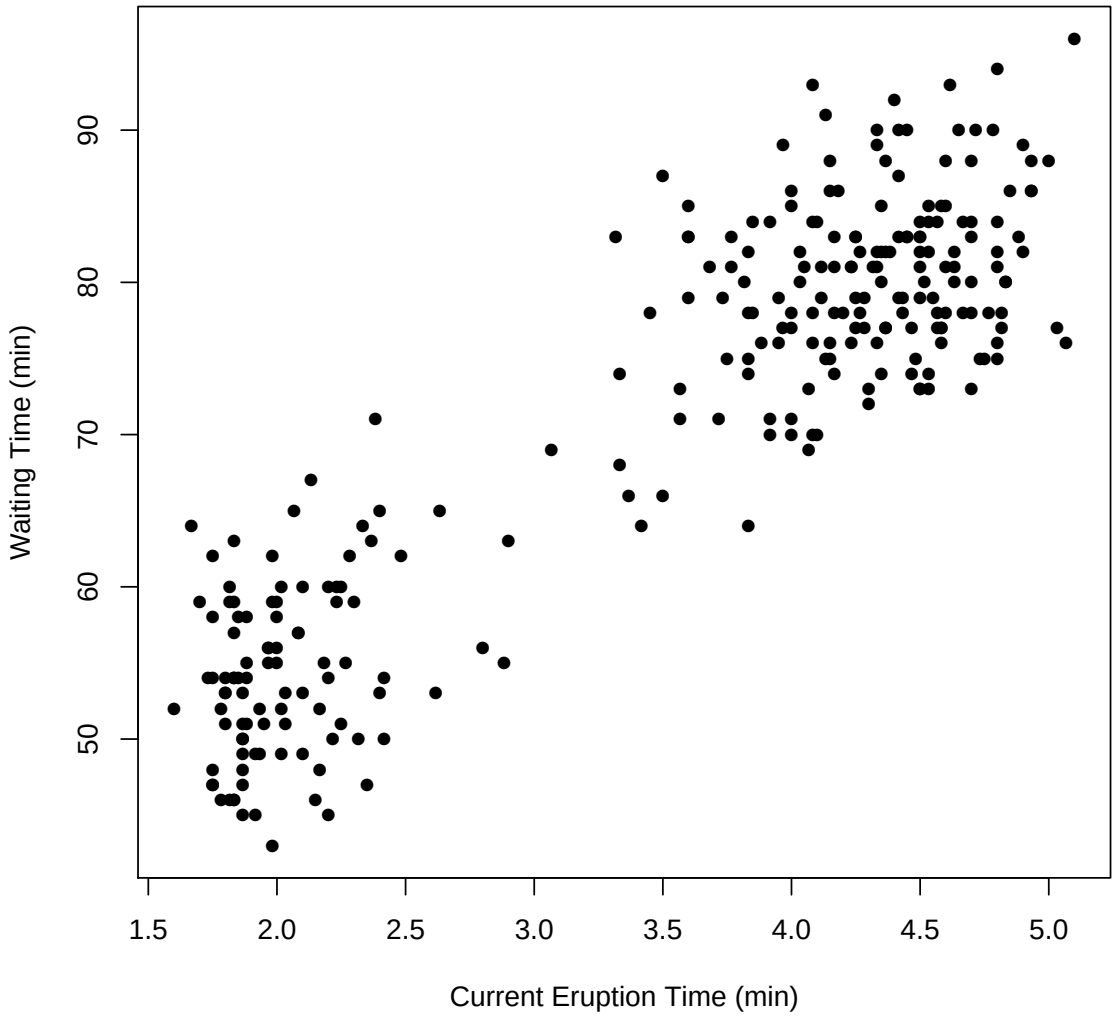
Department of Electrical Engineering
& Data Science Institute

Columbia University

Linear Regression

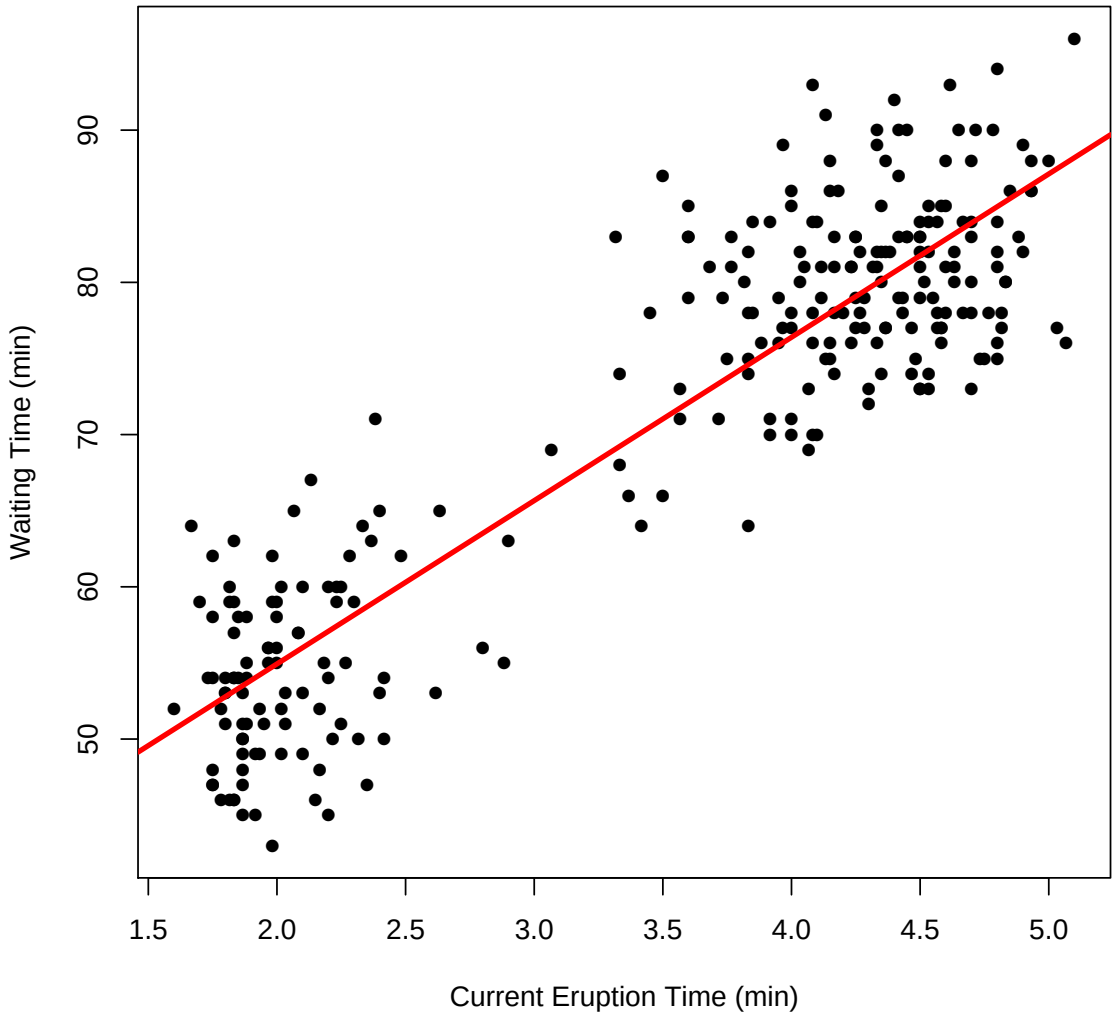
Example: Old Faithful

EXAMPLE: OLD FAITHFUL



Can we meaningfully predict the time between eruptions only using the duration of the last eruption?

Example: Old Faithful



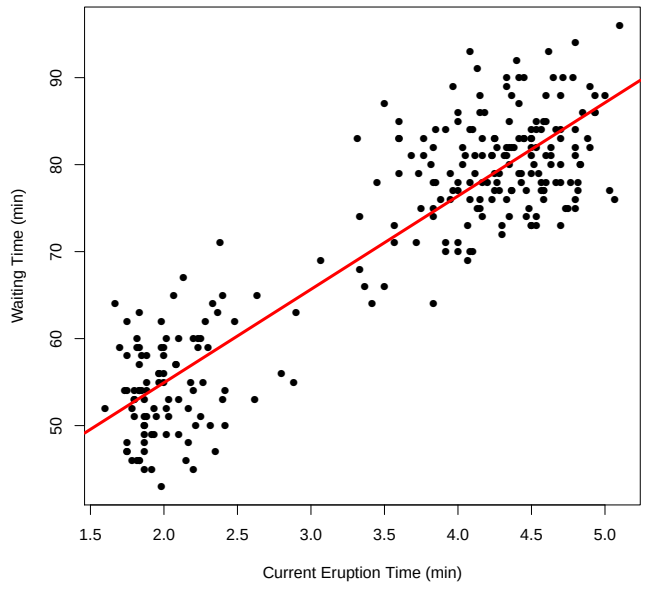
Can we meaningfully predict the time between eruptions only using the duration of the last eruption?

Example: Old Faithful

One model for this

$$\text{(wait time)} \approx w_0 + \text{(last duration)} \times w_1$$

- w_0 and w_1 are to be learned.
- This is an example of linear regression.



Refresher

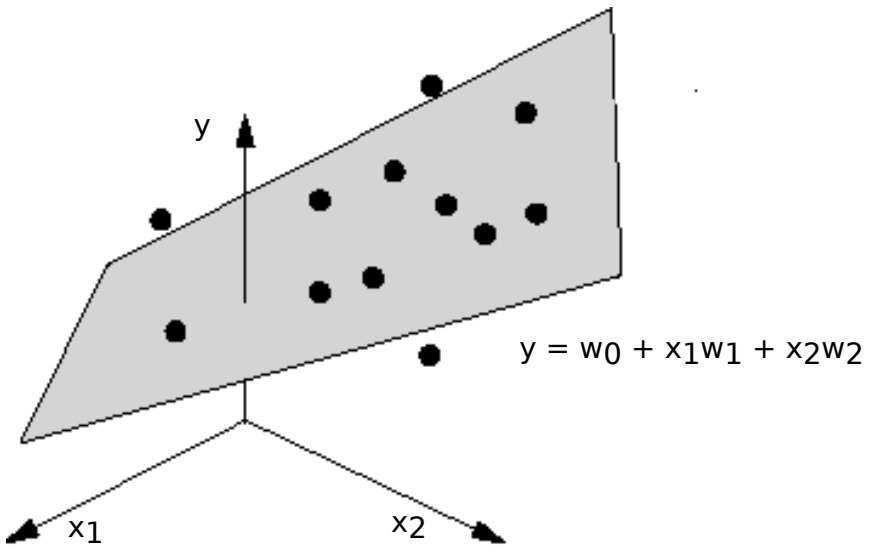
w_1 is the slope, w_0 is called the intercept, bias, shift, offset.

HIGHER DIMENSIONS

Two inputs

$$\text{(output)} \approx w_0 + \text{(input 1)} \times w_1 + \text{(input 2)} \times w_2$$

With two inputs the intuition is the same $\longrightarrow$



Regression with Partial Least Squares - Trial Version of PDFAnnotator - www.PDFAnnotator.com

Data

Input: $x \in \mathbb{R}^d$ (i.e., measurements, covariates, features, indepen. variables)
Output: $y \in \mathbb{R}$ (i.e., response, dependent variable)

Goal

Find a function $f : \mathbb{R}^d \to \mathbb{R}$ such that $y \approx f(x; w)$ for the data pair (x, y).
$f(x; w)$ is called a *regression function*. Its free parameters are w.

Definition of linear regression

A regression method is called *linear* if the prediction f is a linear function of the unknown parameters w.

f is a linear function of unknown parameters (w), does not necessarily mean that 'f' is linear function of covariates (x). → 'w' parameters interact linearly with inputs x to map to output y.

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Model

The linear regression model we focus on now has the form

$$y_i \approx f(x_i; w) = w_0 + \sum_{j=1}^{d} x_{ij} w_j.$$

Model learning

We have the set of *training data* $(x_1, y_1) \dots (x_n, y_n)$. We want to use this data to learn a w such that $y_i \approx f(x_i; w)$. But we first need an *objective function* to tell us what a "good" value of w is.

Least squares

The *least squares* objective tells us to pick the w that minimizes the sum of squared errors

$$w_{\text{LS}} = \arg\min_{w} \sum_{i=1}^{n} (y_i - f(x_i; w))^2 \equiv \arg\min_{w} \mathcal{L}.$$

Least squares in pictures

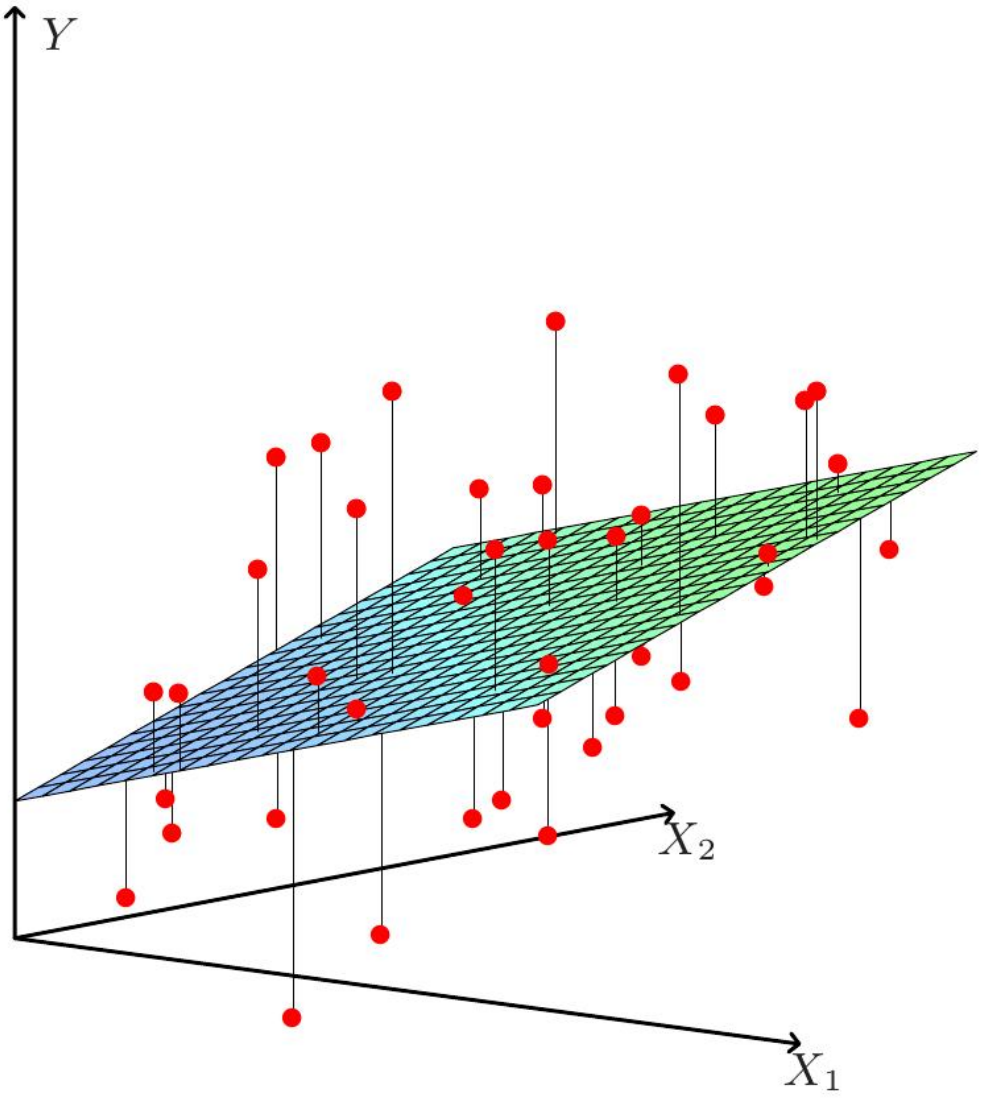
Observations:

Vertical length is error.

The objective function $\mathcal{L}$ is the sum of all the squared lengths.

Find weights (w_1, w_2) plus an offset w_0 to minimize $\mathcal{L}$.

(w_0, w_1, w_2) defines this plane.



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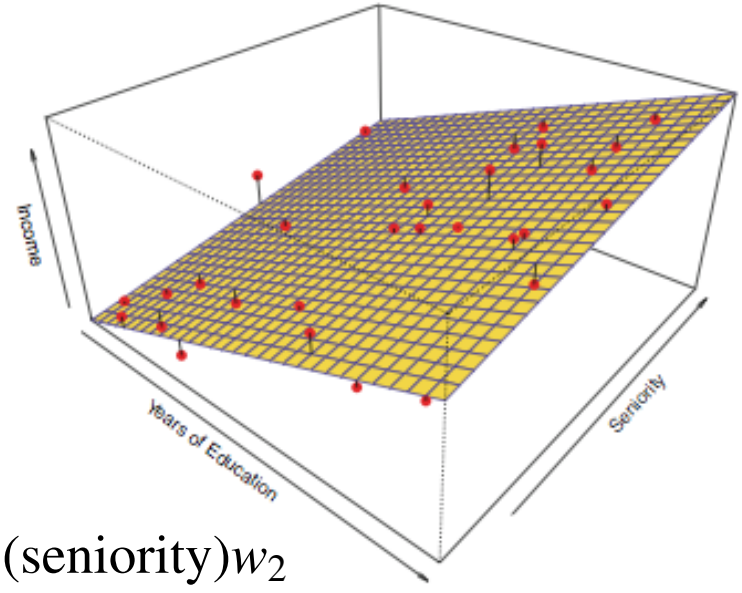
2-dimensional problem



Input: (education, seniority) $\in \mathbb{R}^2$.

Output: (income) $\in \mathbb{R}$

Model: (income) $\approx w_0 + (\text{education})w_1 + (\text{seniority})w_2$

Question: Both $w_1, w_2 > 0$. What does this tell us?

Answer: As education and/or seniority goes up, income tends to go up.

(Caveat: This is a statement about correlation, not causation.)

LEAST SQUARES LINEAR REGRESSION MODEL

Thus far

We have data pairs (x_i, y_i) of measurements $x_i \in \mathbb{R}^d$ and a response $y_i \in \mathbb{R}$.
We believe there is a linear relationship between x_i and y_i,

$$y_i = w_0 + \sum_{j=1}^{d} x_{ij} w_j + \epsilon_i$$

and we want to minimize the objective function

$$\mathcal{L} = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - w_0 - \textstyle\sum_{j=1}^{d} x_{ij} w_j)^2$$

with respect to $(w_0, w_1, \ldots, w_d)$.

Can math notation make this easier to look at/work with?

Notation: Vectors and Matrices

We think of data with d dimensions as a *column* vector:

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix} \quad \text{(e.g.)} \Rightarrow \quad \begin{bmatrix} \text{age} \\ \text{height} \\ \vdots \\ \text{income} \end{bmatrix}$$

A set of n vectors can be stacked into a matrix:

$$\mathbf{X} = \begin{bmatrix} x_{11} & \dots & x_{1d} \\ x_{21} & \dots & x_{2d} \\ \vdots & & \vdots \\ x_{n1} & \dots & x_{nd} \end{bmatrix} = \begin{bmatrix} - x_1^T - \\ - x_2^T - \\ \vdots \\ - x_n^T - \end{bmatrix}$$

Assumptions for now:

- All features are treated as continuous-valued ($x \in \mathbb{R}^d$)
- We have more observations than dimensions ($d < n$)

NOTATION : REGRESSION (AND CLASSIFICATION)

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Usually, for linear regression (and classification) we include an intercept term w_0 that doesn't interact with any element in the vector $x \in \mathbb{R}^d$.

It will be convenient to attach a 1 to the first dimension of each vector x_i (which we indicate by $x_i \in \mathbb{R}^{d+1}$) and in the first column of the matrix X:

$$x_i = \begin{bmatrix} 1 \\ x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1d} \\ 1 & x_{21} & \dots & x_{2d} \\ \vdots & & \vdots & \\ 1 & x_{n1} & \dots & x_{nd} \end{bmatrix} = \begin{bmatrix} 1 - & x_1^T & - \\ 1 - & x_2^T & - \\ & \vdots & \\ 1 - & x_n^T & - \end{bmatrix}.$$

X is (n × (d+1))

We also now view $w = [w_0, w_1, \dots, w_d]^T$ as $w \in \mathbb{R}^{d+1}$.

$$= \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

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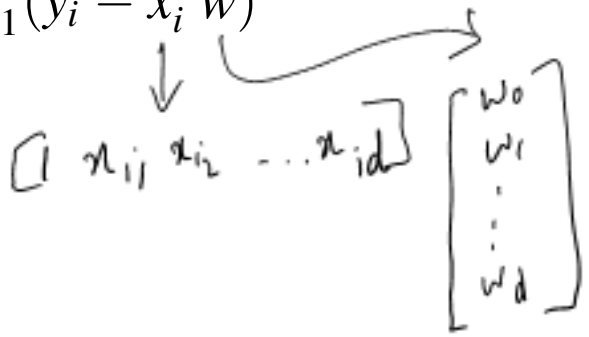
Original least squares objective function: $\mathcal{L} = \sum_{i=1}^{n} (y_i - w_0 - \sum_{j=1}^{d} x_{ij} w_j)^2$

Using vectors, this can now be written: $\mathcal{L} = \sum_{i=1}^{n} (y_i - x_i^T w)^2$



Least squares solution (vector version)

We can find w by setting,

$$\nabla_w \mathcal{L} = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} \nabla_w (y_i^2 - 2w^T x_i y_i + w^T x_i x_i^T w) = 0.$$

Solving gives,

$$-\sum_{i=1}^{n} 2y_i x_i + \Big(\sum_{i=1}^{n} 2x_i x_i^T\Big) w = 0 \quad \Rightarrow \quad w_{\text{LS}} = \Big(\sum_{i=1}^{n} x_i x_i^T\Big)^{-1} \Big(\sum_{i=1}^{n} y_i x_i\Big).$$

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This solution is Numerical Analytic.
Other solution is Gradient descent.
(Read in next slide)

Least squares solution (matrix version)

Least squares in matrix form is even cleaner.

Start by organizing the y_i in a column vector, $y = [y_1, \ldots, y_n]^T$. Then

$$\mathcal{L} = \sum_{i=1}^{n} (y_i - x_i^T w)^2 = \|y - Xw\|^2 = (y - Xw)^T (y - Xw).$$

If we take the gradient with respect to w, we find that

$$\nabla_w \mathcal{L} = 2X^T X w - 2X^T y = 0 \quad \Rightarrow \quad w_{\text{LS}} = (X^T X)^{-1} X^T y.$$

is a solution assuming $X^T X$ is invertible. i.e. Non-singular

Notes - ML-class (NMC)

Any matrix that can be written as $X^T X$ is +ive semi-definite, hence can be inversed. ?

can have eigen values = 0, ⇒ Singular

Doubt:- is $X^T X$ also +ive definite?

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Gradient descent: Minimizing $J(\theta)$ cost function, trying to find a solution iteratively -

Solving for 'n' → ⑤ / ②

② Gradient Descent	⑤ Normal Equations
• Need to choose α (learning rate)	• no need to choose α
• Need many iterations to converge	• no iterations
• Works well 'n' is large	• Need to compute $(X^T X)^{-1}$
	• Slow if 'n' is large

$\Rightarrow$ n = 100, 1000 is fine, inverting

$10^6 \times 10^6$ we should go for Gradient descent $\leftarrow$ { $\Rightarrow$ Inverting $10k \times 10k$ matrix is still doable but anything like $10^6 \times 10^6$

Note:- Gradient points in the direction of the greatest rate of increase of the function & it's magnitude is the slope of the graph in that direction.

Recall from linear algebra

Recall: Matrix $\times$ vector $\left(X^T y = \sum_{i=1}^n y_i x_i\right)$

$$\begin{bmatrix} | & | & & | \\ x_1 & x_2 & \dots & x_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = y_1 \begin{bmatrix} | \\ x_1 \\ | \end{bmatrix} + y_2 \begin{bmatrix} | \\ x_2 \\ | \end{bmatrix} + \cdots + y_n \begin{bmatrix} | \\ x_n \\ | \end{bmatrix}$$

Recall: Matrix $\times$ matrix $\left(X^T X = \sum_{i=1}^n x_i x_i^T\right)$

$$\begin{bmatrix} | & | & & | \\ x_1 & x_2 & \dots & x_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} - & x_1^T & - \\ - & x_2^T & - \\ & \vdots & \\ - & x_n^T & - \end{bmatrix} = x_1 x_1^T + \cdots + x_n x_n^T.$$

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Two notations for the *key equation*

$$w_{\text{LS}} = \Big(\sum_{i=1}^{n} x_i x_i^T\Big)^{-1}\Big(\sum_{i=1}^{n} y_i x_i\Big) \quad \Longleftrightarrow \quad w_{\text{LS}} = (X^T X)^{-1} X^T y.$$

Making Predictions

We use w_{LS} to make predictions.

Given x_{new}, the least squares prediction for y_{new} is

$$y_{\text{new}} \approx x_{\text{new}}^T w_{\text{LS}}$$

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Andrew Ng (Normal Equation: Non-invertibility)

What if $(X^T X)^{-1}$ is non-invertible?

→ could be due ① Redundant features (linearly dependent)

② Too many features ($m \leq n$)
samples ↓ features
- delete some features, or use regularization.

A **matrix** is **full** row **rank** when each of the rows of the **matrix** are linearly independent and **full** column **rank** when each of the columns of the **matrix** are linearly independent. For a square **matrix** these two concepts are equivalent and we say the **matrix** is **full rank** if all rows and columns are linearly independent. Jan 29, 2013

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Potential issues

Calculating $w_{\text{LS}} = (X^T X)^{-1} X^T y$ assumes $(X^T X)^{-1}$ exists.

When doesn't it exist?

Answer: When $X^T X$ is not a full rank matrix.

When is $X^T X$ full rank?

Answer: When the $n \times (d+1)$ matrix X has at least $d+1$ *linearly independent* rows. This means that any point in $\mathbb{R}^{d+1}$ can be reached by a weighted combination of $d+1$ rows of X.

Obviously if $n < d+1$, we can't do least squares. If $(X^T X)^{-1}$ doesn't exist, there are an infinite number of possible solutions.

Takeaway: We want $n \gg d$ (i.e., X is "tall and skinny").

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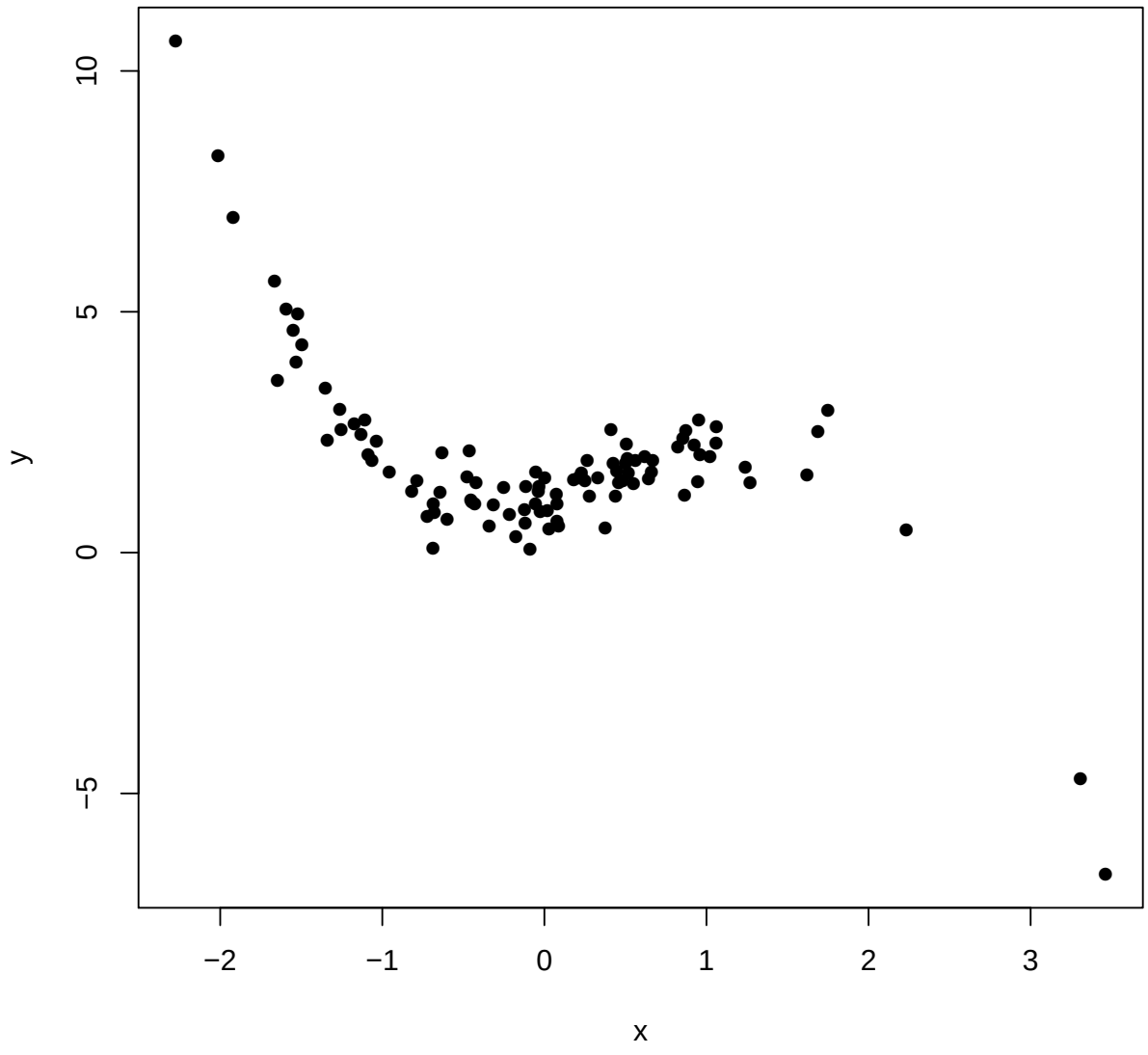
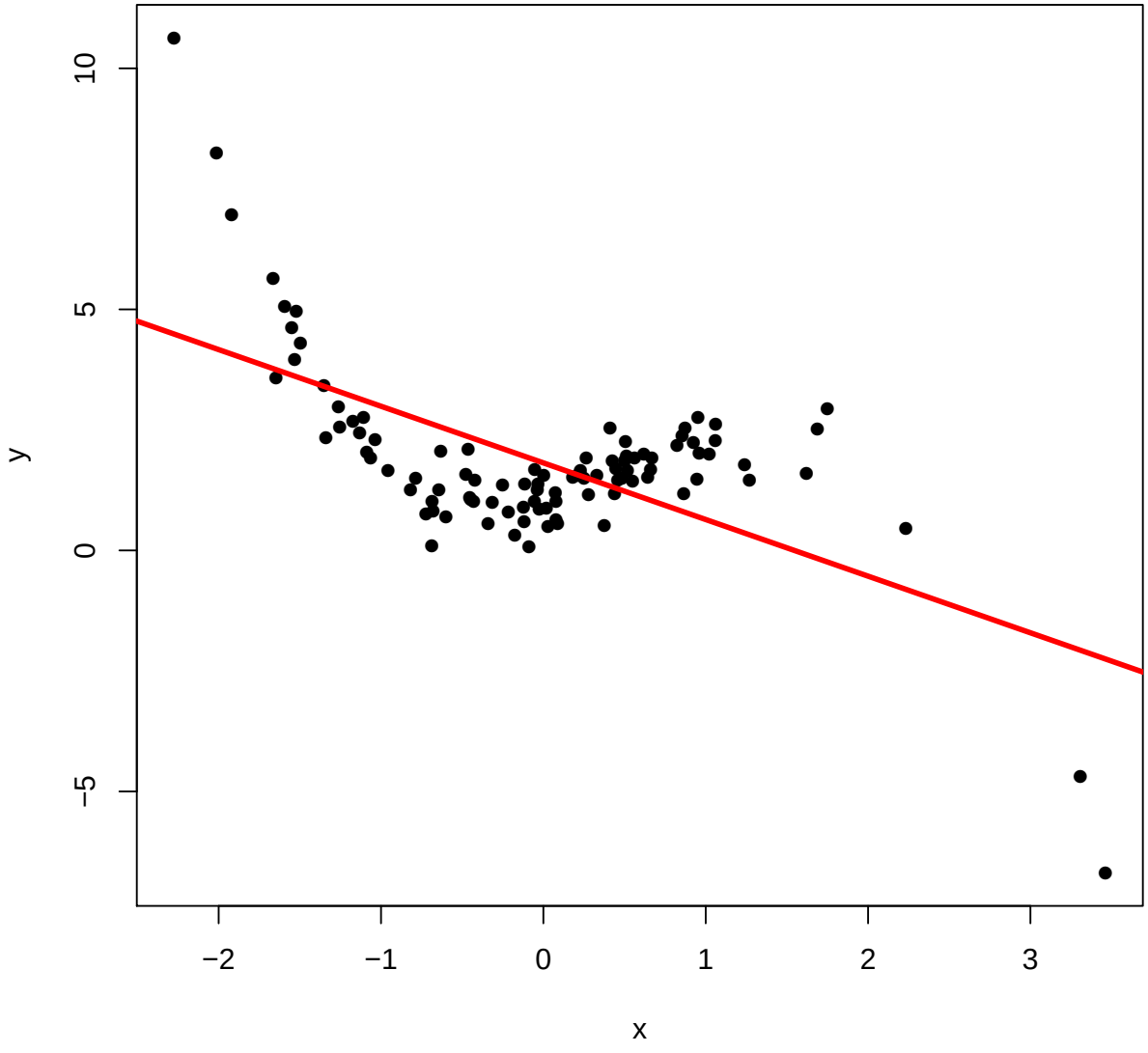
output is linear in weights, not necessarily in input x.



Broadening linear regression

$$y = w_0 + w_1 x$$



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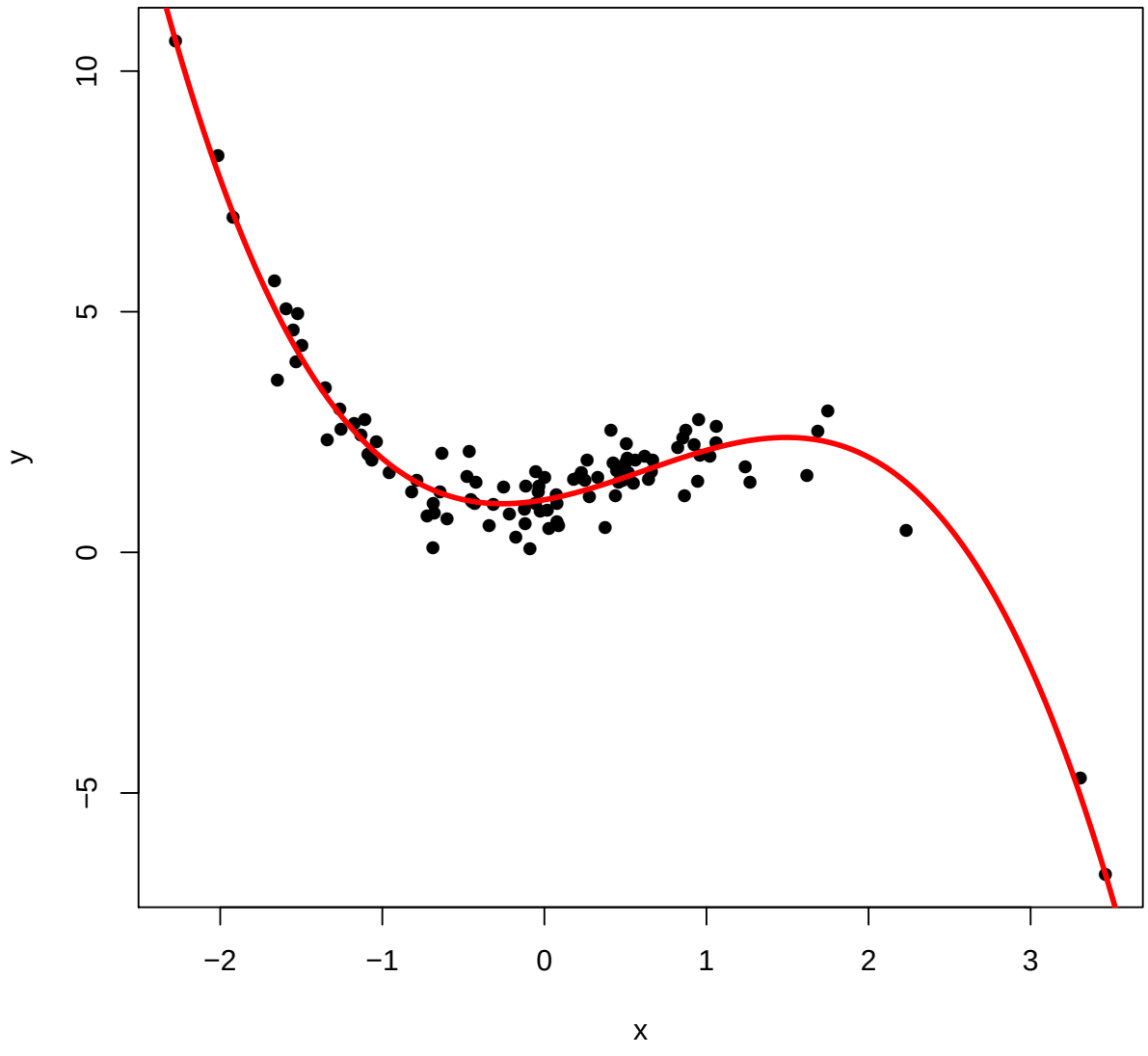
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$ → still linear regression (Read Next slide)



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Recall: Definition of linear regression

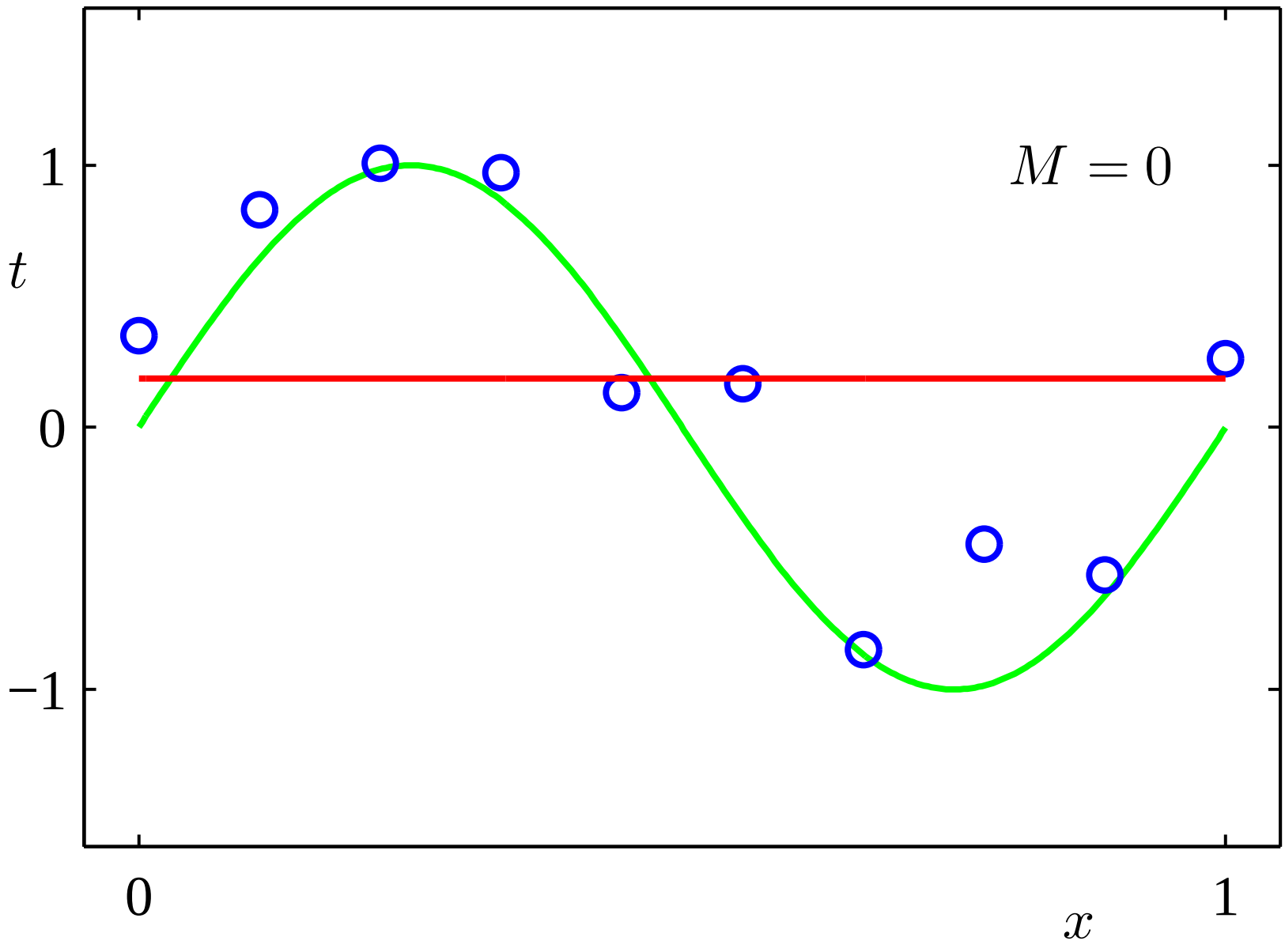
A regression method is called *linear* if the prediction f is a linear function of the unknown parameters w.

- Therefore, a function such as $y = w_0 + w_1 x + w_2 x^2$ is *linear* in w. The LS solution is the same, only the preprocessing is different.
- E.g., Let $(x_1, y_1) \ldots (x_n, y_n)$ be the data, $x \in \mathbb{R}$, $y \in \mathbb{R}$. For a pth-order polynomial approximation, construct the matrix

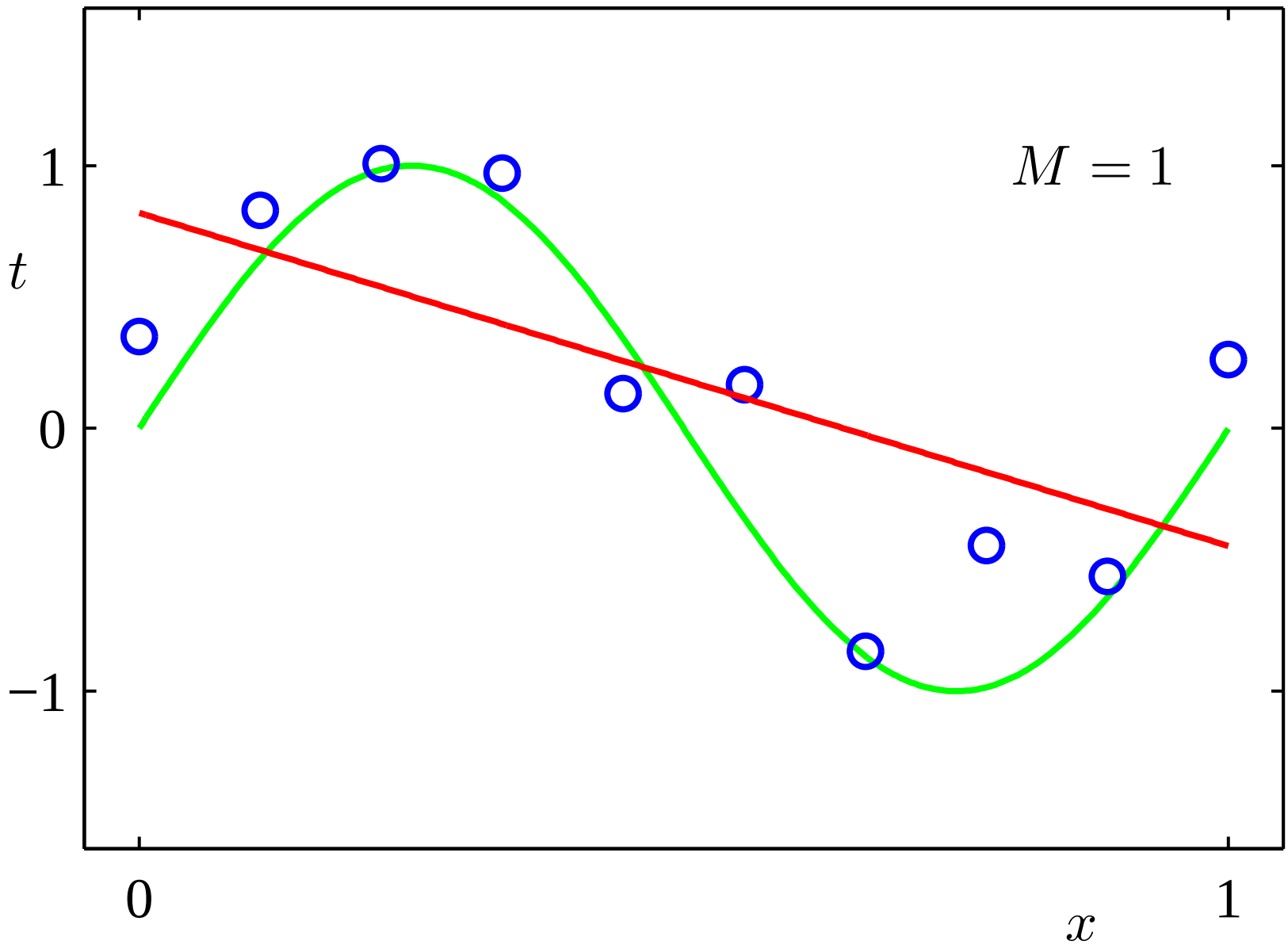
$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^p \\ 1 & x_2 & x_2^2 & \ldots & x_2^p \\ \vdots & & & \vdots & \\ 1 & x_n & x_n^2 & \ldots & x_n^p \end{bmatrix}$$

- Then solve exactly as before: $w_{\text{LS}} = (X^T X)^{-1} X^T y$.

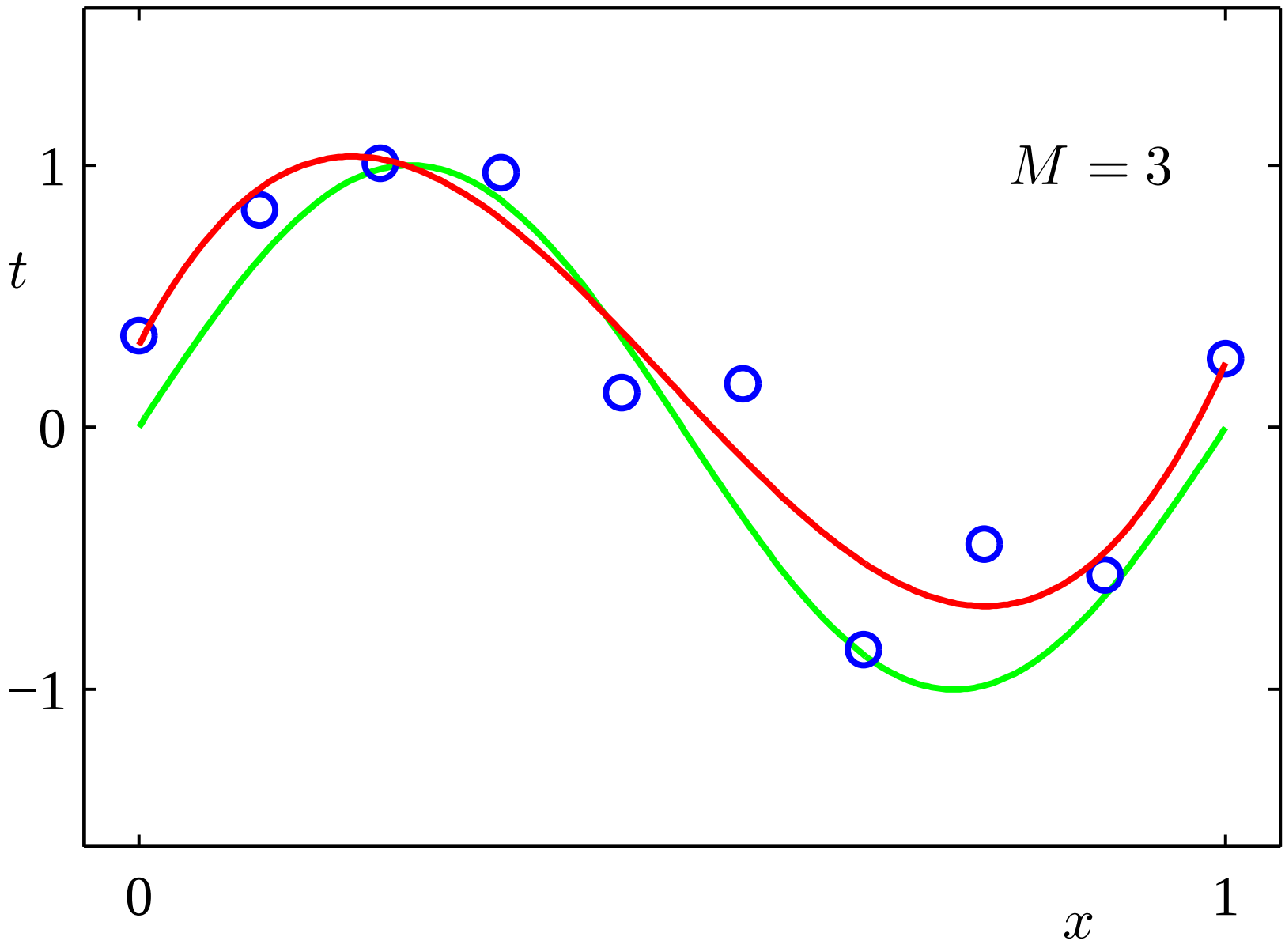
Polynomial regression (Mth order)



POLYNOMIAL REGRESSION (MTH ORDER)



Polynomial regression (Mth order)



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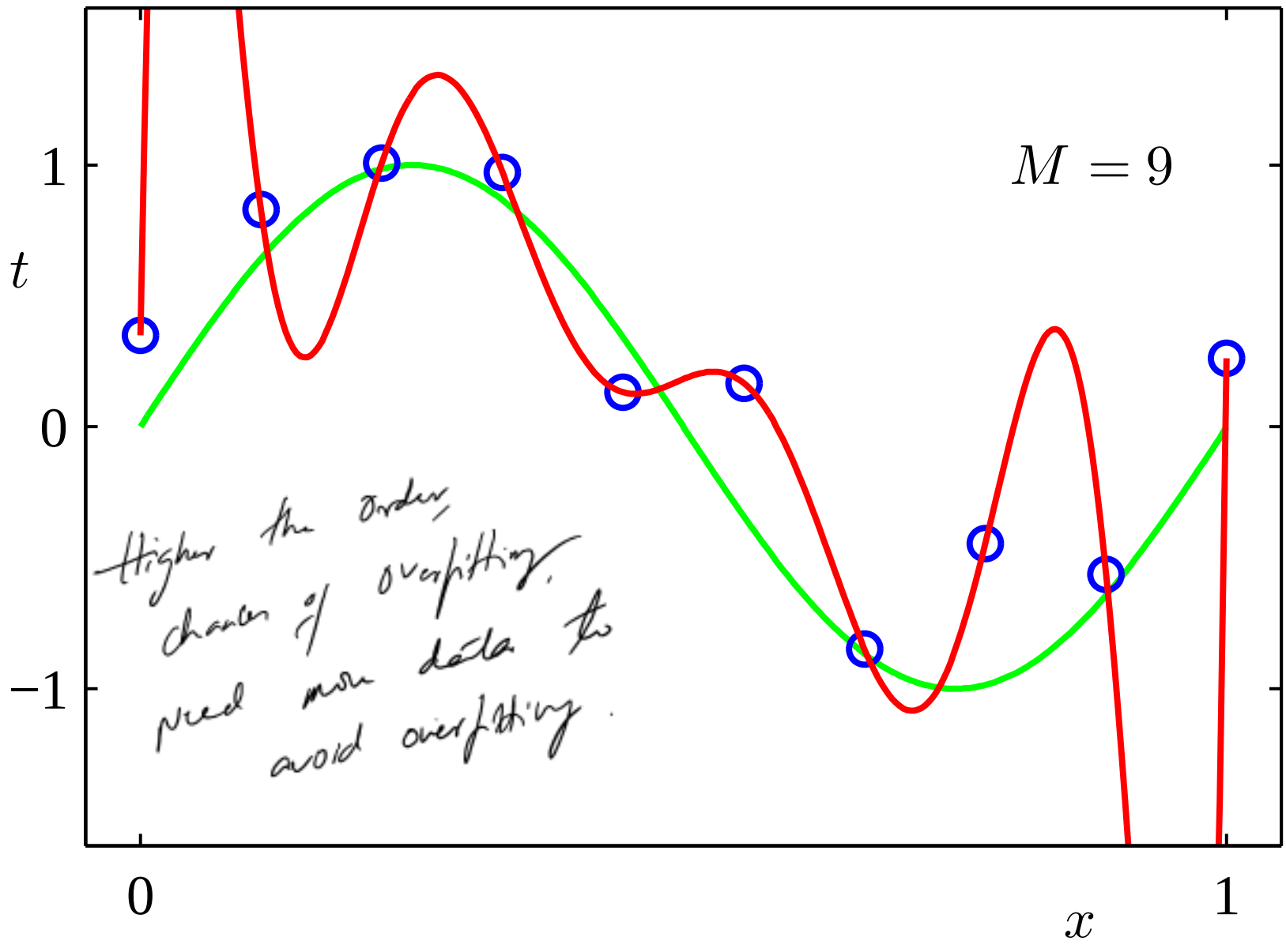


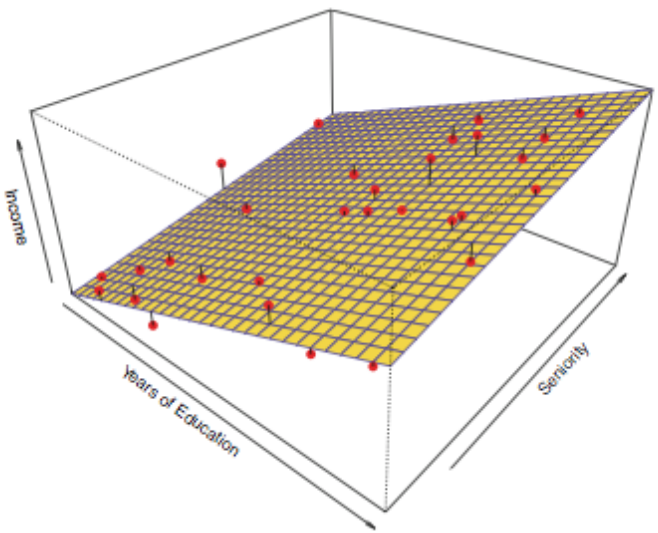
POLYNOMIAL REGRESSION IN TWO DIMENSIONS

Example: 2nd and 3rd order polynomial regression in $\mathbb{R}^2$

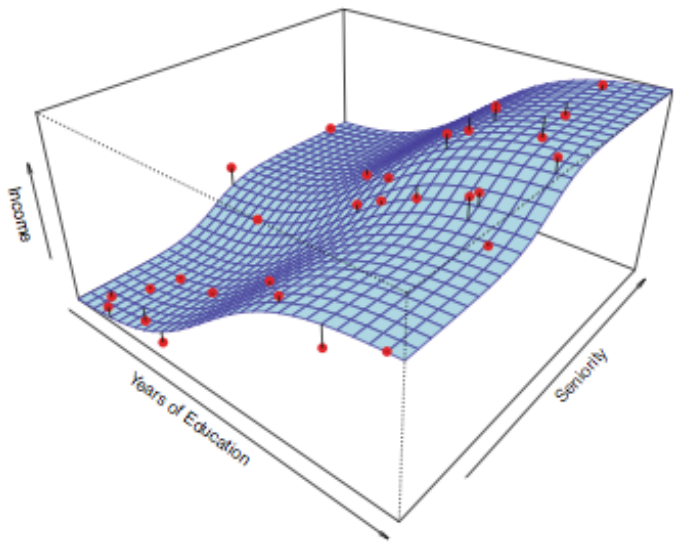
The width of X grows as (order) $\times$ (dimensions) + 1.

2nd order: $y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + w_3 x_{i1}^2 + w_4 x_{i2}^2$

3rd order: $y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + w_3 x_{i1}^2 + w_4 x_{i2}^2 + w_5 x_{i1}^3 + w_6 x_{i2}^3$



(a) 1st order



(b) 3rd order

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More generally, for $x_i \in \mathbb{R}^{d+1}$ least squares linear regression can be performed on functions $f(x_i; w)$ of the form

$$y_i \approx f(x_i, w) = \sum_{s=1}^{S} g_s(x_i) w_s.$$

For example,

$$\begin{aligned} g_s(x_i) &= x_{ij}^2 \\ g_s(x_i) &= \log x_{ij} \\ g_s(x_i) &= \mathbb{I}(x_{ij} < a) \\ g_s(x_i) &= \mathbb{I}(x_{ij} < x_{ij'}) \end{aligned}$$

these functions are generally based on domain knowledge.

As long as the function is *linear* in $w_1, \ldots, w_S$, we can construct the matrix X by putting the transformed x_i on row i, and solve $w_{\text{LS}} = (X^T X)^{-1} X^T y$.

One caveat is that, as the number of functions increases, we need more data to avoid overfitting.

GEOMETRY OF LEAST SQUARES REGRESSION

Thinking geometrically about least squares regression helps a lot.

- We want to minimize $\|y - Xw\|^2$. Think of the vector y as a point in $\mathbb{R}^n$. We want to find w in order to get the product Xw close to y.
- If X_j is the jth *column* of X, then $Xw = \sum_{j=1}^{d+1} w_j X_j$.
- That is, we weight the columns in X by values in w to approximate y.
- The LS solutions returns w such that Xw is as close to y as possible in the Euclidean sense (i.e., intuitive "direct-line" distance).

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$$\arg\min_w \|y - Xw\|^2 \quad \Rightarrow \quad w_{\text{LS}} = (X^T X)^{-1} X^T y.$$

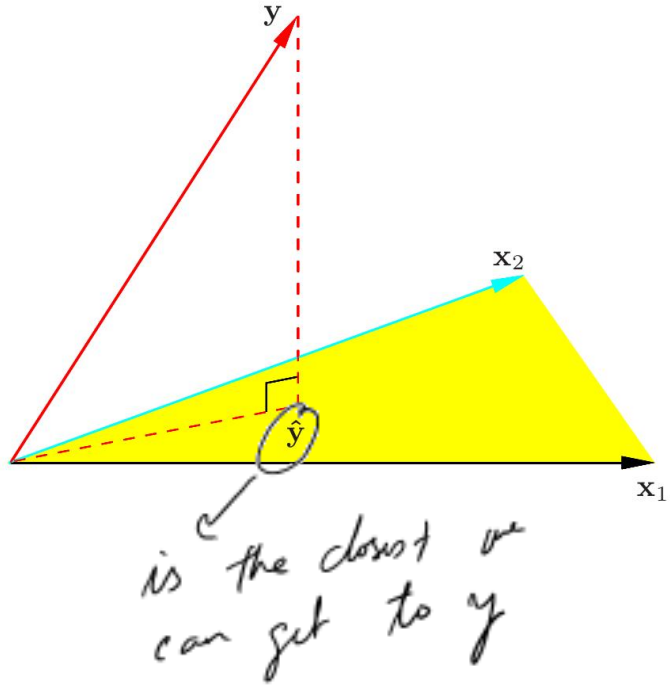
The columns of X define a $d+1$-dimensional subspace in the higher dimensional $\mathbb{R}^n$.

The closest point in that subspace is the *orthonormal projection* of y into the *column space* of X.

Right: $y \in \mathbb{R}^3$ and data $x_i \in \mathbb{R}$.

$$X_1 = [1,1,1]^T \text{ and } X_2 = [x_1, x_2, x_3]^T$$

The approximation is $\hat{y} = Xw_{\text{LS}} = X(X^T X)^{-1} X^T y$.



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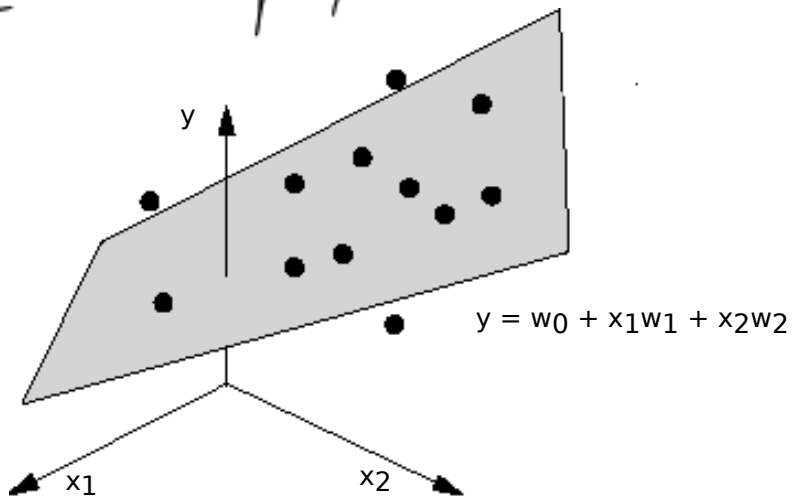
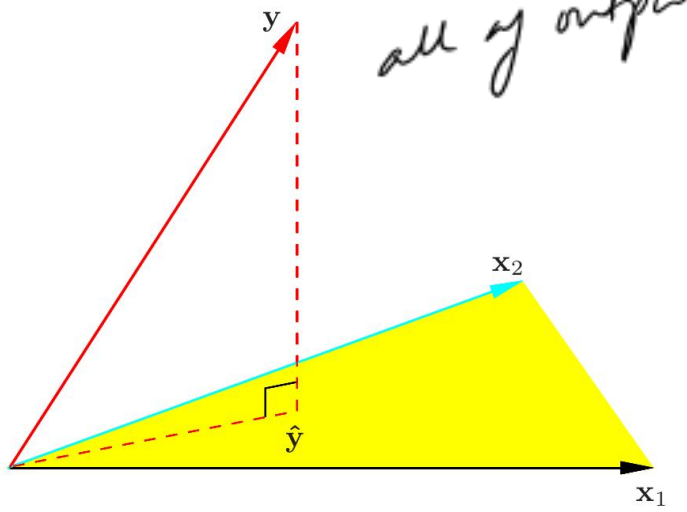
[Didn't fully understand the difference]



(a) $y_i \approx w_0 + x_i^T w$ for $i = 1, \ldots, n$

→ Here we stack all y outputs together



(b) $y \approx Xw$

There are some key difference between (a) and (b) worth highlighting as you try to develop the corresponding intuitions.

for any number of points

(a) Can be shown for all n, but only for $x_i \in \mathbb{R}^2$ (not counting the added 1).

(b) This corresponds to $n = 3$ and one-dimensional data: $X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix}$.

X_1 X_2