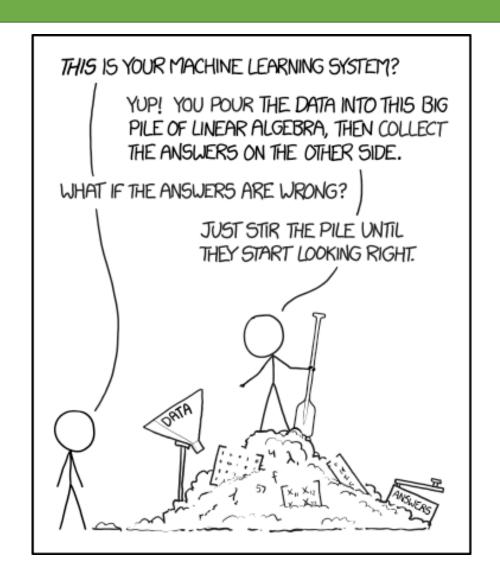


Machine learning in Oil&Gas Industry

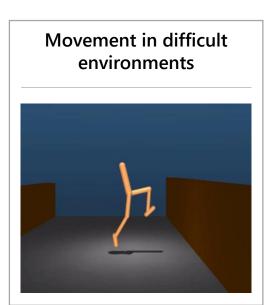
Andrey Murachev

What is Machine learning?

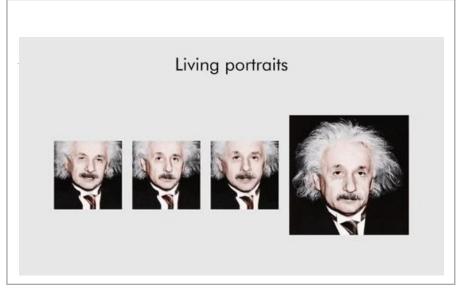


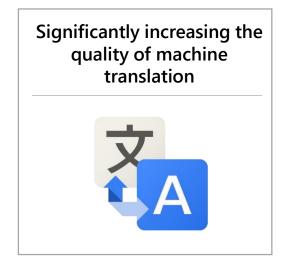
Amazing machine learning

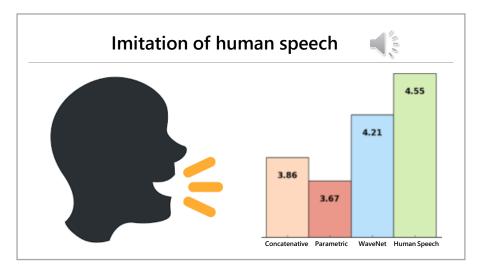


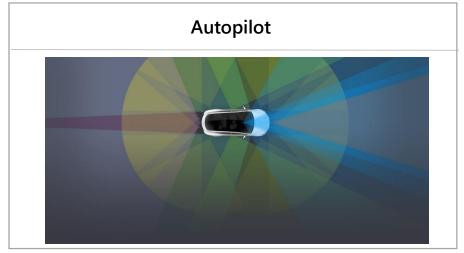








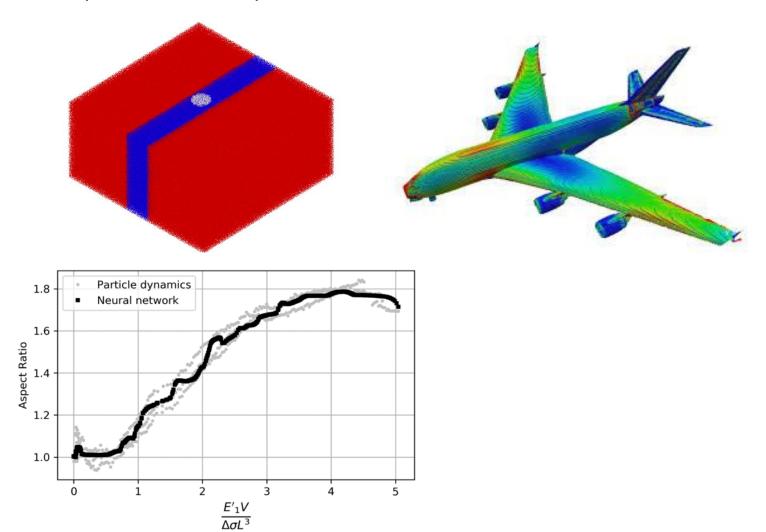




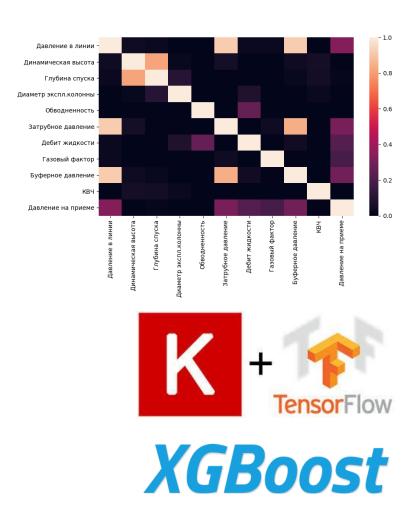
ML in science



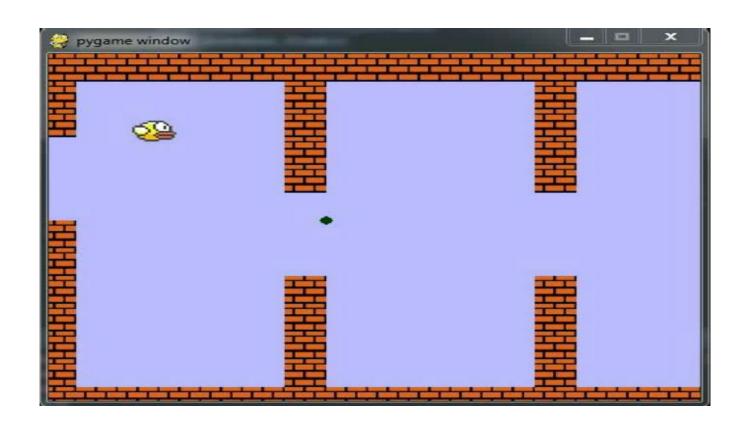
Surrogate modelling approach for optimization complex calculations



Oil well pressure prediction











- A computer program is said to learn from experience 'E', 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'.
- The extraction of learning from data
- Put simply, if a computer program improves itself with experience then we can say that it has learned.



Learning is based on precedents



X is the set of objects

(X, Y) is dataset

Y is the set of answers

 $g: X \to Y$ is unknow function (target function)

Data

$$\{x_1, x_2, ..., x_n\} \subset X$$
 are samples $y_i = y(x_i), i = 1 ... n$, are known answers

000	000	000	00	0000
111	1/1	1/1	1)	1111
222	223	227	22	2220
333	333	333	33	3333
444	4 4 4	444	44	4444
555	555	155	55	5555
6 6 6	666	666	66	6666
777	177	177	77	77)1
888	888	888	8 8	8888
999	999	999	89	9999

Goal

 $a: X \to Y$ is algorithm that approximates function g on dataset X, decision function

Learning is based on precedents

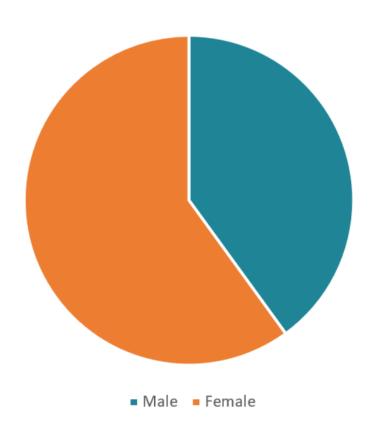
 $f_j: X \to D_j$, $j = 1 \dots n$, is features of objects (numbers, result of measurement)

Types of features:

- $D_i = \{0,1\}$ is binary feature (true/false)
- D_i is categorical feature (race, pet breed, name)
- $D_i < \infty$ is ordinal feature. There is a clear ordering of the variables.
- $D_i = \mathbb{R}$ is Interval feature

$$(f_1(x), ..., f_m(x))$$
 – feature vector

$$F = \begin{pmatrix} f_1(x_1) & \dots & f_m(x_1) \\ \dots & \dots & \dots \\ f_1(x_n) & \dots & f_m(x_n) \end{pmatrix} \text{ is feature matrix or Data frame}$$



Iris classification

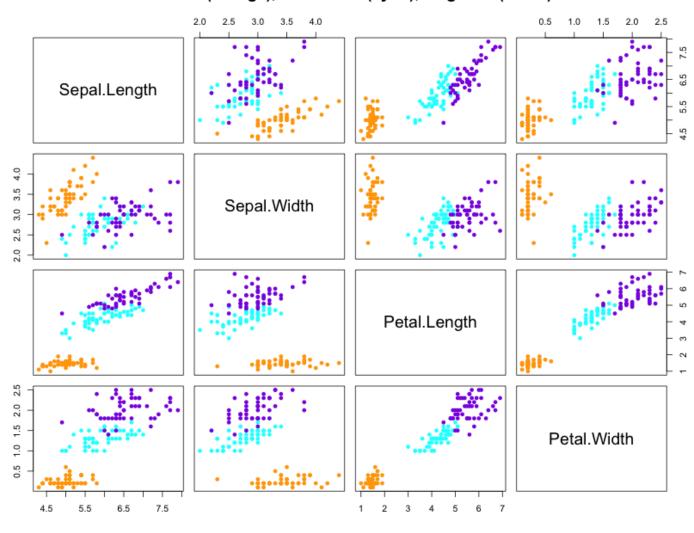


Fisher's Iris Data Set Setosa (orange), Versicolor (cyan), Virginica (violet)





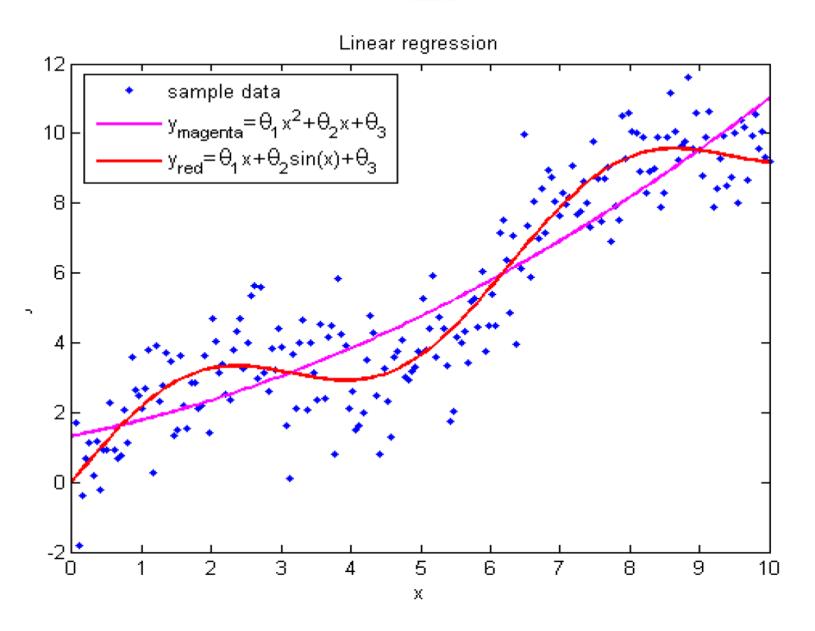




Regression



Different models produce different results





Learning steps

Train

The learning algorithm builds the decision function based on the train data

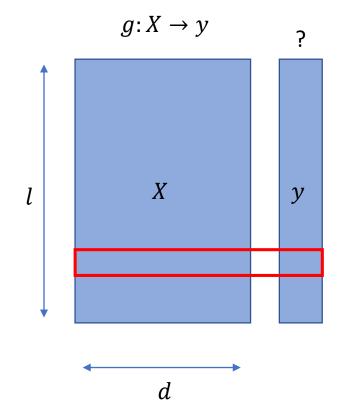
$$\begin{bmatrix}
f_1(x_1) & \dots & f_m(x_1) \\
\dots & \dots & \dots \\
f_1(x_n) & \dots & f_m(x_n)
\end{bmatrix} \xrightarrow{y} \begin{pmatrix} y_1 \\ \dots \\ y_n \end{pmatrix} \xrightarrow{\mu} a$$

Test

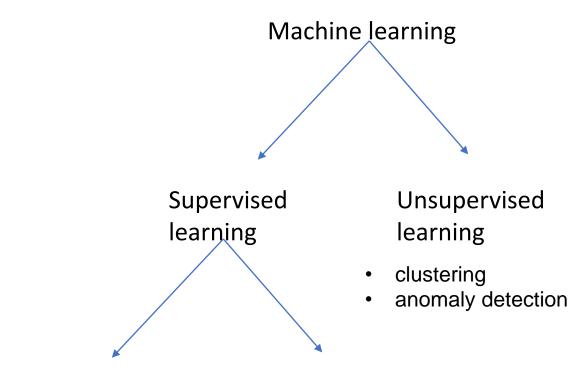
The decision function is used on new data x' (test data)

$$\begin{pmatrix} f_1(x'_1) & \dots & f_m(x'_1) \\ \dots & \dots & \dots \\ f_1(x'_k) & \dots & f_m(x'_k) \end{pmatrix} \stackrel{\mathsf{a}}{\longrightarrow} \begin{pmatrix} \mathsf{a}(x'_1) \\ \dots \\ \mathsf{a}(x'_k) \end{pmatrix}$$

70% 30%



- •clustering is identifying partitions of instances based on the features of these instances so that the members within the groups are more similar to each other than those in the other groups;
- •anomaly detection is search for instances that are "greatly dissimilar" to the rest of the sample or to some group of instances



classification

classification of an instance to one of the categories based on its features

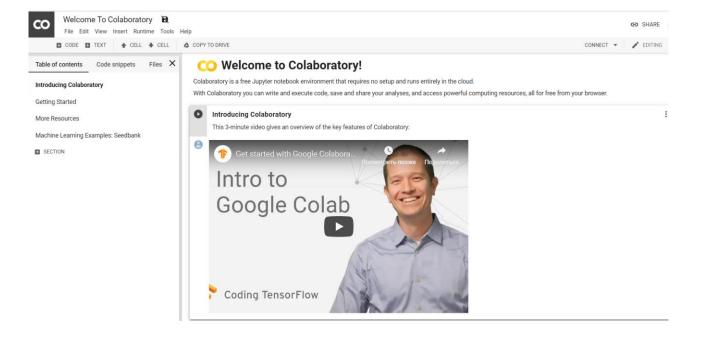
regression

prediction of a numerical target feature based on other features of an instance

Programming

Google colaboratory

https://colab.research.google.com/



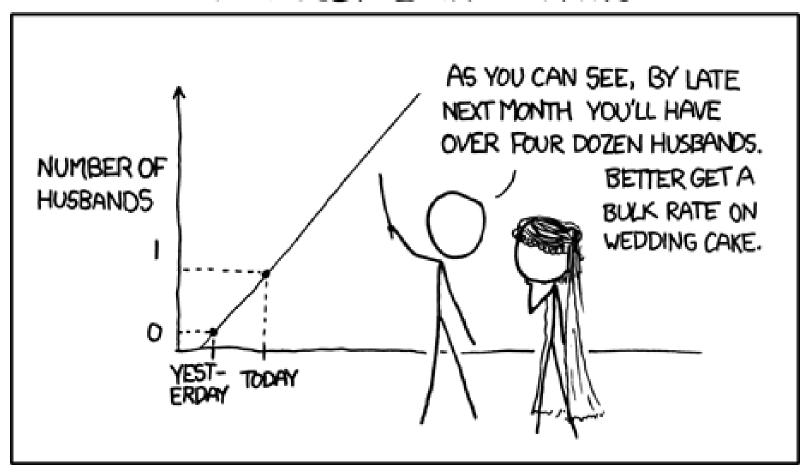


JetBrains PyCharm + Anaconda

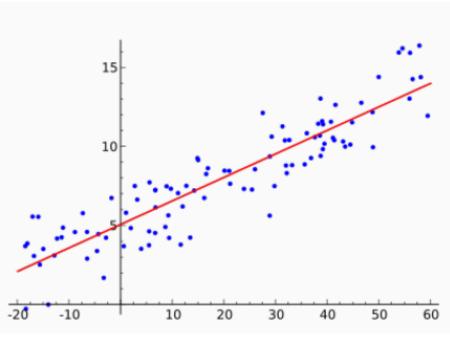


Linear regression

MY HOBBY: EXTRAPOLATING



Model



The liner regression model

$$y(x, w) = w_0 + \sum_{j=1}^{n} x^{(j)} w_j = x^T w,$$
 $x = (1, x^{(1)}, ..., x^{(n)})$

• We want to predict y as function of vector x

$$h(x) = w_0 + \sum_{j=1}^{n} x^{(j)} w_j = x^T w$$

• $y \in \mathbb{R}^n$ is the target variable;

$$y^{(i)} = y(x^{(i)}), i = 1, ..., m$$

- w is the vector of the model parameters (in machine learning, these parameters are often referred to as weights);
- x is a matrix of features, x.size()=[m,n]

Liner regression

 x_1

 x_2

 x_3

 χ_4

y

• • •

	Area	Number of rooms	Number of floors	Age	Price (в \$1000)
	2104	5	1	45	460
$x^{(2)}$	1416	3	2	40	232
	1534	3	3	30	315
	852	2	1	36	178

$$x^{(2)} = \begin{bmatrix} 1416 \\ 3 \\ 2 \\ 40 \end{bmatrix} \qquad x_3^{(2)} = 2$$

Liner regression

$$h_{\theta}(x) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4$$

$$XW^{T} = \begin{bmatrix} x_{0} \\ x_{1} \\ x_{2} \\ x_{3} \\ x_{4} \end{bmatrix} [w_{0} \ w_{1} \ w_{2} \ w_{3} \ w_{4}] = w_{0}x_{0} + w_{1}x_{1} + w_{2}x_{2} + w_{3}x_{3} + w_{4}x_{4} = h_{w}(x)$$

$$x_{0} = 1$$

$$X = \begin{bmatrix} 2104 & 5 & 1 & 45 \\ 1416 & 3 & 2 & 40 \\ 1534 & 3 & 3 & 30 \\ 852 & 2 & 1 & 36 \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 3 & 30 \\ 1 & 852 & 2 & 1 & 36 \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 3 & 30 \\ 1 & 852 & 2 & 1 & 36 \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 3 & 30 \\ 1 & 852 & 2 & 1 & 36 \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}$$

Ordinary Least Squares

- How to find the best parameters **w** for training data $(x_i, y_i)_{i=1}^m$?
- Ordinary Least Squares. Let's minimize

$$RSS(w) = \sum_{i=1}^{m} (y^{(i)} - x^{(i)T}w)^{2}$$

• How can we do it?

Accurate solution

• To order obtain an accurate solution let's represent RSS(w) in the following form

$$\mathrm{RSS}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^{\top}(\mathbf{y} - \mathbf{X}\mathbf{w}),$$

To solve this optimization problem, we need to calculate derivatives with respect to the model parameters. We set them to zero and solve the resulting equation for \mathbf{w}

$$\hat{\mathbf{w}} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

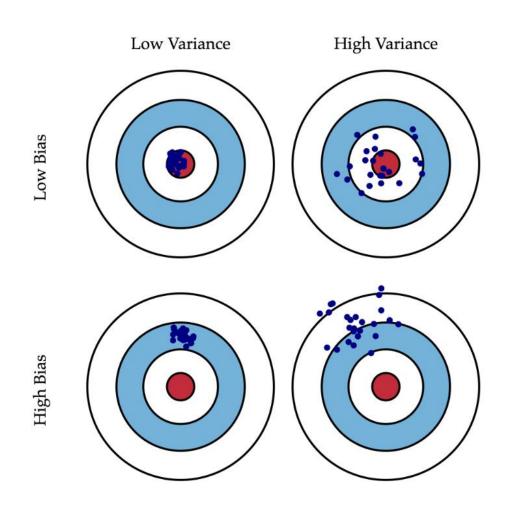
Notes:

- We do not need to scale data
- The solution is difficult to calculate when the number of features is very large $n \approx 10^6$
- The matrix X^TX is irreversible when $m \leq n$
- The matrix X^TX is irreversible when linearly dependent features exist

Bias-Variance Decomposition

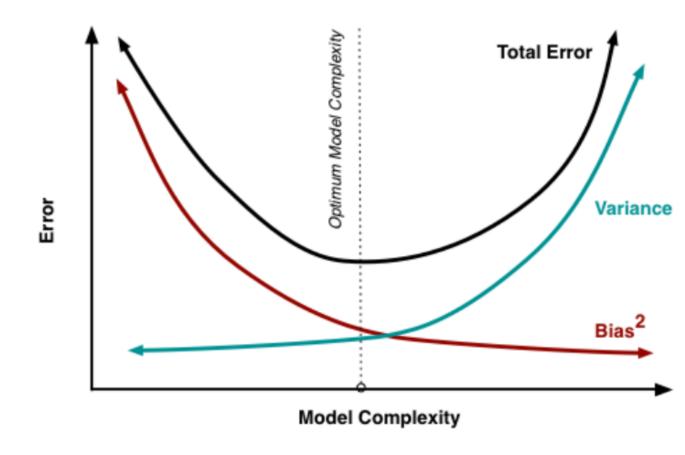
$$Err(x) = Bias(h)^2 + Var(h) + \sigma^2$$

- Bias(h) is the average error for all sets of data
- Var(h) is error variability, or by how much error will vary if we train the model on different sets of data;
- irremovable error: σ^2



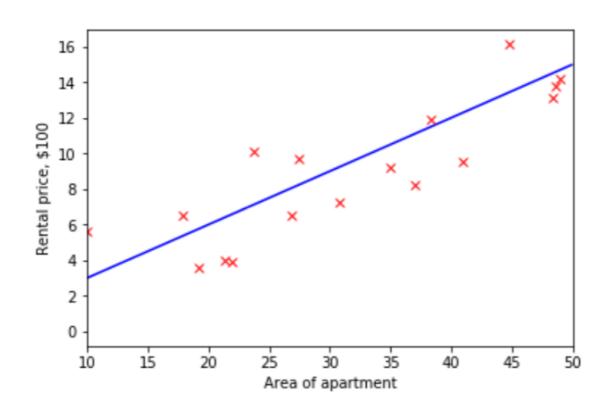
Bias-Variance Decomposition

- Generally, as the model becomes more computational (e.g. when the number of free parameters grows), the variance of the estimate also increases, but bias decreases. The model learns well the training data, but it is incapable of generalization. Therefore, there are surprises in the test set.
- On the other side, if the model is too simple, it will not be able to learn the pattern.
- the OLS estimator of parameters of the linear model is the best for the class of linear unbiased estimator (The Gauss-Markov theorem).



Example. Cost function (MSE)

Area of apartment	Rental price
26.80	6.50
35.00	9.25
44.80	16.12
38.30	11.92
40.90	9.53
23.70	10.08



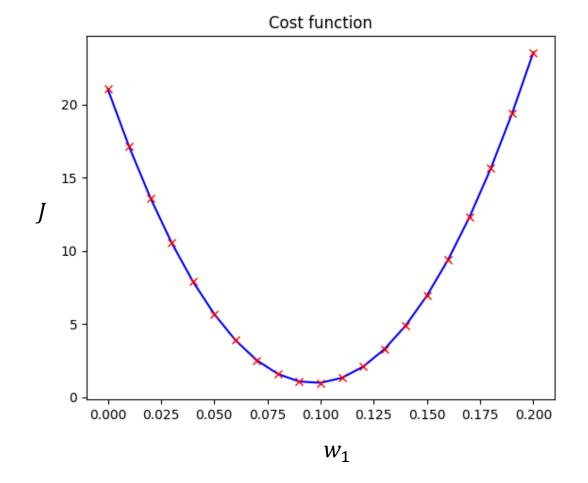
Hypothesis: $h_{\rm w} = w_0 + w_1 x$ – one-dimensional linear regression

Git:

Cost function

$$J(w_0, w_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\mathbf{w}}(x^{(i)}) - y^{(i)})^2$$

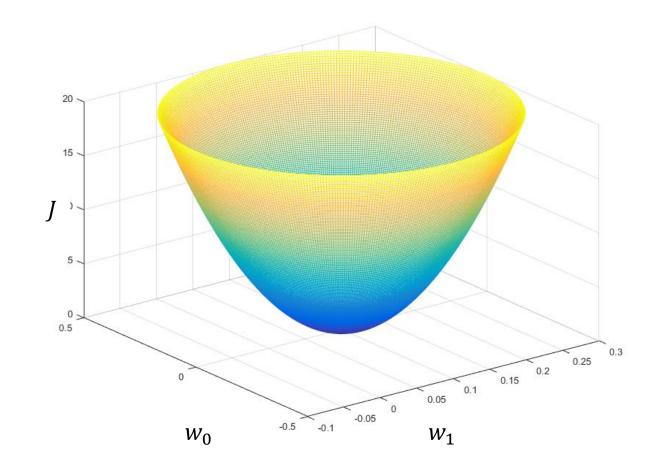
The learning task is the minimization $J(w_0, w_1)$.



Cost function

$$J(w_0, w_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)})^2$$

The learning task is the minimization $J(w_0, w_1)$.



Let the function $J(w_0, w_1)$ is arbitrary function.

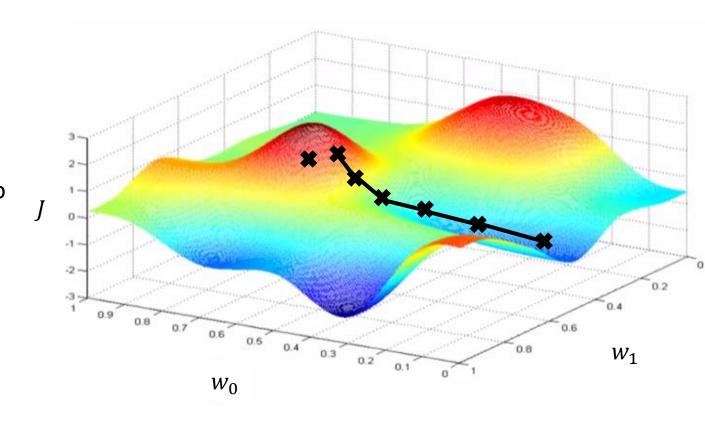
Our goal is to find a minimum $J(w_0, w_1)$.

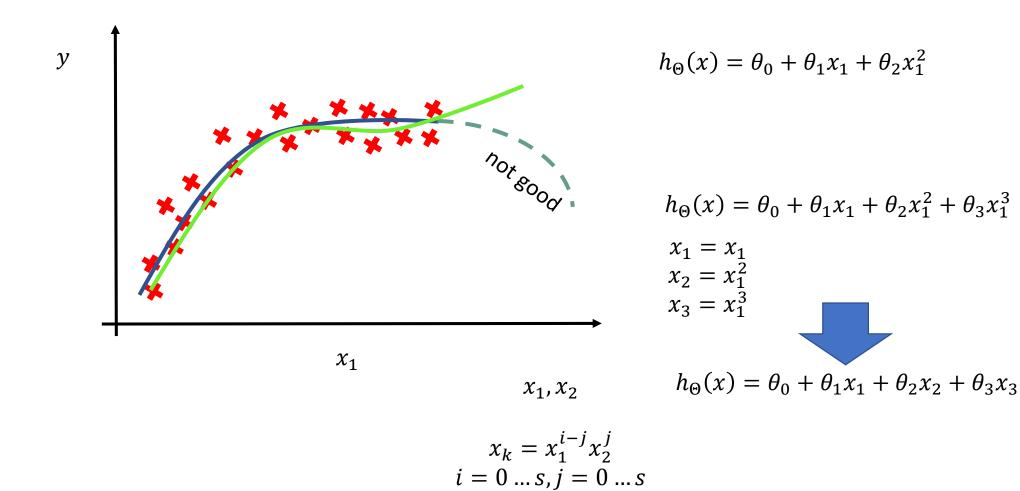
Main idea:

Initial values w_0 and w_1 is chosen randomly.

Usually $w_0 = w_1 = 0$.

We change the values of w_0 and w_1 in order to reduce $J(w_0, w_1)$.





repeat until convergence { $w_j\coloneqq w_j-\alpha\,\frac{\partial}{\partial w_j}J(w_0,w_1) \qquad \text{(for }j=0,\;j=1\text{)}.$ } $\alpha-\text{learning rate}.$ $w_0,w_1 \text{ are updated simultaneously!}$

Correct!

$$temp0 := w_0 - \alpha \frac{\partial}{\partial w_0} J(w_0, w_1)$$

$$temp1 := w_1 - \alpha \frac{\partial}{\partial w_1} J(w_0, w_1)$$

$$w_0 := temp0$$

$$w_1 := temp1$$

Incorrect!

$$temp0 \coloneqq w_0 - \alpha \frac{\partial}{\partial w_0} J(w_0, w_1)$$

$$w_0 \coloneqq temp0$$

$$temp1 \coloneqq w_1 - \alpha \frac{\partial}{\partial w_1} J(w_0, w_1)$$

$$w_1 \coloneqq temp1$$

$$h_w(x) = w_0 + w_1 x$$

$$\frac{\partial}{\partial w_j} J(w_0, w_1) = \frac{\partial}{\partial w_j} \frac{1}{2m} \sum_{i=1}^m \left(w_0 + w_1 x^{(i)} - y^{(i)} \right)^2$$

$$w_0$$
: $\frac{\partial}{\partial w_0} J(w_0, w_1) = \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)})$

$$w_1: \frac{\partial}{\partial w_1} J(w_0, w_1) = \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)}) x^{(i)}$$

repeat until convergence { $w_j \coloneqq w_j - \alpha \frac{\partial}{\partial w_j} J(\theta_0, \theta_1)$ }

$$J(w_0, w_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_{\mathbf{w}}(x^{(i)}) - y^{(i)})^2$$

$$J(W) = \frac{1}{2m} \sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)})^{2}$$

Repeat until convergence {

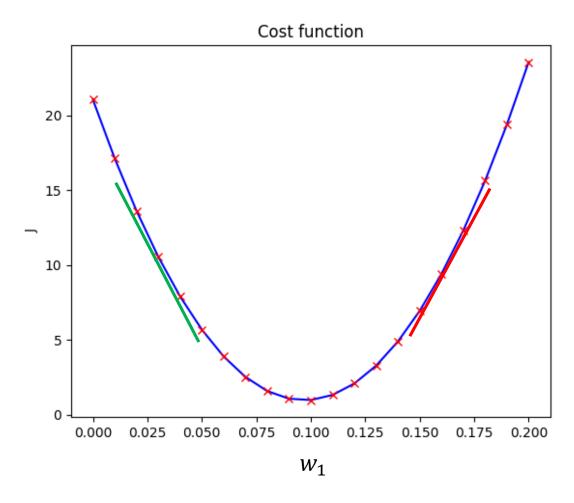
$$w_{j} \coloneqq w_{j} - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_{w}(x^{(i)}) - y^{(i)} \right) x_{j}^{(i)}$$

$$\partial$$

$$w_0 \coloneqq w_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_w(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$w_1 \coloneqq w_1 - \alpha \frac{1}{m} \sum_{i=1}^m (h_w(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

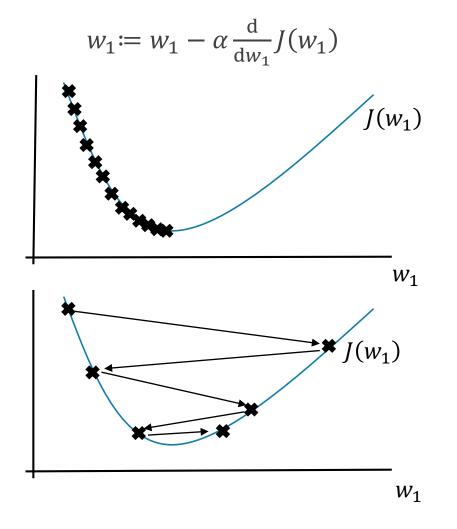
$$w_2 \coloneqq w_2 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_w(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

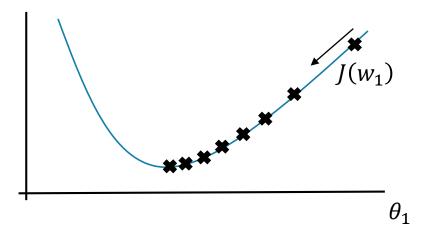


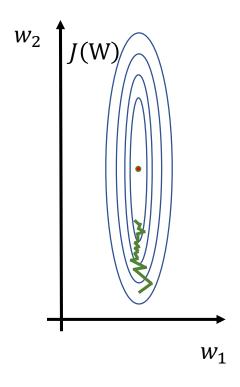
$$w_1 \coloneqq w_1 - \alpha \boxed{\frac{\mathrm{d}}{\mathrm{d}w_1} J(w_1)} \ge 0$$

 $w_1 - decrease$

 $w_1 - increase$

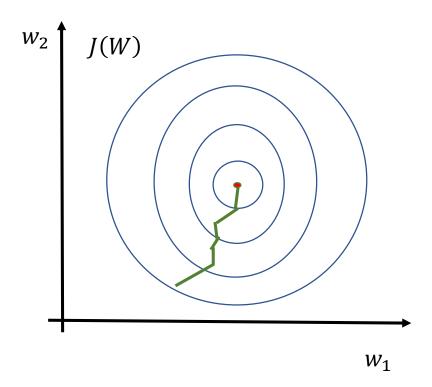






$$x_1 = 500 \dots 2000$$

 $x_2 = 1 \dots 5$

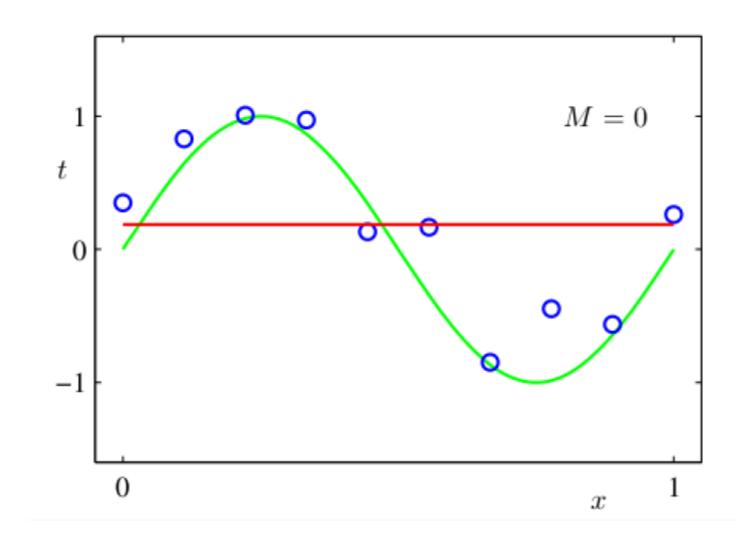


for
$$j \ge 1$$

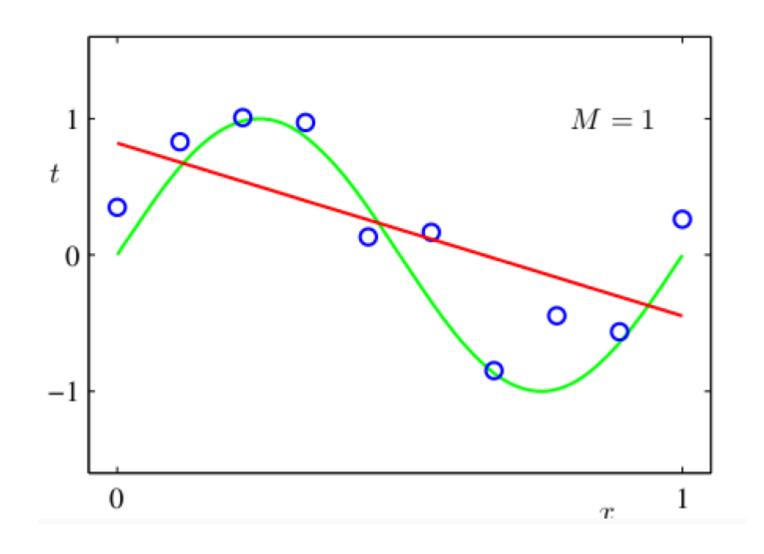
$$x_j = \frac{x_j - \mu}{\sigma}$$

$$\mu$$
 – mean value x_i

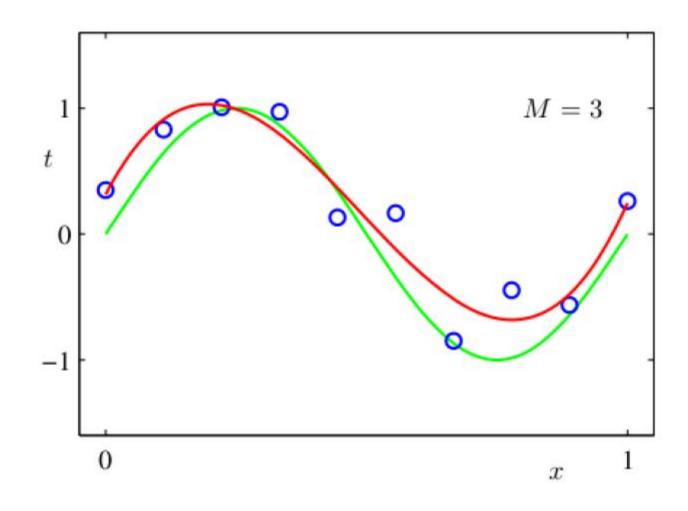
Polynomial regression



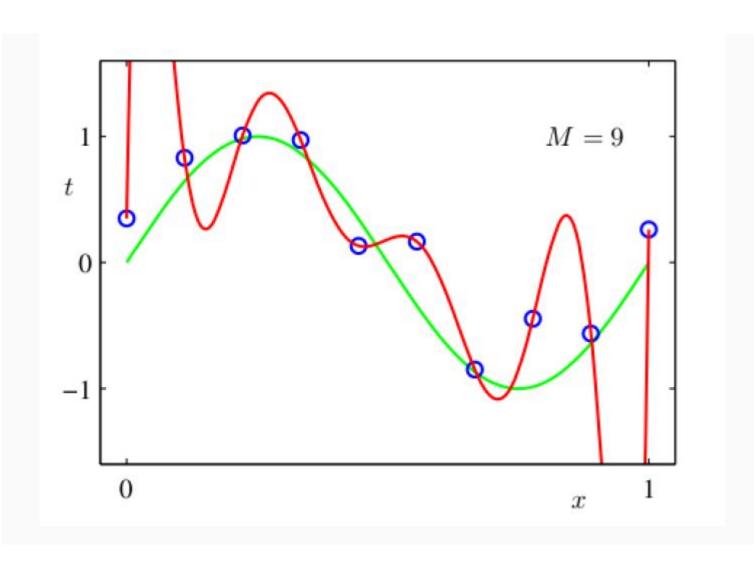
Polynomial regression



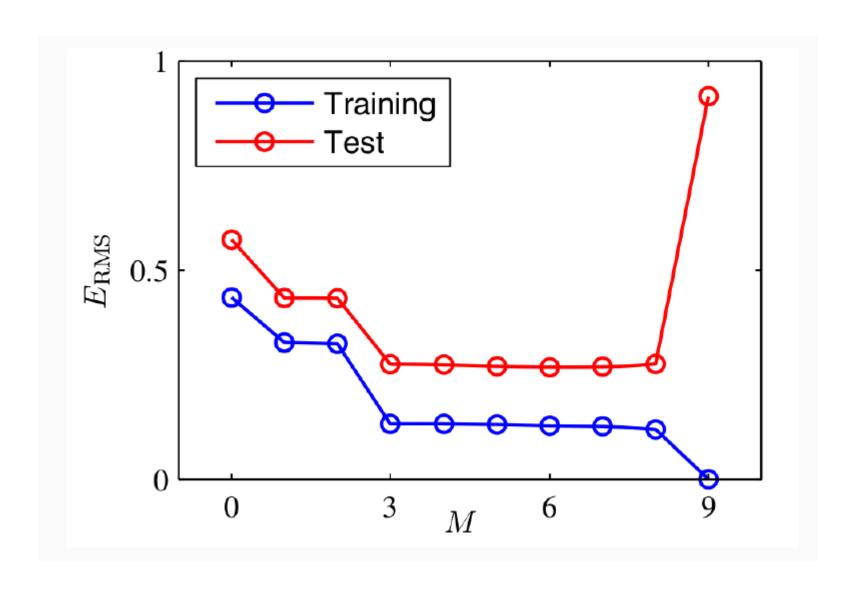
Polynomial regression



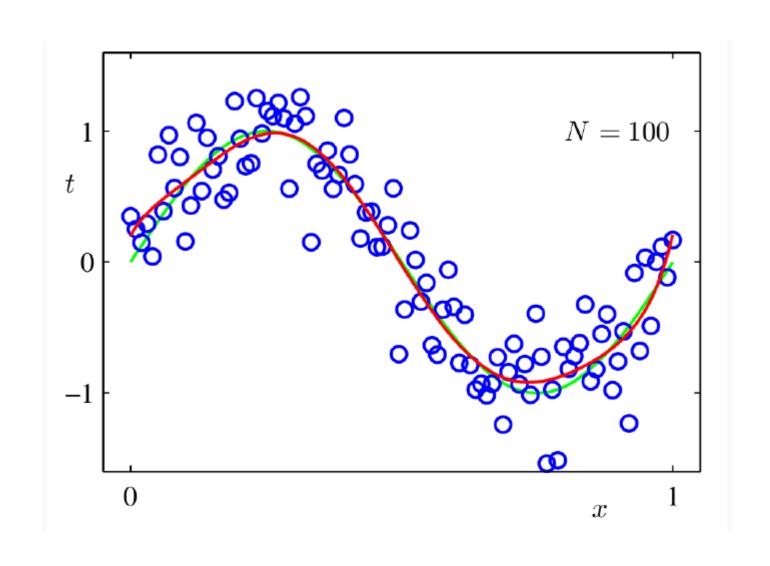
Polynomial regression



Root mean square Error



How to deal with it? Add data

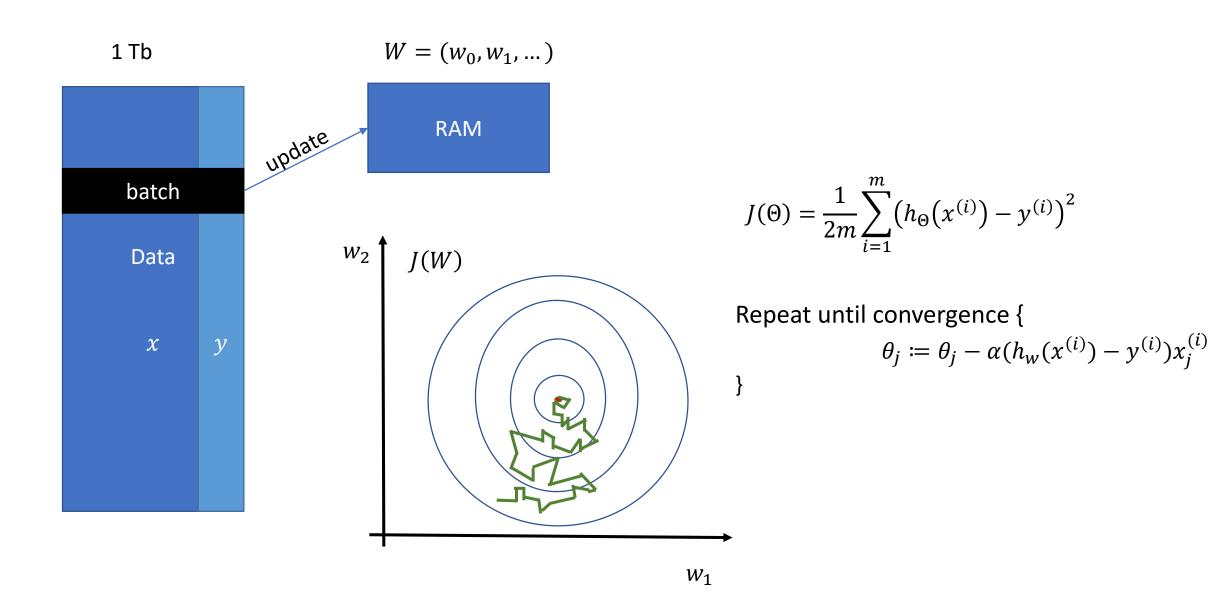


Regulirization

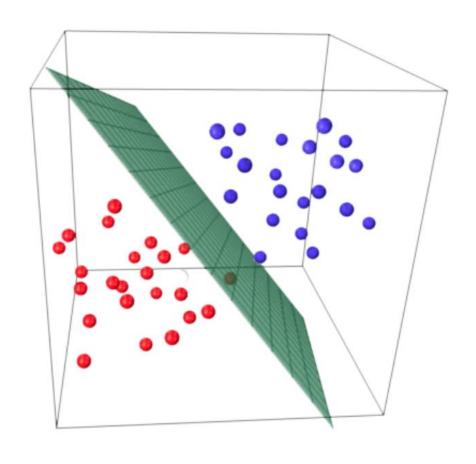
OLD:
$$J(W) = \frac{1}{2m} \sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)})^{2}$$

NEW:
$$J(W) = \frac{1}{2m} \sum_{i=1}^{m} (h_{w}(x^{(i)}) - y^{(i)})^{2} + \frac{\lambda}{2} ||w^{2}||$$

Stochastic gradient descent (SGD)







Email: Spam / Not Spam

Online transactions: Fraud (Yes / No)

Tumor: Benign / Malignant

Classes can be many:

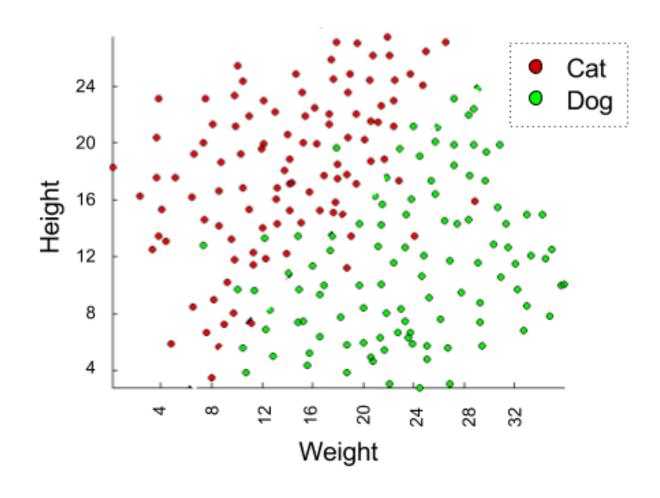
$$y \in \{0,1,2,3,...\}$$

The basic idea behind the linear classifier is that the two values of the target class can be separated by a hyperplane in the feature space.

Data Schema

Discrete Continuous Variables Variable Height (in) Weight (lb) Species 20.4, 28.4, Dog, 10.2, 8.9, Cat, ...197 more entries... 18.0, 0.0, Cat,

Data Visualization



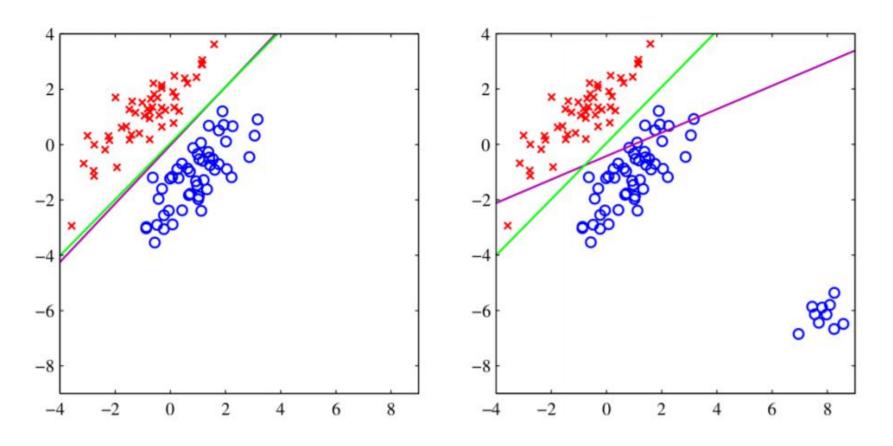
- Our task is to compare the vector of features **x** with one of the known classes
- Feature space is somehow divided into classes
- We are actually want to find a decision surface (or decision boundary).
- How to code classes? If we have two classes, then it is done in a very natural way. We define the variable y.

$$y = 0$$
 corresponds to C_1 ; $y = 1$ corresponds to C_2

- The value y can be interpreted as the probability
- If there are several classes, it is convenient to enter a vector

$$y = (0,0,...1,...,0,0)$$

Binary classification. OLS



Why does least squares work so badly?

The ordinary least squares implies Gaussian error distribution. But binary vectors are not distributed in Gauss

Logistic regression

Let's P(x) - the probability of an event x

The odds ratio

$$OR(x) = \frac{P(x)}{1 - P(x)}$$

is the ratio of the probabilities of whether or not an event will happen.

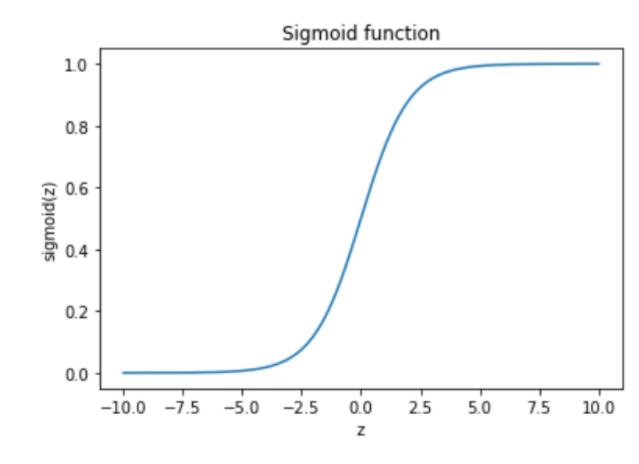
why?

$$P(x) = (0,1)$$

$$OR(x) = (0, \infty)$$

profit!

we predict $\log(OR(x)) \in \mathbb{R}$



How logistic regression will make a prediction?

 $p^{(i)} = P(y_i = 1 \mid x_i, w)$, let's assume that we have somehow obtained weights W

$$\log(OR) = \log\left(\frac{p^{(i)}}{1 - p^{(i)}}\right) = w_0 + w_1 x_1 + w_2 x_2 = W^T X^{(i)}$$

some algebra...

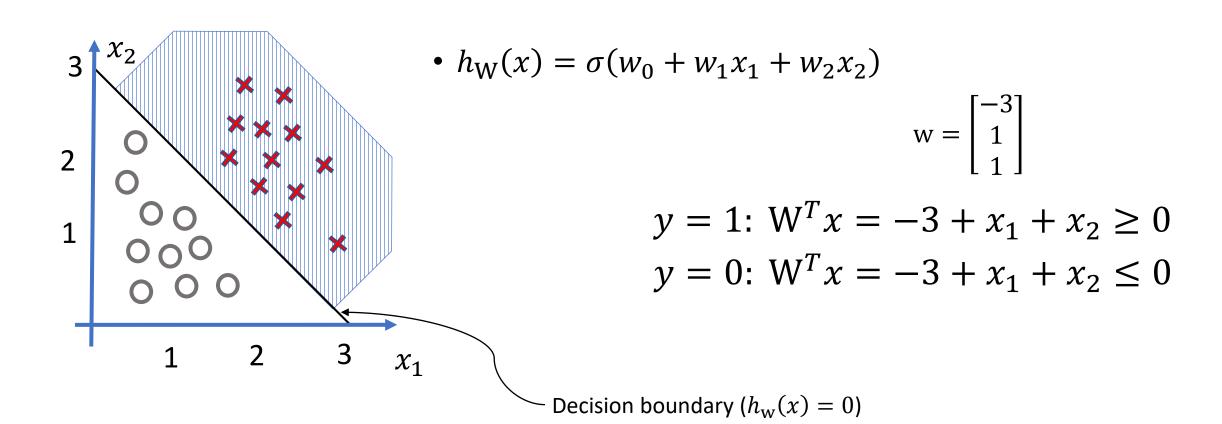
$$h_{\mathbf{W}}(x) = p^{(i)} = \frac{e^{\mathbf{W}^T X^{(i)}}}{1 + e^{\mathbf{W}^T X^{(i)}}} = \frac{1}{1 + e^{-\mathbf{W}^T X^{(i)}}} \stackrel{\text{def}}{=} \sigma(\mathbf{W}^T X^{(i)})$$
the sigmoid function.

Logistic regression

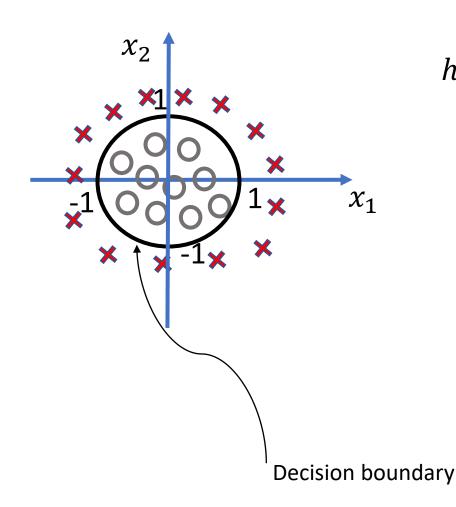
So, logistic regression predicts the probability of assigning an example to the "+" class (assuming that we know the features and weights of the model) as a sigmoid transformation of a linear combination of the weight vector and the feature vector:

$$p^+(x) = P(y_i = 1 \mid x_i, w) = \sigma(w^T x_i).$$

Decision boundary



Decision boundary



$$h_{w}(x) = g(w_0 + w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_2^2)$$

$$y = 1$$
: $w^T x = -1 + w_1^2 + w_2^2 \ge 0$
 $y = 0$: $w^T x = -1 + w_1^2 + w_2^2 \le 0$

$$W = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

51

Likelihood maximization

Lets there is the dataset

$$D = \{\bar{x}_n, y_n\}, y_n \in \{0,1\}$$

How to find the likelihood of Data p(D|w) ?

$$p(D|w) = \prod p(d|w) = \prod_{d \in C_1} p(C_1|w) \cdot \prod_{d \in C_2} p(C_2|w)$$

Use the trick:

$$p(d|w) = \frac{p(C_1|w)}{1 - p(C_1|w)} = p(C_1|w)^y (1 - p(C_1|w))^{1-y}$$

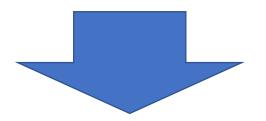
When:

$$p(D|w) = \prod_{n} p(C_1|w)^y (1 - p(C_1|w))^{1-y} = \prod_{n} \sigma(w^T x_n)^{y_n} (1 - \sigma(w^T x_n))^{1-y_n}$$
Maximize by w

Cost function

$$J(w) = \frac{1}{m} \sum_{i=1}^{m} \operatorname{Cost}(h_{w}(x^{(i)}), y^{(i)})$$

$$\operatorname{Cost}(h_{\operatorname{w}}(x),y) = \begin{cases} -\log(h_{\operatorname{w}}(x)), \text{ если } y = 1 \\ \log(1-h_{\operatorname{w}}(x)), \text{ если } y = 0 \end{cases}$$

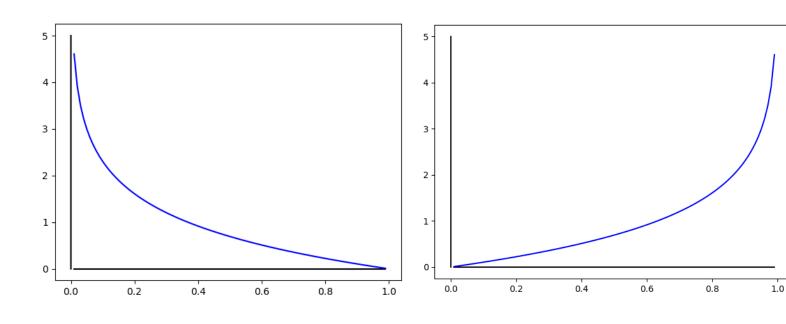


$$h_{\mathbf{w}}(x) = \sigma(\mathbf{w}^T x) = \frac{1}{1 + e^{-\mathbf{w}^T x}}$$

$$J(w) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}(h(x), y) = -\frac{1}{m} \left[\sum_{i=1}^{m} y^{(i)} \log \left(h_{w}(x^{(i)}) \right) + (1 - y^{(i)}) \log \left(1 - h_{w}(x^{(i)}) \right) \right]$$

Cost function

$$Cost = \begin{cases} -\log(h_{w}(x)) & \text{if } y = 1\\ \log(1 - h_{w}(x)) & \text{if } y = 0 \end{cases}$$



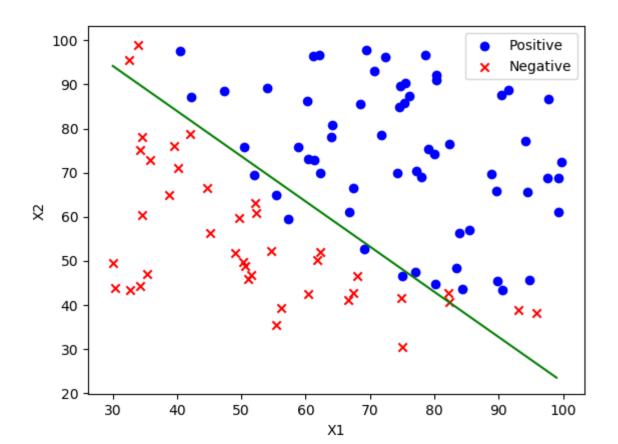
If
$$y = 1$$

$$Cost = 0 \text{ if } h_{W}(x) = 1$$

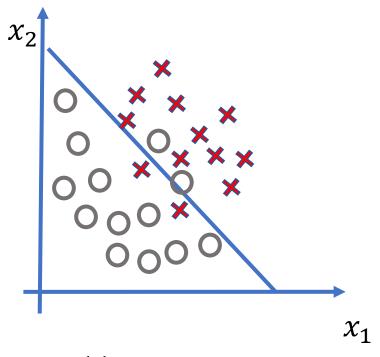
$$Cost \rightarrow \infty \text{ if } h_{W}(x) \rightarrow 0$$

We use gradient dissent to minimize cost function

$$J'(\mathbf{w}) = \sum (y_n - \sigma(\mathbf{w}^T \bar{x})) \bar{x}$$

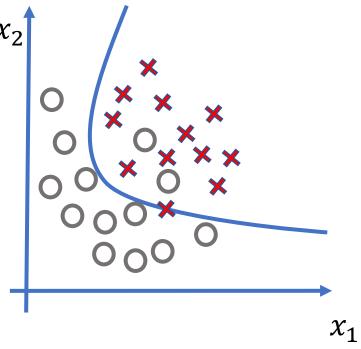


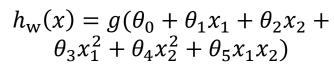
Overfitting

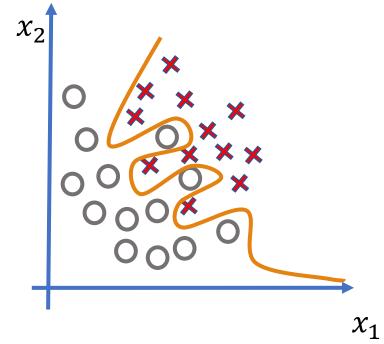


$$h_{\mathbf{w}}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$





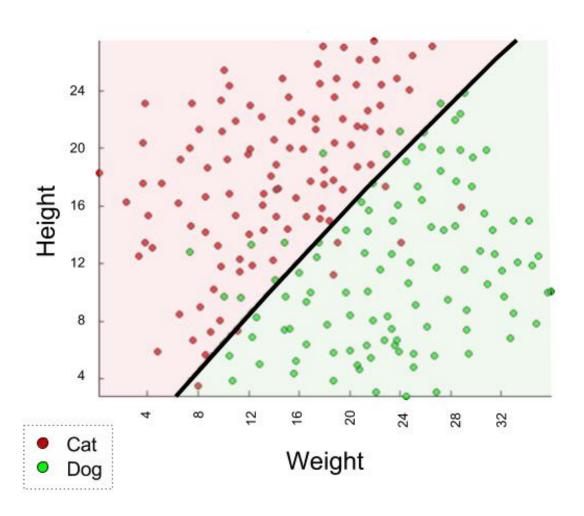


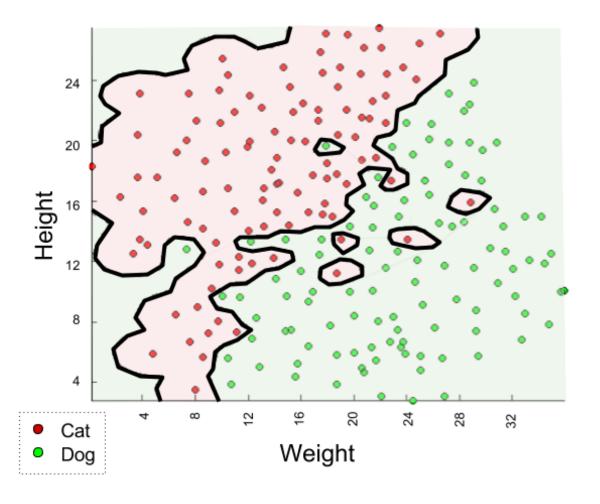


 $h_{w}(x) = g(\theta_{0} + \theta_{1}x_{1} + \theta_{2}x_{1}^{2}x_{2} + \theta_{3}x_{1}^{2}x_{2}^{2} + \theta_{4}x_{2}^{2}x_{3}^{2} + \theta_{5}x_{1}^{3}x_{2} + \cdots)$

<u>Overfit</u>

Overfitting





Regularization

The goal is to reduce the value of parameters $w_0, w_1 \dots w_n$

$$J(w) = \frac{1}{2m} \left[\sum_{i=0}^{m} (h_w(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n} w_j^2 \right]$$

• λ is a regularization parameter

if
$$\lambda\gg 1$$
 ($\lambda\approx 10^{10}$), to $w_1\approx 0$, $w_2\approx 0$, $w_3\approx 0$, ... $h_{\rm w}(x)\approx w_0$

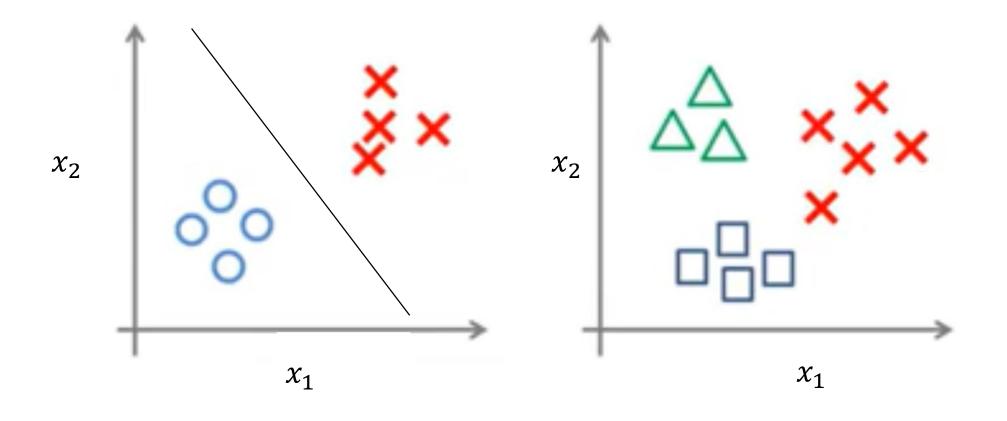
Gradient descent

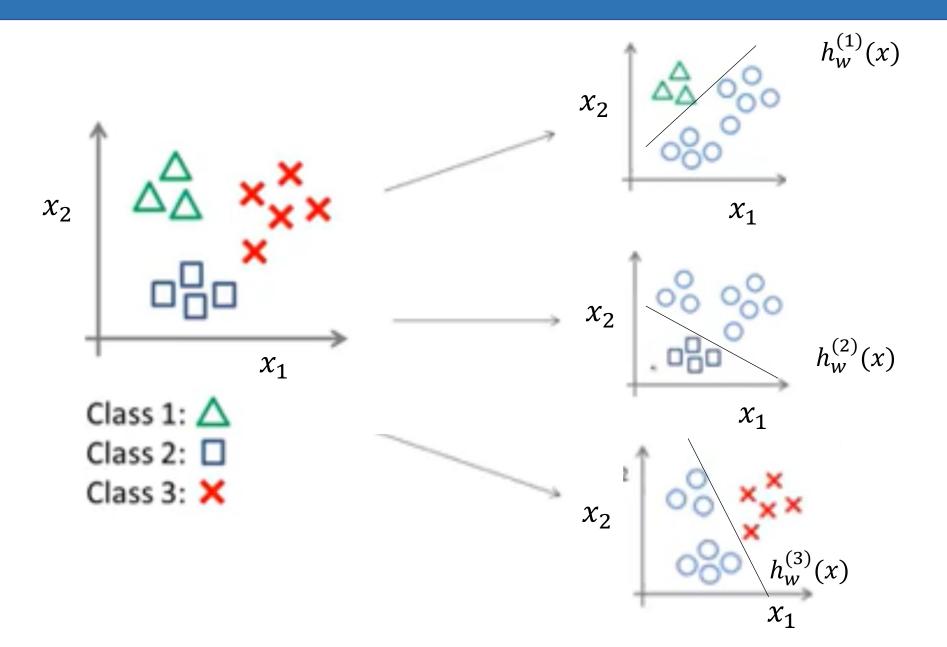
repeat until convergence {

$$w_0 \coloneqq w_0 - \frac{\alpha}{m} \sum_{i=1}^{m} (h_w(x^{(i)}) - y^{(i)}) x^{(i)}$$

$$w_j := w_j - \frac{\alpha}{m} \sum_{i=1}^m \left[(h_w(x^{(i)}) - y^{(i)}) x^{(i)} + \frac{\lambda}{m} w_j \right]$$

$$w_j := w_j \left(1 - \frac{\lambda}{m} \right) - \frac{\alpha}{m} \sum_{i=1}^m \left(h_w(x^{(i)}) - y^{(i)} \right) x^{(i)}$$





Train the logistic regression classifier $h_w(x)$ for each class i to predict the probability that y=i

On a new input x to make a prediction, pick the class i that maximizes

$$\max_{i} h_{w}^{(i)}(x)$$









We want:

$$h_{\mathrm{w}}(x) pprox egin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad h_{\mathrm{w}}(x) pprox egin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$
 man car

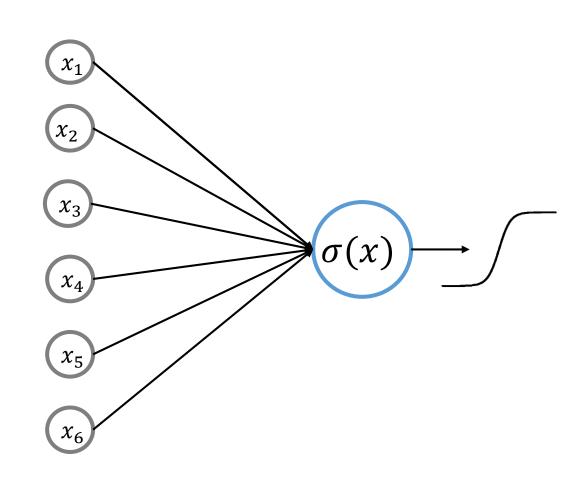
$$h_{\rm w}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \qquad h_{\rm w}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
 bike

One-vs-all

Data train:

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$$

$$y^{(j)} = [0,1]$$



One-vs-all

Data train:

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$$

$$y^{(j)} \in \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

