Introduction to Artificial Intelligence: Methods, Models, Algorithms

Aleksandr I. Panov and Konstantin S. Yakovlev

National Research University Higher School of Economics

20 July 2018 – Summer University

apanov@hse.ru

Nearest-neighbor method

- It is a task of classification
- Data: $X = (x_i, y_i)_{i=1}^{l}$
- Learning process: we just remember the data

Nearest-neighbor method

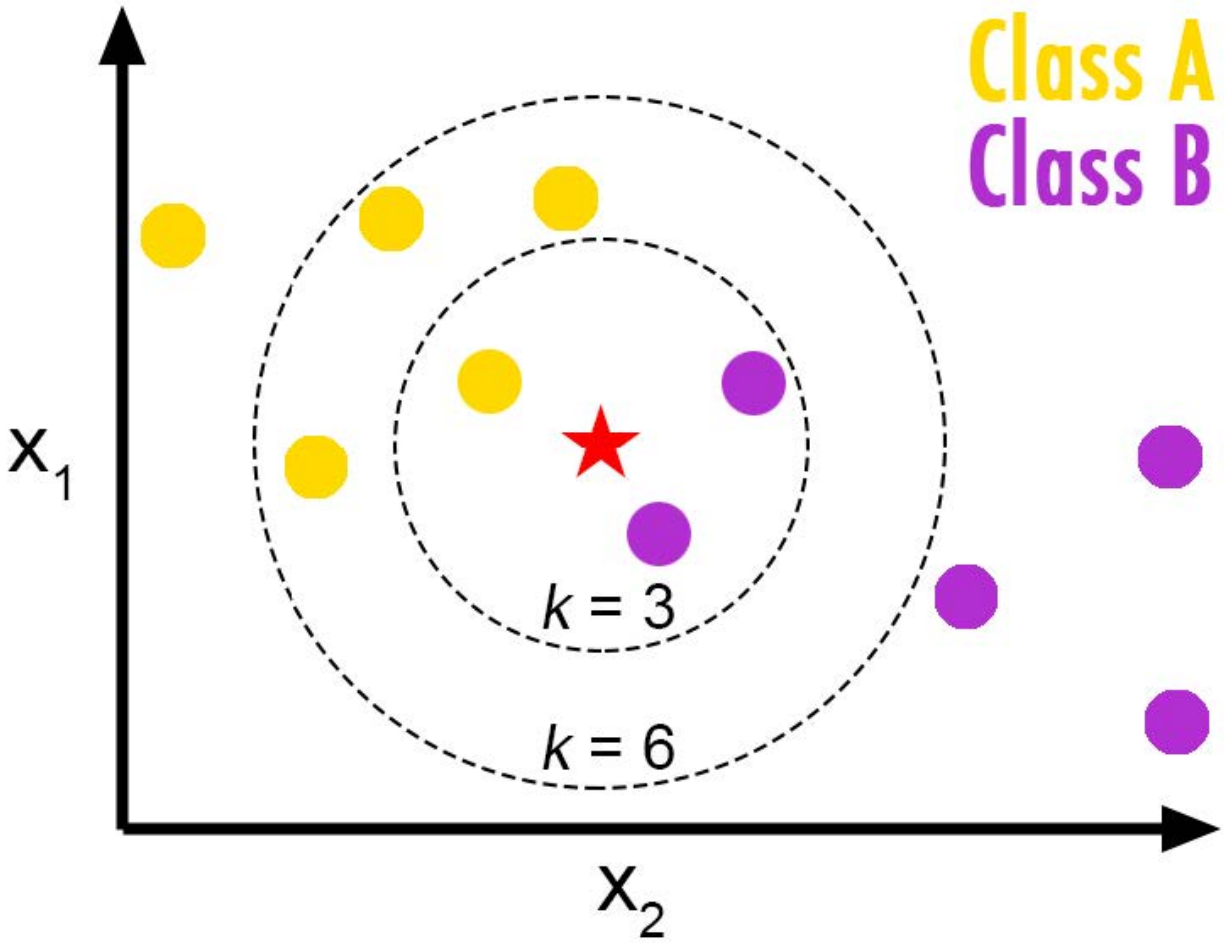
- New object x
- Sorting objects of training data by distance from x:

$$\rho(x, x_{(1)}) \leq \cdots \leq \rho(x, x_{(l)})$$

- Choose class that is most popular among k nearest neighbors:

$$a(x) = arg \min_{y \in \mathbb{Y}} \sum_{i=1}^{k} [y_{(i)} = y]$$

Nearest-neighbor method

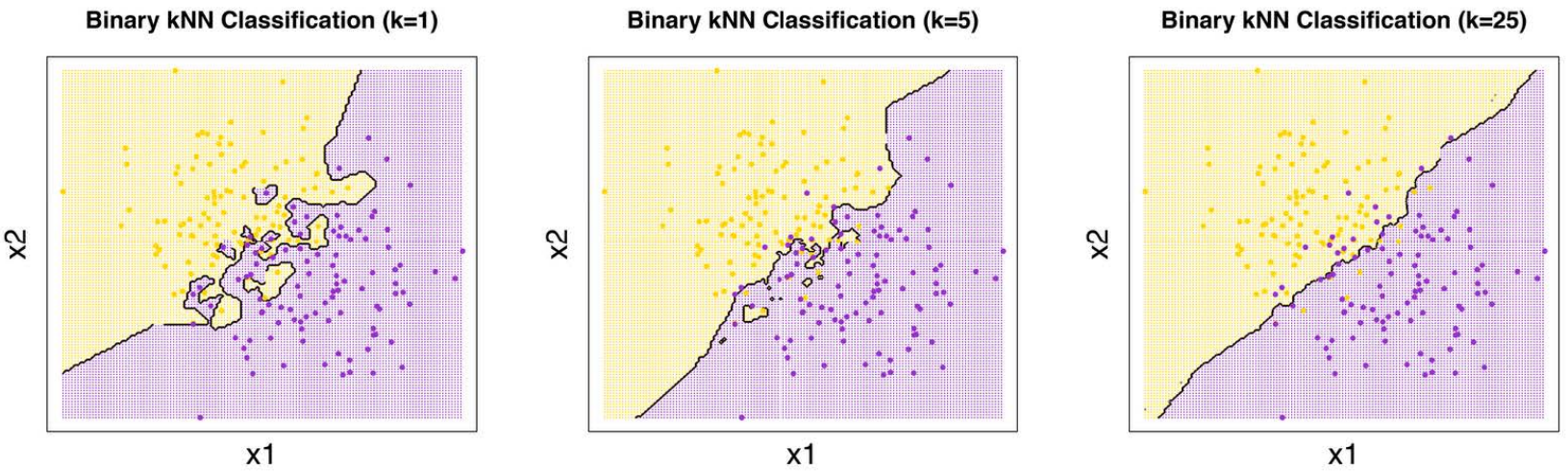


Nearest-neighbor method

$$a(x) = arg \min_{y \in \mathbb{Y}} \sum_{i=1}^{k} [y_{(i)} = y]$$

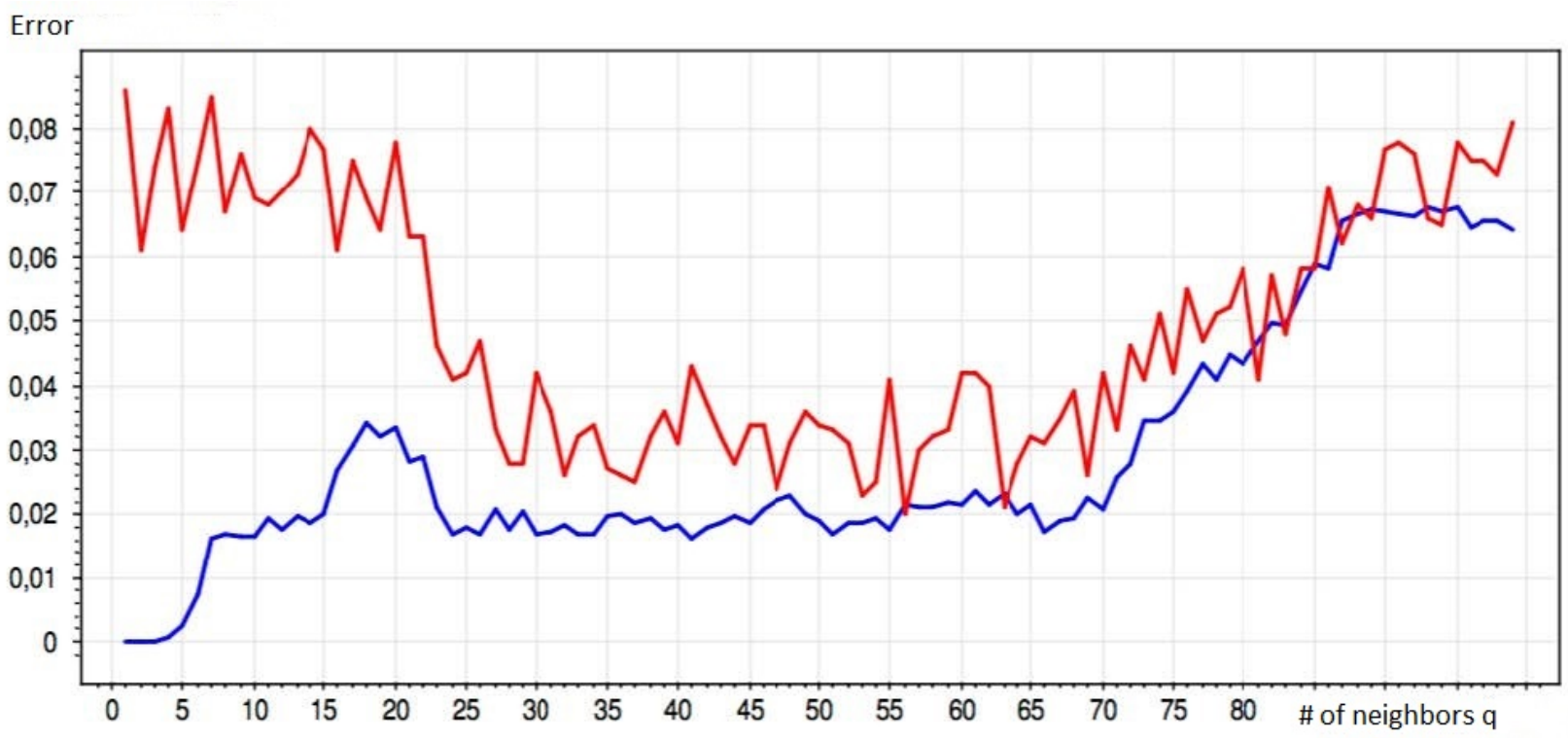
- k - hyperparameter of the algorithm
- we can select it via using of hold-out dataset and cross-validation
- The larger k, the easier the separating surface

How to choose number of neighbors?

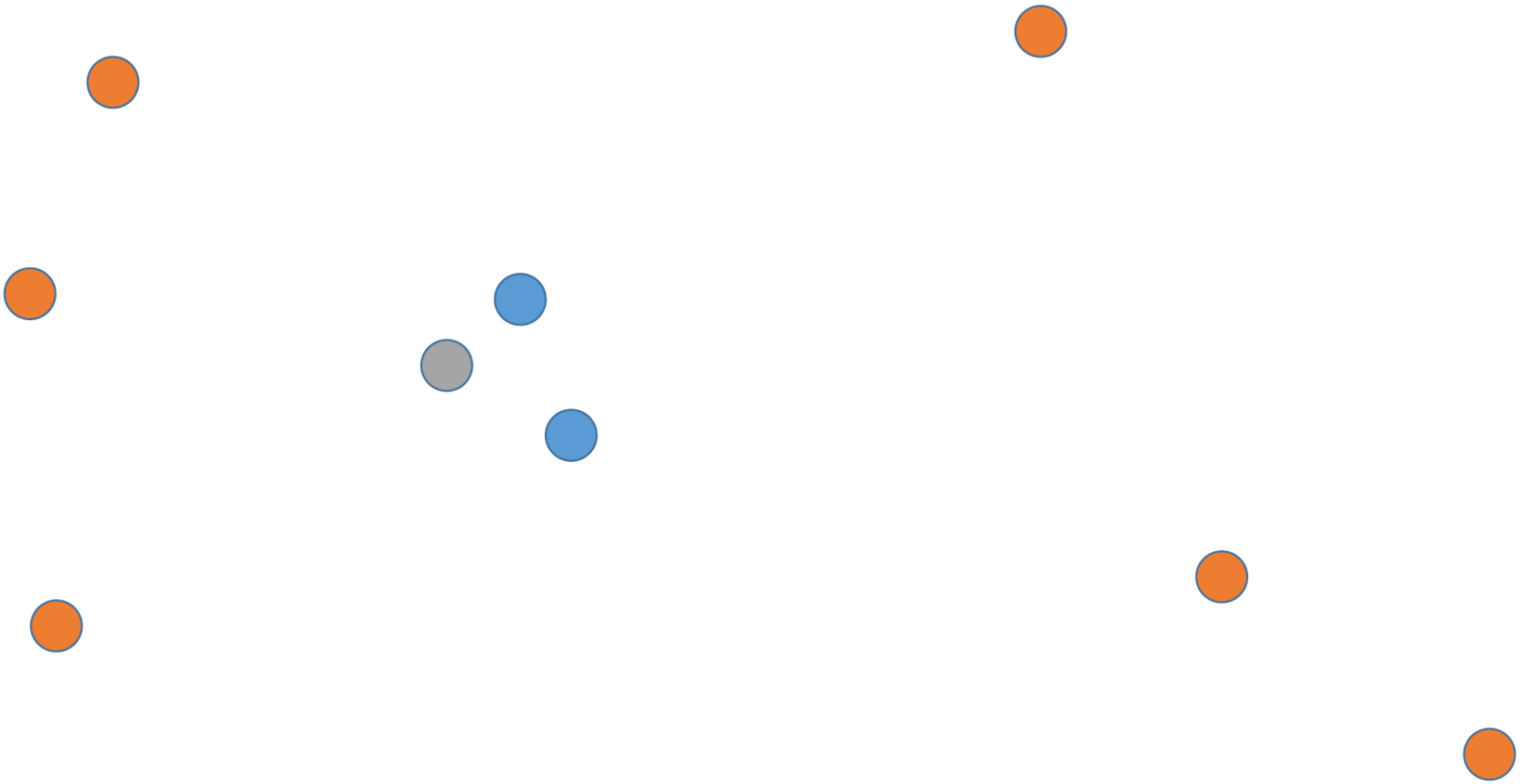


How to choose number of neighbors?

- Blue - learning error
- Red - cross-validation error



Problem of k-NN



Nearest-neighbor method

- Do not take into account the distances to k nearest neighbors
- Closer neighbors should be more important

k-NN with weights

$$a(x) = arg \min_{y \in \mathbb{Y}} \sum_{i=1}^{k} w_i [y_{(i)} = y]$$

Options:

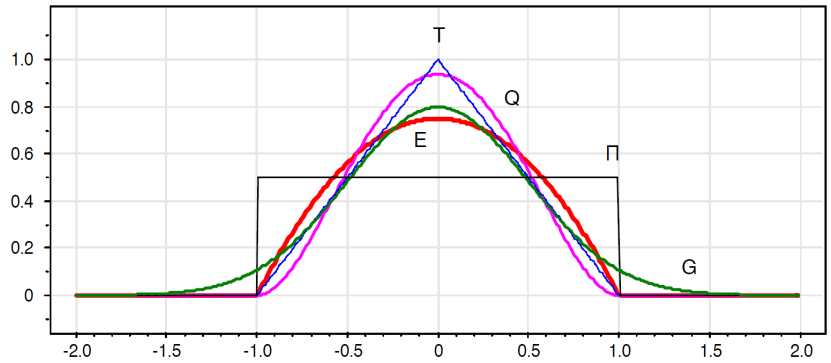
- $w_i = \frac{k+1-1}{k}$
- $w_i = q^i$
- Not a distance weight

k-NN with weights

$$a(x) = arg \min_{y \in \mathbb{Y}} \sum_{i=1}^{k} w_i [y_{(i)} = y]$$

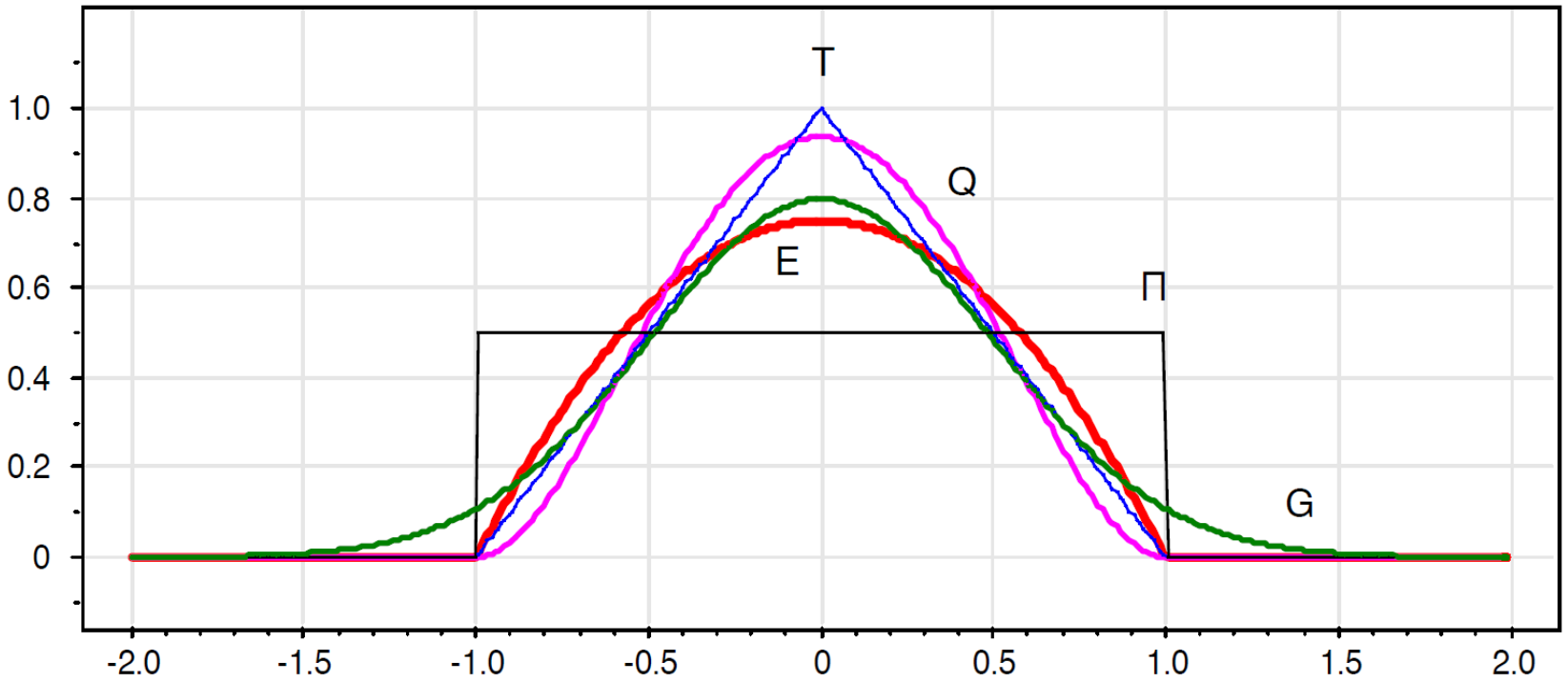
The Parzenov window:

- $w_i = K(\frac{\rho(x, x_{(i)})}{h})$
- K - kernel
- h - width of the window

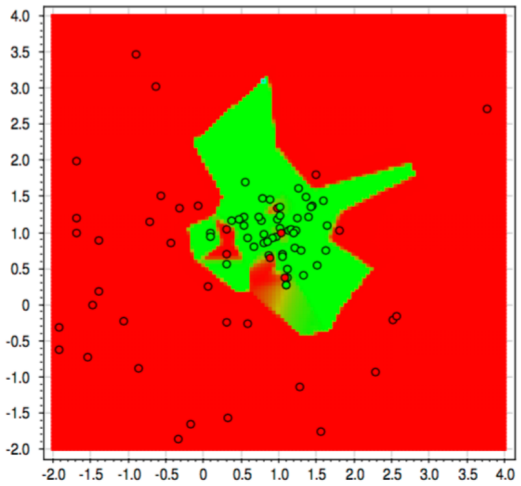


Nearest-neighbor method

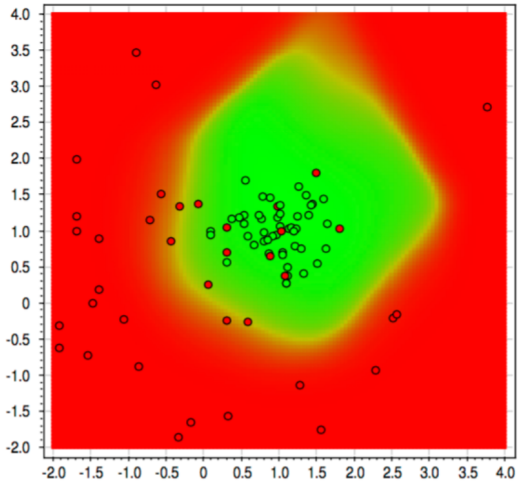
- Gaussian kernel: $K(z) = (2\pi)^{-0.5} \exp^{-\frac{1}{2}z}$
- And many others



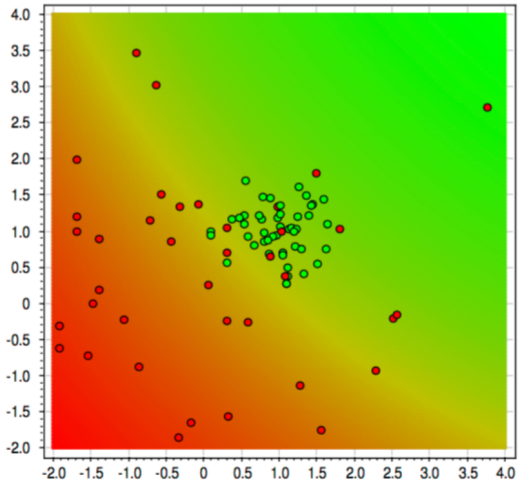
Kernels



$h = 0.05$



$h = 0.5$



$h = 5$

Properties of kNN

- Training is absent - it is only necessary to memorize the training sample
- To apply the model, you need to calculate the distances from the new object to all the training objects
- Application requires $l \times d$ operations
- There are special methods for finding nearest neighbors

kNN for regression

- Classification:

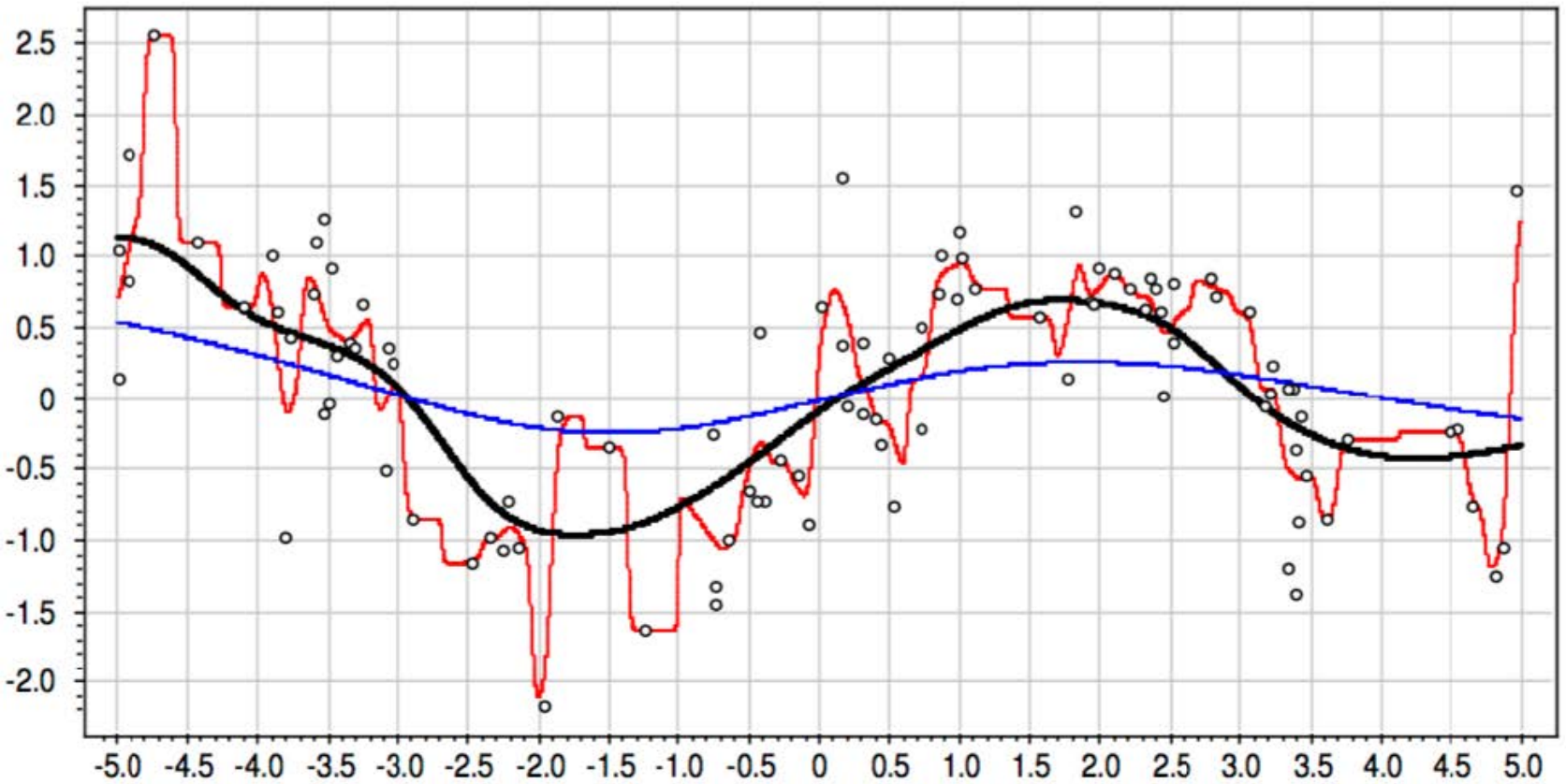
$$a(x) = arg \min_{y \in \mathbb{Y}} \sum_{i=1}^{k} [y_{(i)} = y]$$

- Regression:

$$a(x) = \frac{\sum_i^k w_i y_{(i)}}{\sum_{i=1}^k w_i}$$

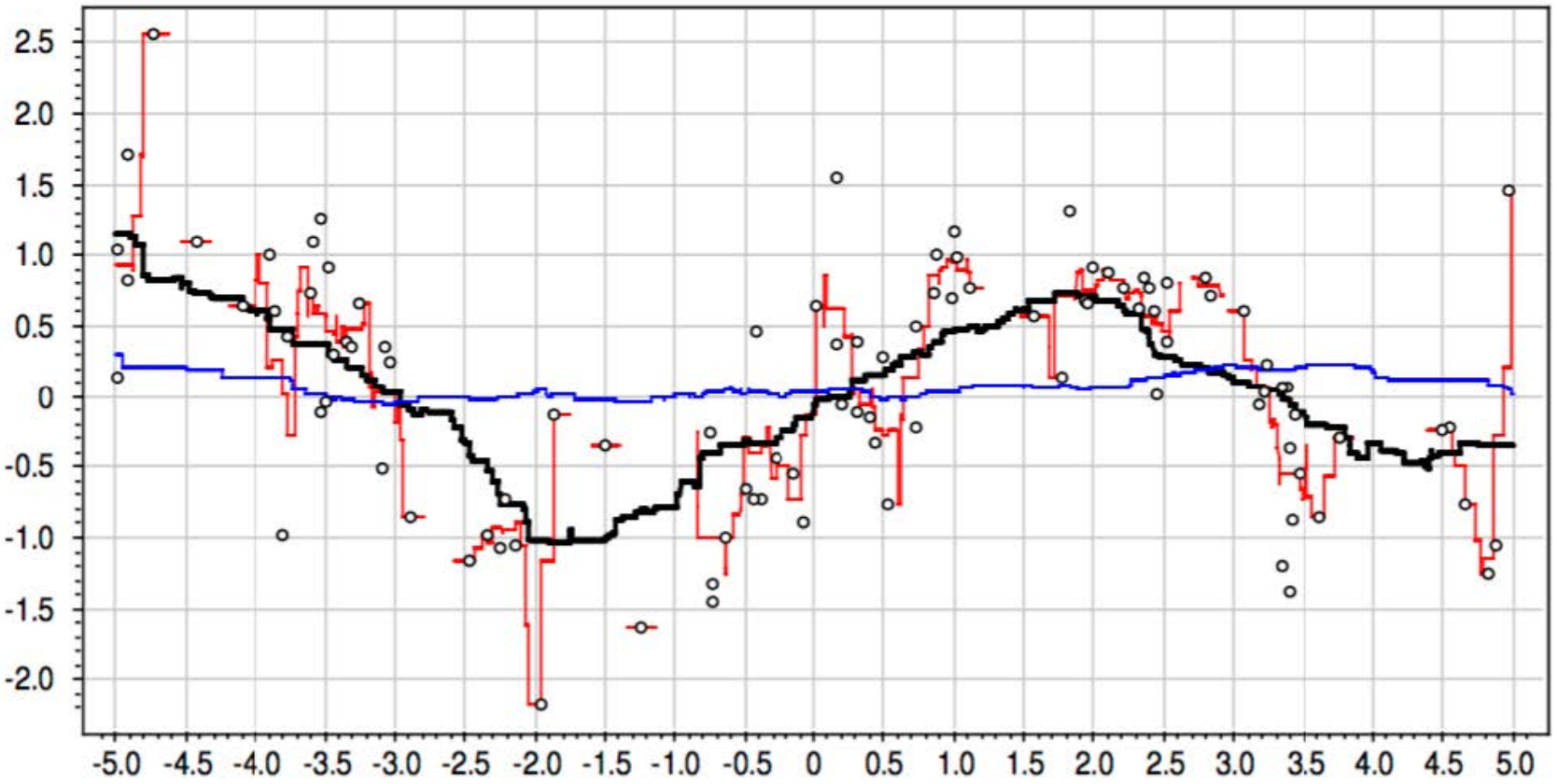
kNN for regression

- Gaussian kernel
- $h \in \{0.1, 1.0, 3.0\}$

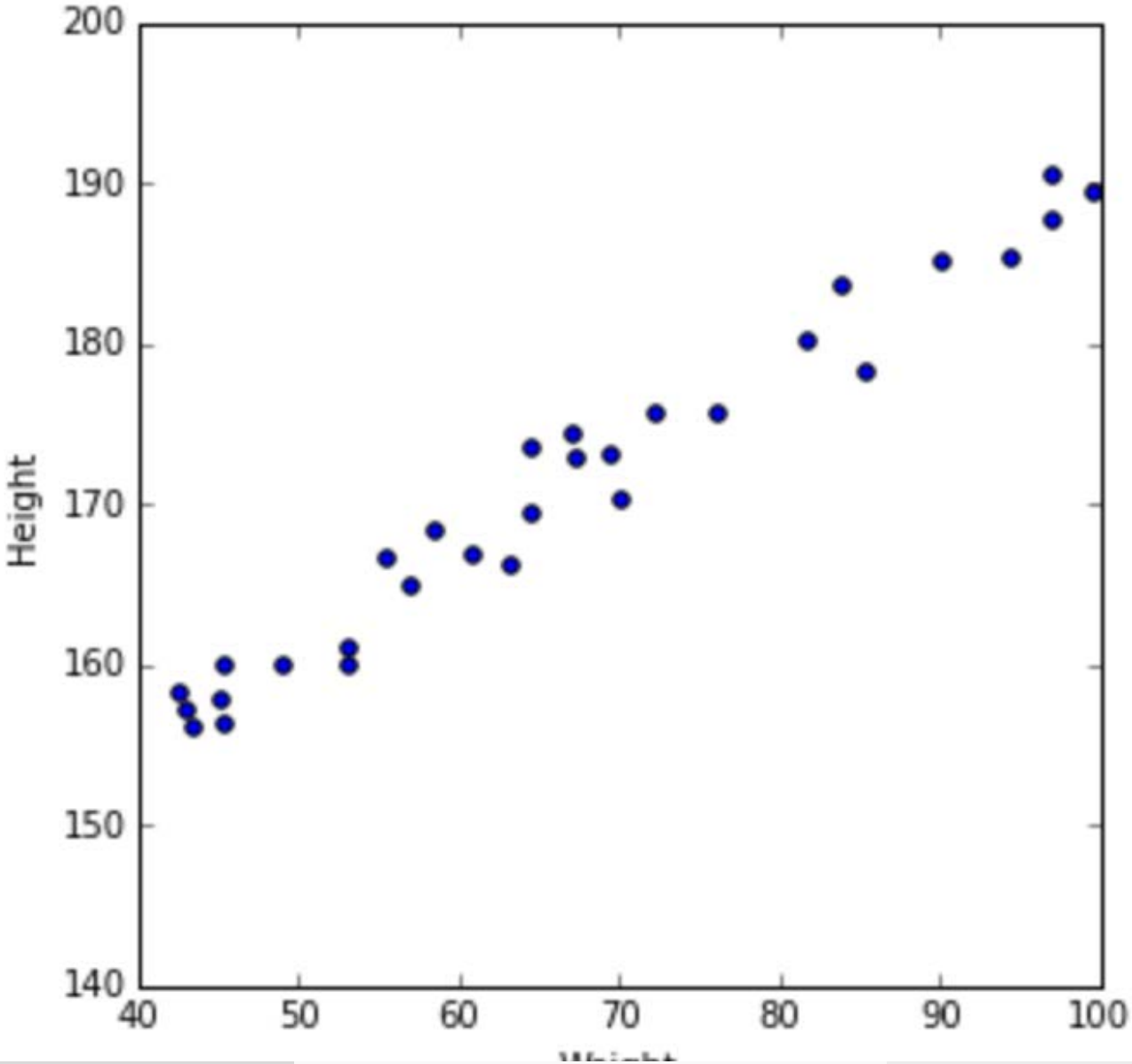


kNN for regression

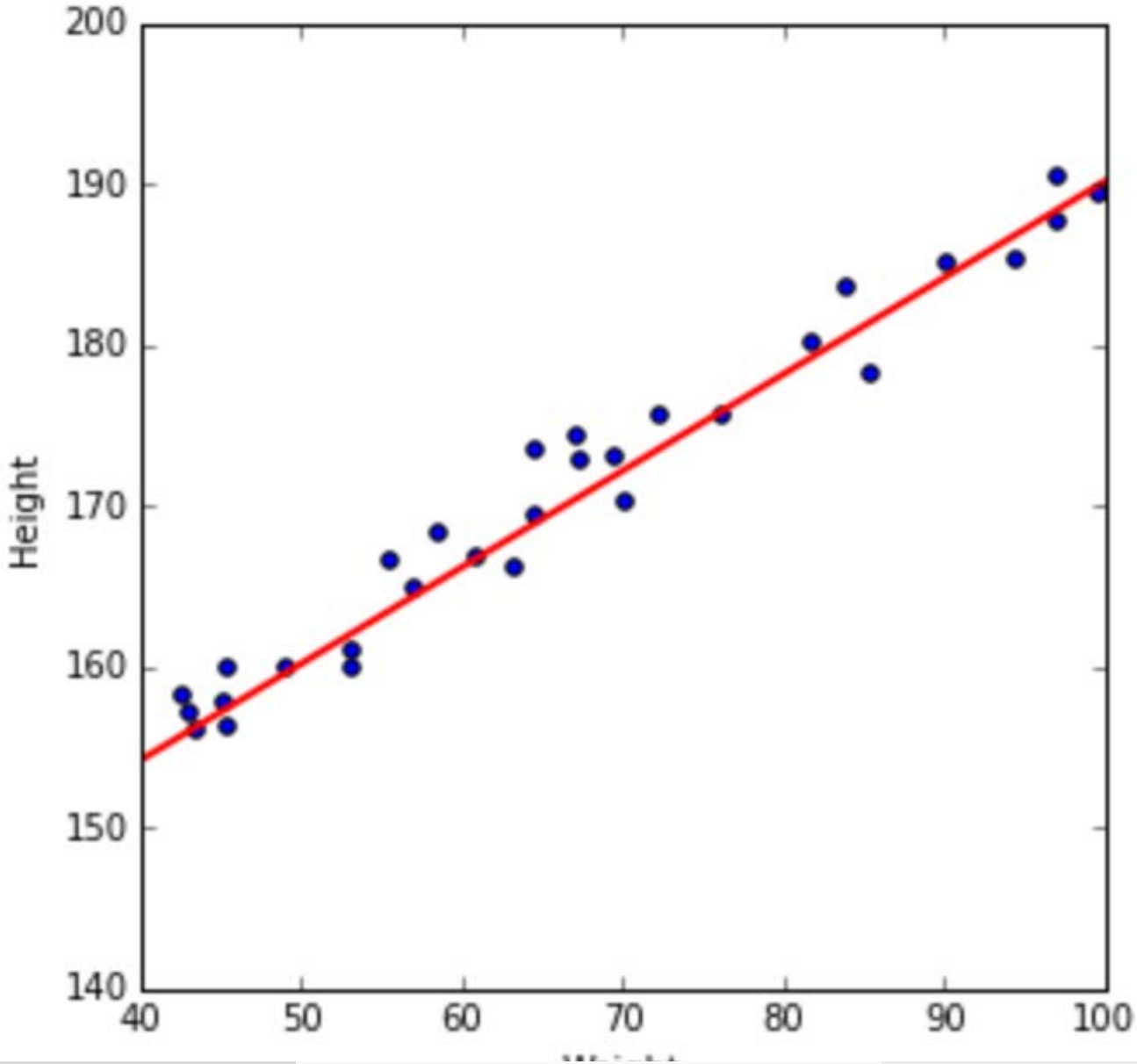
- Rectangle kernel $K(z) = [|z| \leq 1]$
- $h \in \{0.1, 1.0, 3.0\}$



One-dimension sample



One-dimension sample



Paired regression

- The simplest case: only one feature
- Model: $a(x) = w_0 + w_1 x$
- Tow parameters: w_0 and w_1
- The simplest model

Linear regression

- Weighted sum of features

$$a(x) = w_0 + w_1 x^1 + \cdots + w_d x^d$$

- $x^1, x^2, \ldots, x^d$ - values of features
- $w_0, w_1, \ldots, w_d$ - parameters
- w_0 - bias

Linear regression

$$a(x) = w_0 \times 1 + w_1 x^1 + \cdots + w_d x^d$$

- w_0 - as a coefficient with a single feature
- and if we add it:

$$\begin{pmatrix} x_{11} & \cdots & x_{1d} & 1 \\ \vdots & & \vdots & \vdots \\ x_{l1} & \cdots & x_{ld} & 1 \end{pmatrix}$$

Linear regression

- It gives as scalar product

$$a(x) = w_0 \times 1 + w_1 x^1 + \cdots + w_d x^d = \langle w, x \rangle$$

- Learning:

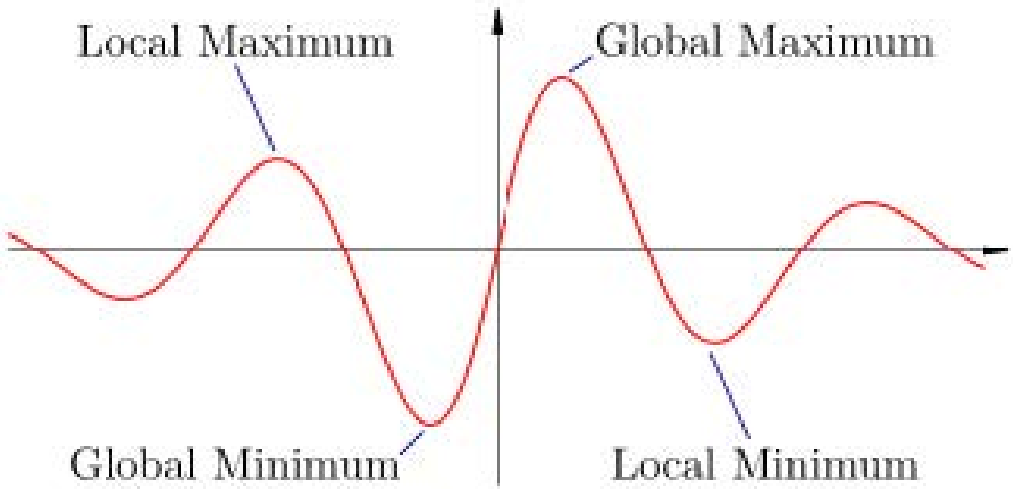
$$\sum_{i=1}^{l} (\langle w, x_i \rangle - y_i)^2 \to \min_w$$

- In vector form:

$$Q(w, X) = \frac{1}{q} \|Xw - y\|^2$$

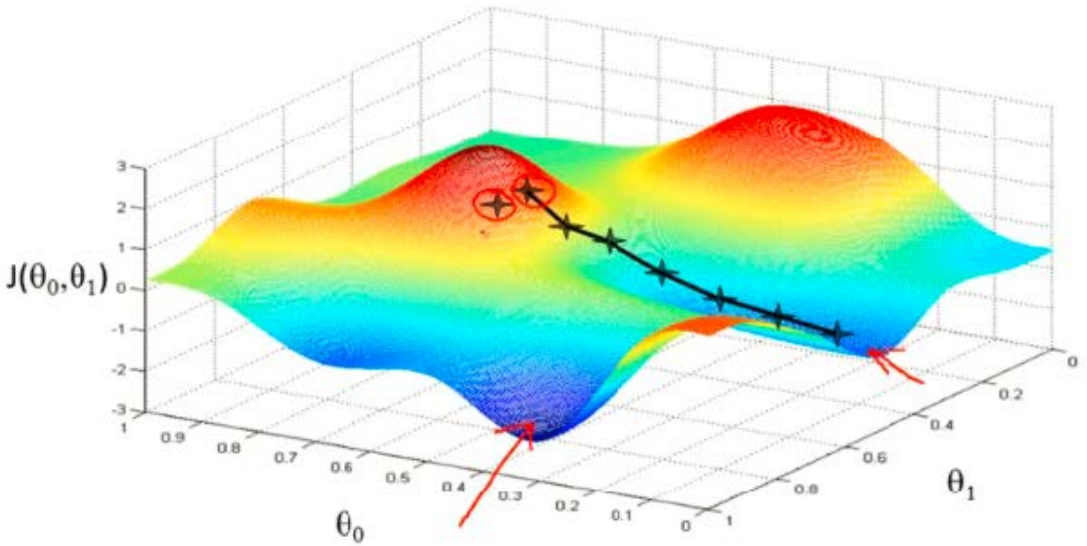
Extremes

- Extreme - minimum or maximum
- The local minimum is less than all values in some neighborhood
- Global minimum - the least of all values



Extremes

- Local minima are one of the main problems in machine learning



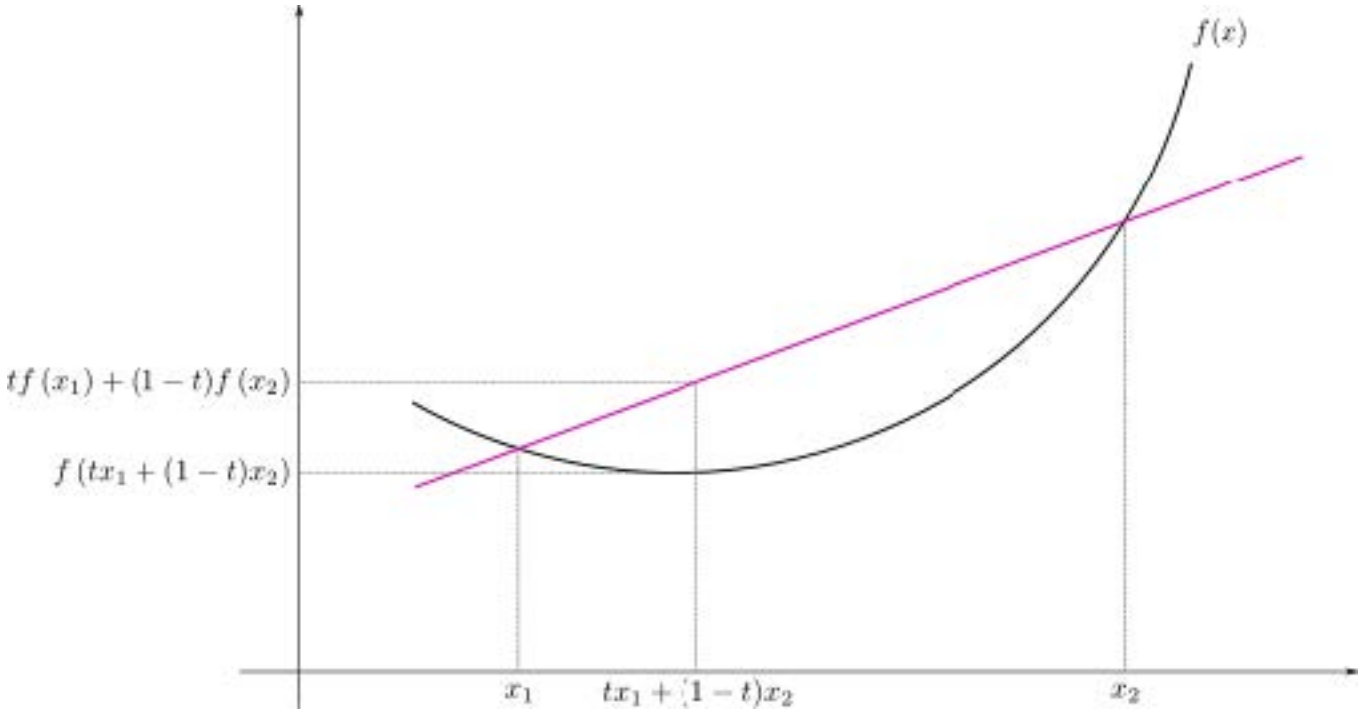
Andrew Ng

The optimality condition

- How do we know if the point x_0 is an extremum?
- Fermat's theorem: if the point x_0 is an extremum, and there is a derivative in it, then $f'(x_0) = 0$
- If the function has a derivative everywhere: we need to solve $f'(x) = 0$
- If there is a problem with the derivative: no luck
- Even if there is a derivative, then what to do with local extremes?

Convex functions

- A convex function if its graph lies below any segment joining two points



Convex functions

- The function is convex if, at all points $f''(x) > 0$
- An important property: any local extremum of a convex function is global
- Solving the equation $f'(x) = 0$, we obtain global extrema
- Conclusion: we will try to choose convex functionals!

An example

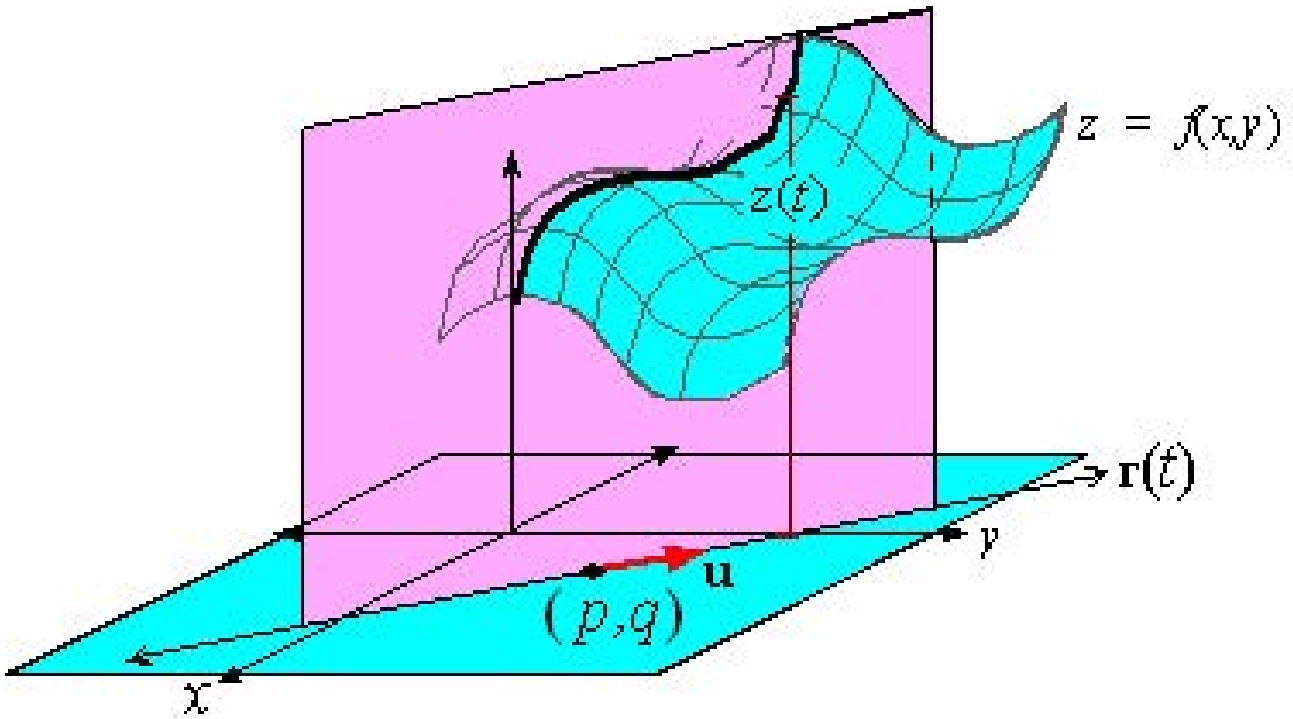
- Quality functional for linear regression:

$$Q(w_1, \ldots, w_d) = \sum_{i=1}^{l} (w_1 x^1 + \cdots + w_d x^d - y_i)^2$$

- How to search for its minimum?

Derivative in direction

- How fast is the function growing in a particular direction?



Derivative in direction

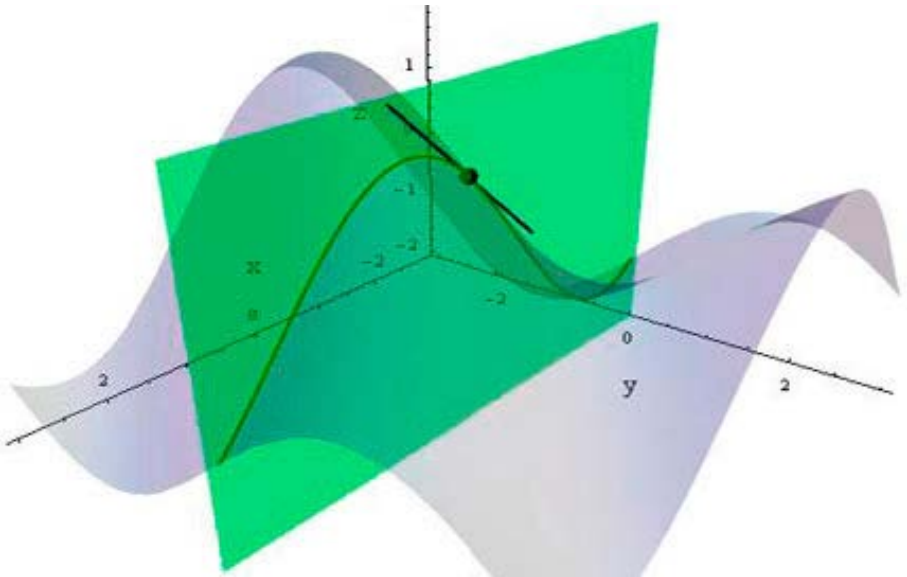
- Direction: v and $\|v\| = 1$
- Derivative:

$$f'_v(x_0) = \lim_{t \to 0} \frac{f(x_0 + tv) - f(x_0)}{t}$$

Partial derivative

- How fast is the function changing along the variable x_i?
- The partial derivative with respect to x_i:

$$\frac{\partial f}{\partial x_i} = \lim_{t \to 0} \frac{f(x_1, \ldots, x_i + t, \ldots, x_d) - f(x_1, \ldots, x_i, \ldots, x_d)}{t}$$



Gradient

- Gradient is vector of partial derivatives:

$$\nabla f(x) = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_d} \right)$$

- Gradient has a very important property!

Gradient

- Lets fix a point x_0
- In which direction is the function growing fastest?

$$f'_v(x_0) \to \max_v$$

- Relationship of directional derivative and gradient:

$$f'_v(x_0) = \langle \nabla f(x_0, v) \rangle = \|\nabla f(x_0)\| \times \|v\| \times \cos\phi$$

Gradient

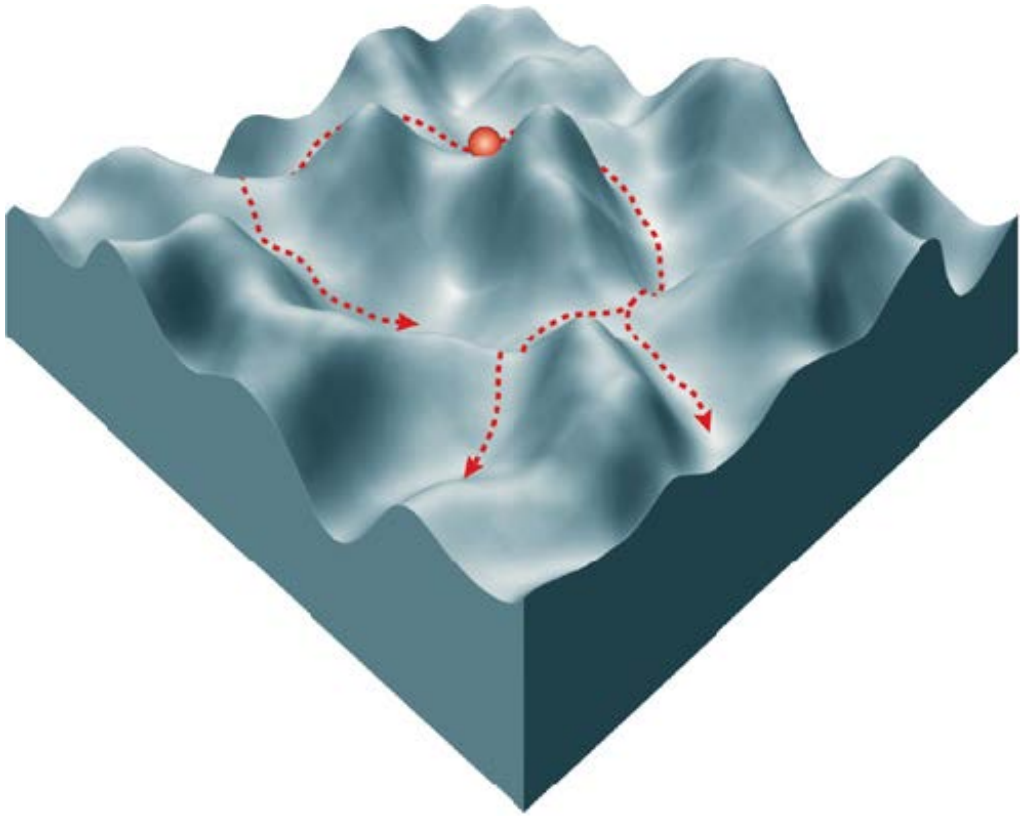
- An arbitrary direction is maximal if the direction coincides with the gradient!
- **Gradient - the direction of the steepest growth of the function**
- Antigradient - the direction of steepest descent

The optimality condition

- How do we know if the point x_0 is an extremum?
- Fermat's theorem: if the point x_0 is an extremum, and there is a gradient in it, then $\nabla f(x_0) = 0$
- If the function has a gradient everywhere: we need to solve $\nabla f(x) = 0$
- If there is a problem with the gradient: no luck

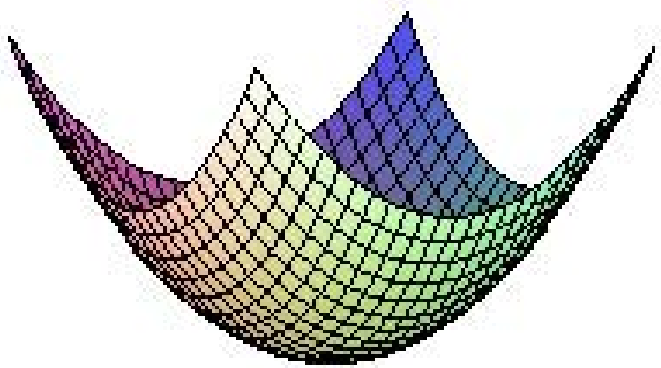
Extremes

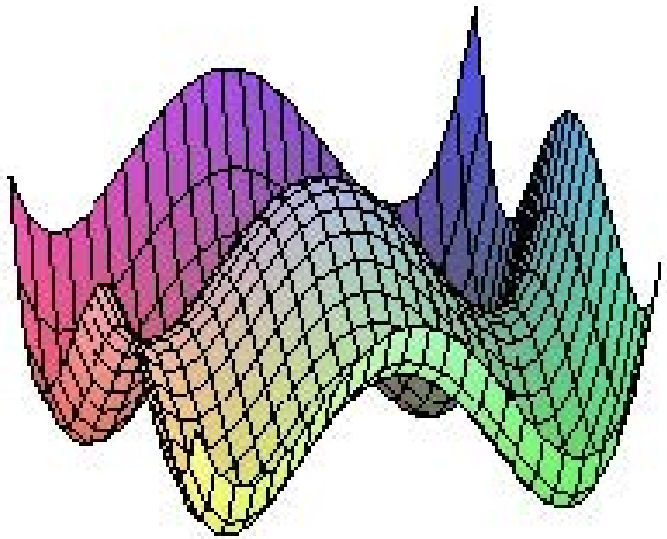
- The problem with local extremes is still relevant



Convex functions

The function is convex if its graph lies below the segment joining any two points





Optimization problem

$$Q(w, X) = \frac{1}{l} \sum_{i=1} l(\langle w, x_i \rangle - y_i)^2 - \to min_w$$

- A gradient exists at any point
- Convex function
- The only minimum (not always)

Optimization problem

$$\nabla Q(w, X) = \left(\frac{\partial Q}{\partial w_1}, \ldots, \frac{\partial Q}{\partial w_d} \right)$$

Derivatives:

$$\frac{\partial Q}{\partial w_j} = \frac{2}{l} \sum_{i=1} l x_i^j (, \langle w, x_i \rangle - y_i)$$

Learning linear regressor

- In a vector form:

$$Q(w, X) = \frac{1}{l}\|Xw - y\|^2$$

- Condition of minimum:

$$\nabla Q(w, X) = 0$$

- What if we try to solve this system of equations?

Learning linear regressor

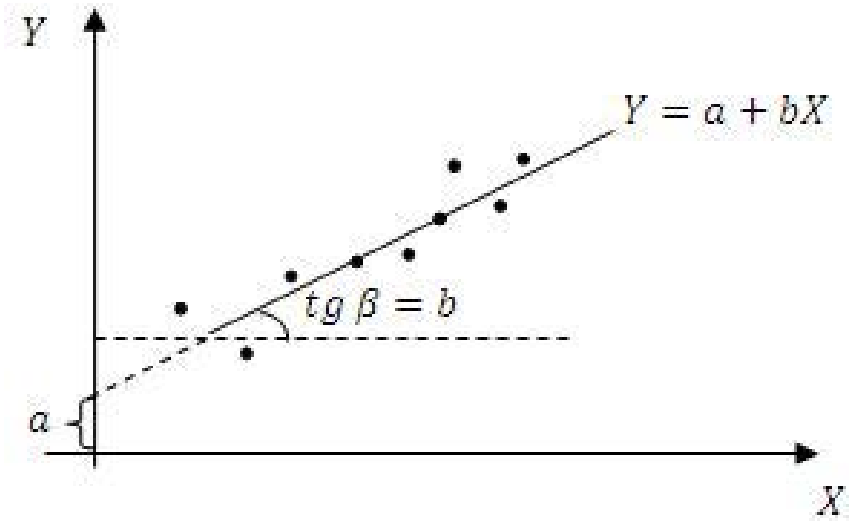
- We can solve it analytically:

$$w = (X^T X)^{-1} X^T y$$

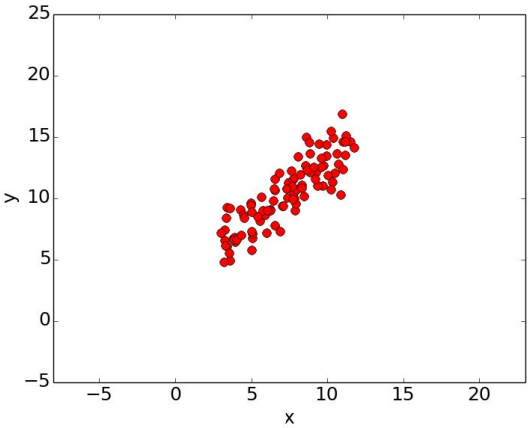
- But the matrix inversion is a very complicated operation
- Gradient descent much faster

Paired regression

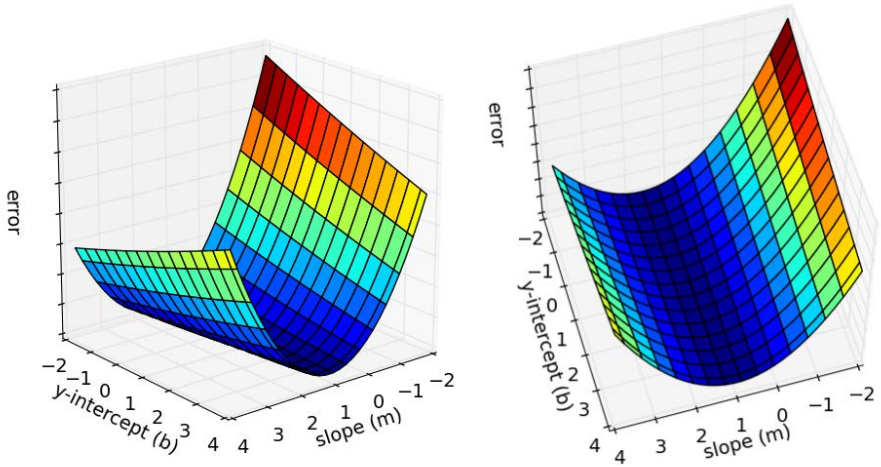
- The simplest case: only one feature
- Model: $a(x) = w_0 + w_1 x$
- Tow parameters: w_0 and w_1
- Quality functional: $Q(w_0, w_1) = \sum_{i=1}^{l} (w_1 x_i + w_0 - y_i)^2$



Paired regression



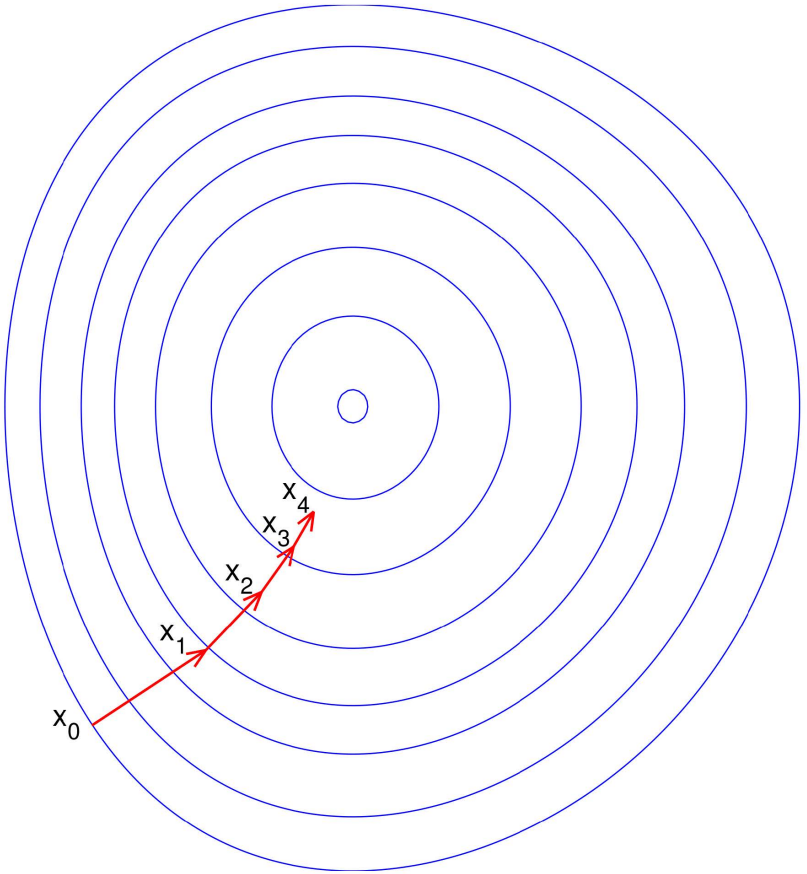
Sample



Quality functional

Gradient descent

- Suppose we have chosen the initial approximation $w^0 = (w_0^0, w_1^0)$
- How to improve it?
- Stepping towards the steepest descent
- That is, towards the anti-gradient!



Gradient descent

- Repeat until convergence

$$w^t = w^{t-1} - \eta \nabla Q(w^{t-1})$$

- convergence: $\|w^t - w^{t-1} < \epsilon\|$

Gradient for pair regression

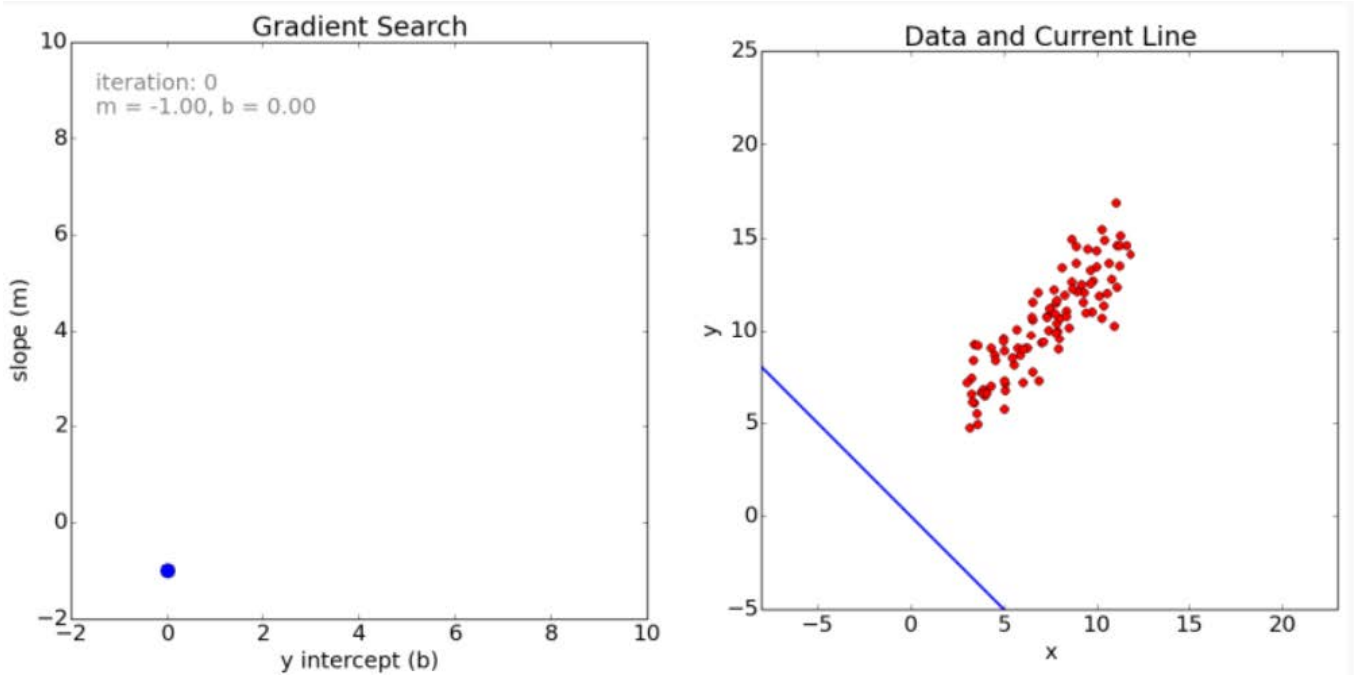
$$Q(w_0, w_1) = \sum_{i=1}^{l} (w_1 x_i + w_0 - y_i)^2$$

Partial derivatives:

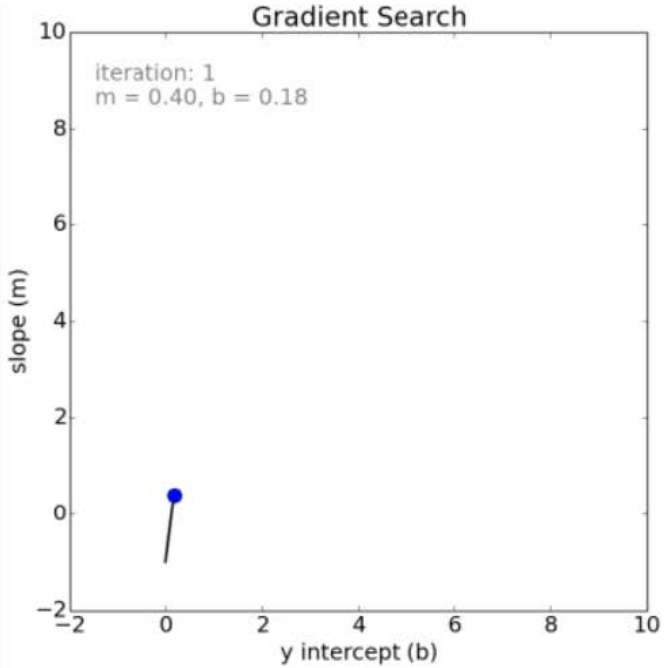
$$\frac{\partial Q}{\partial w_1} = 2 \sum_{i=1}^{l} (w_1 x_i + w_0 - y_i) x_i$$

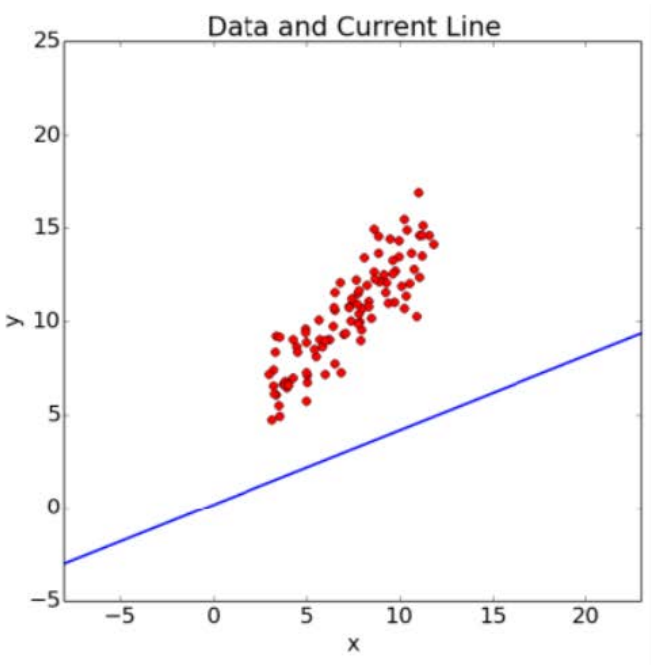
$$\frac{\partial Q}{\partial w_0} = 2 \sum_{i=1}^{l} (w_1 x_i + w_0 - y_i)$$

Paired regression

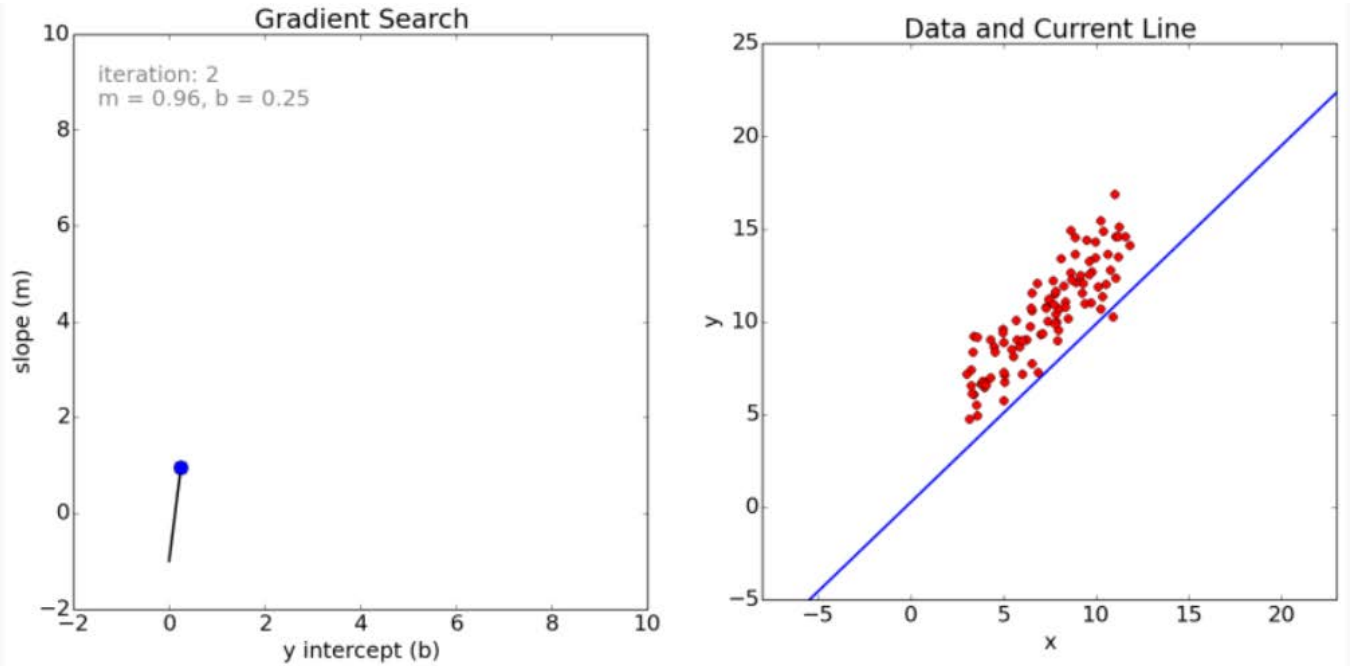


Paired regression

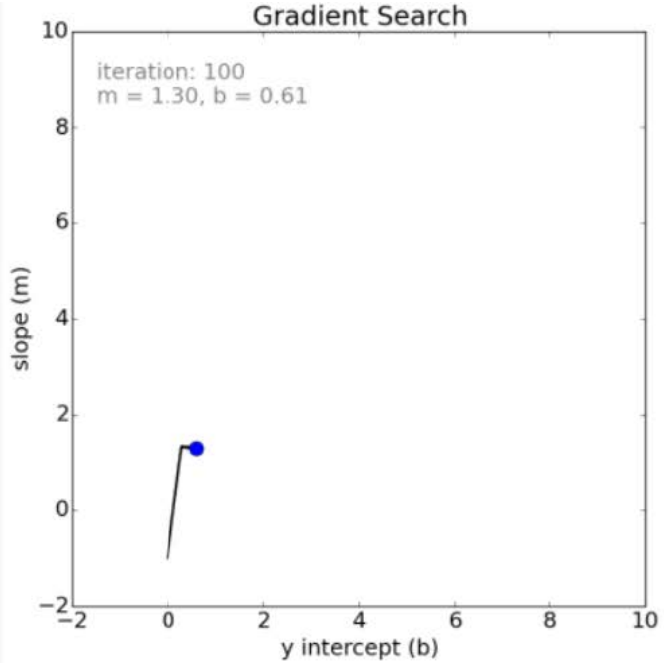


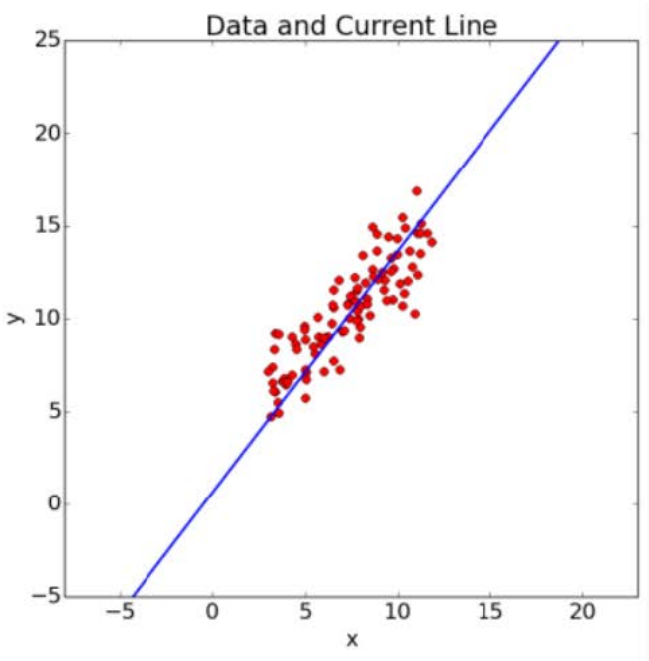


Paired regression

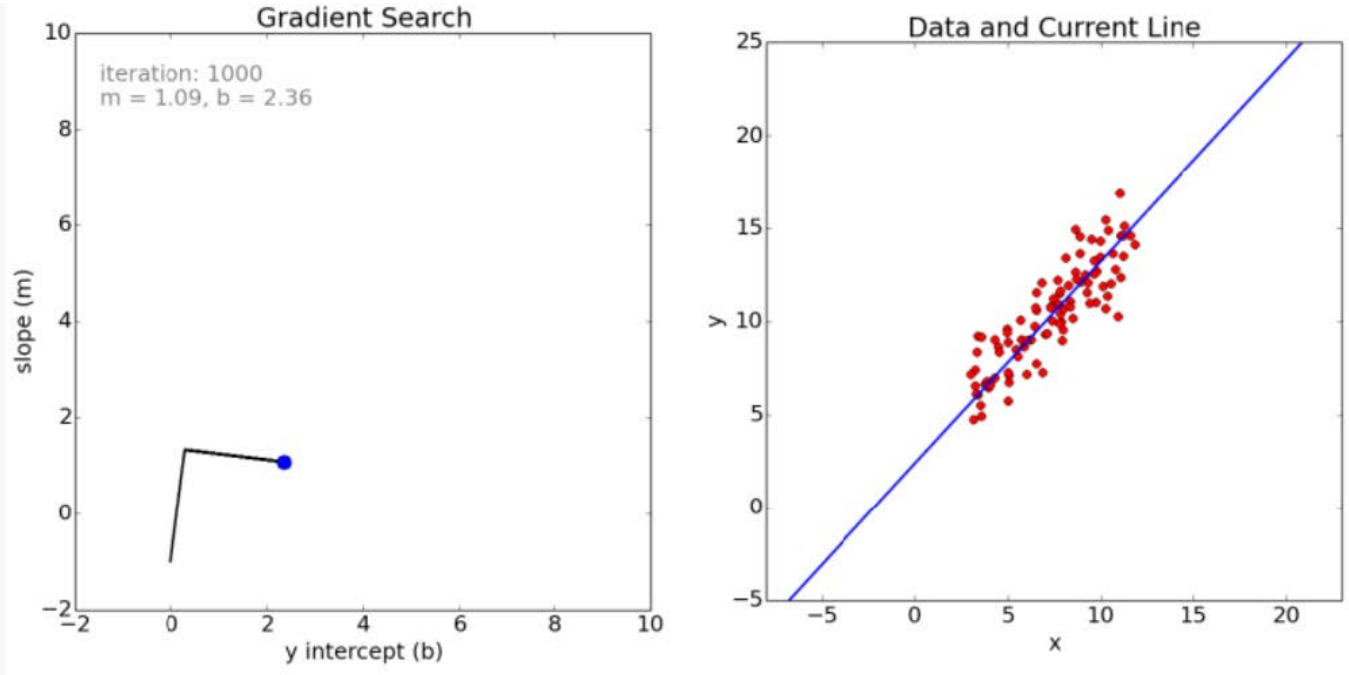


Paired regression

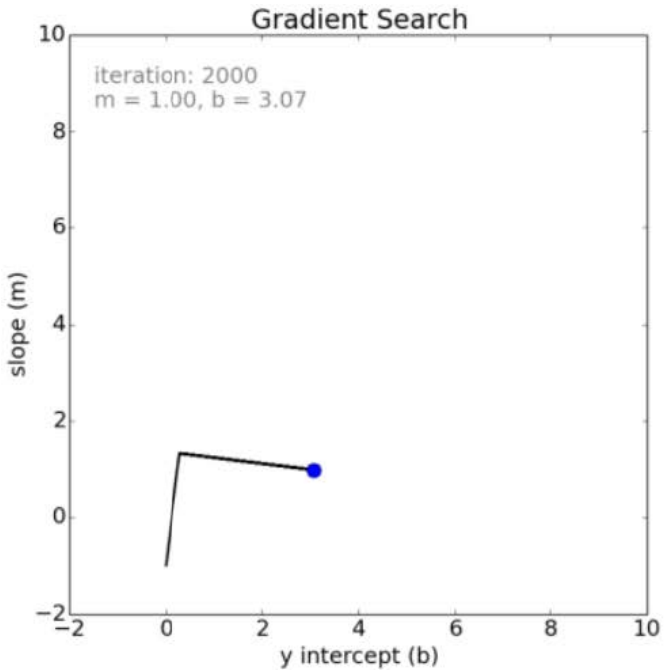


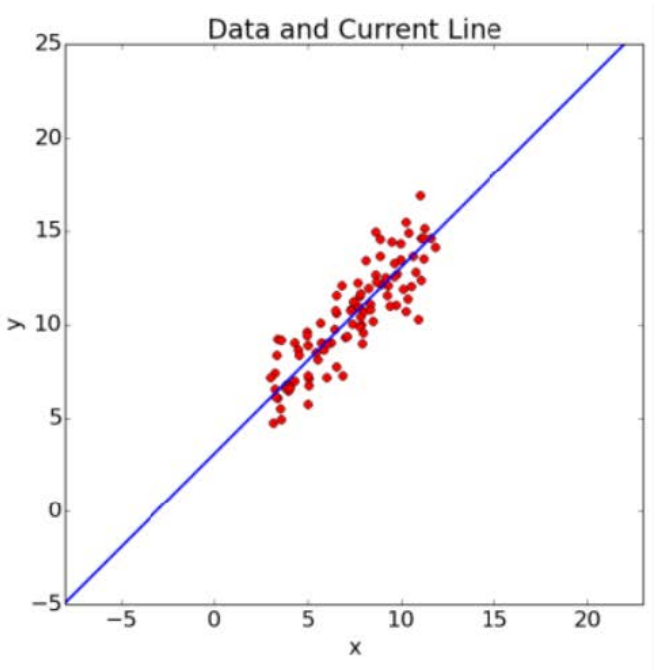


Paired regression

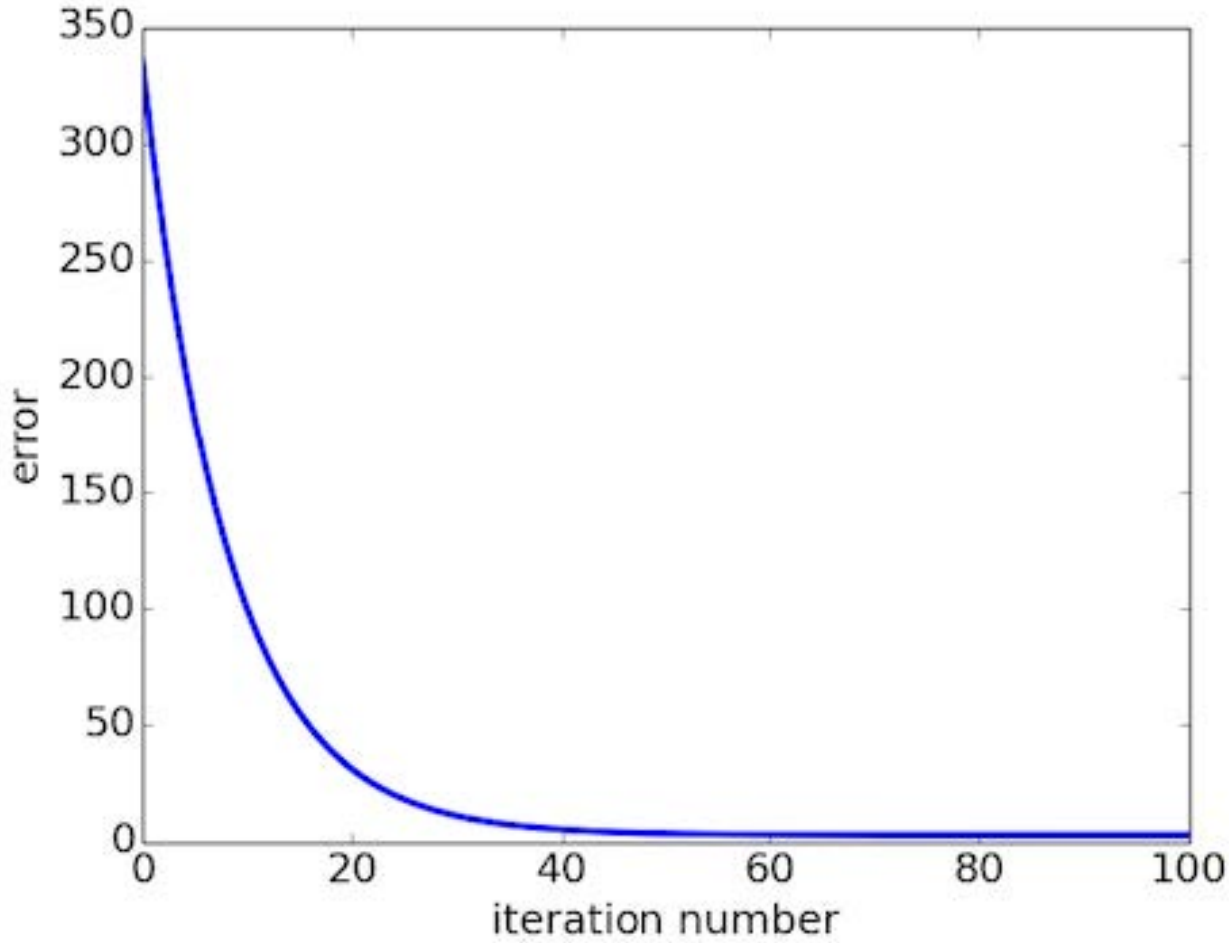


Paired regression



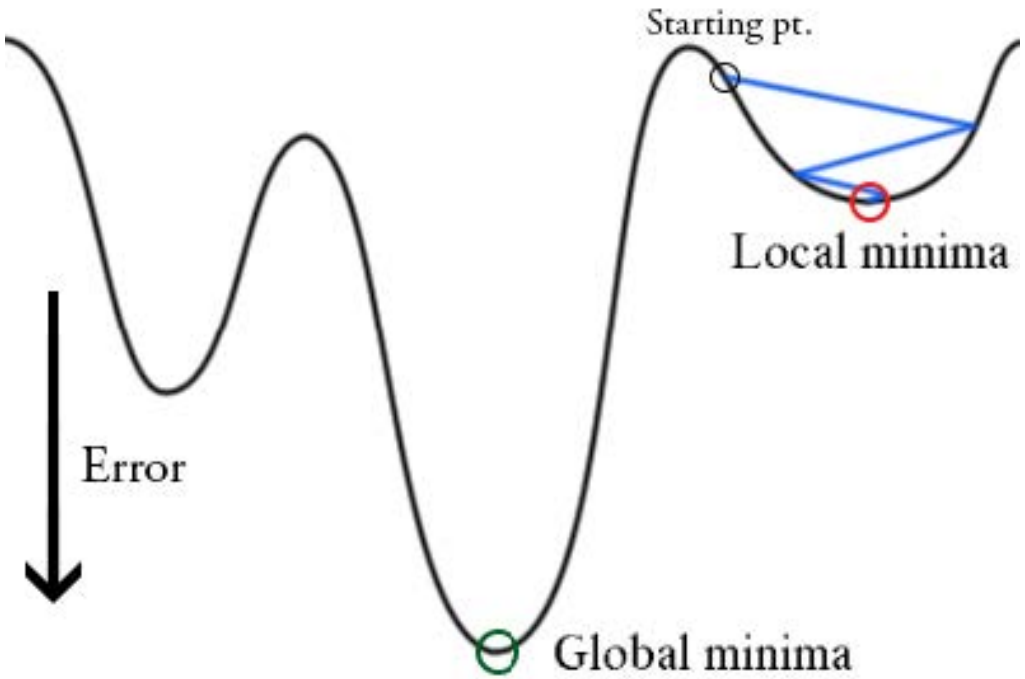


Paired regression



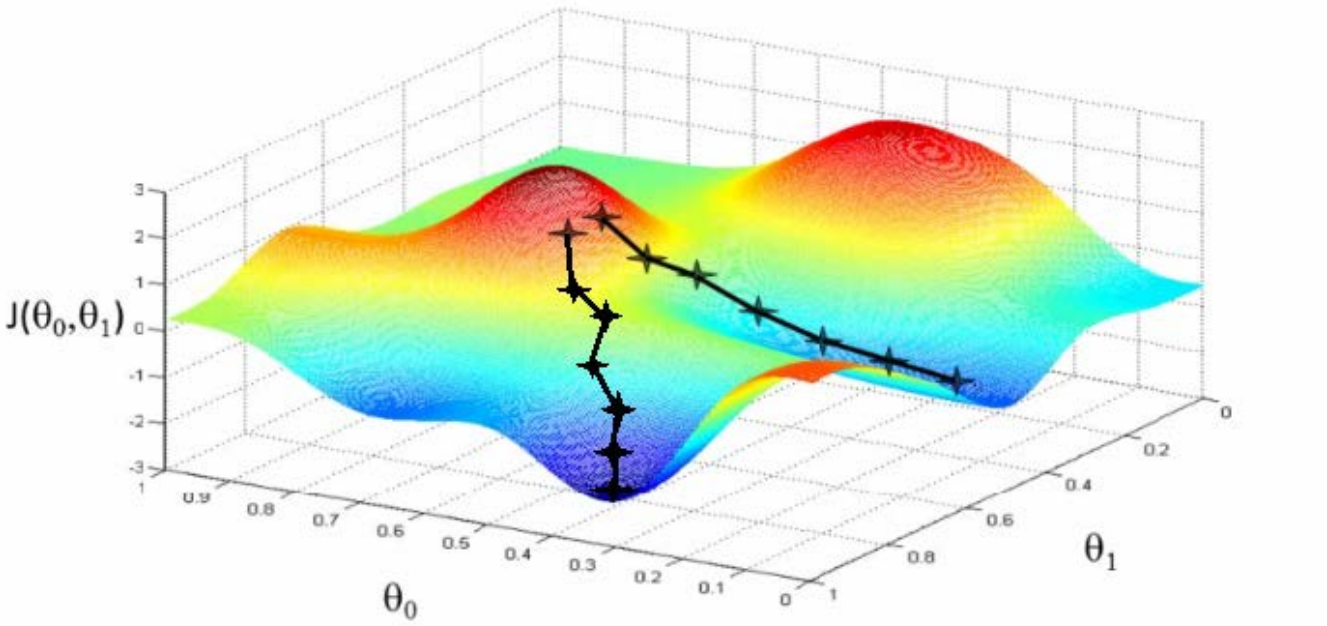
Local minima

Gradient descent can find only local minima



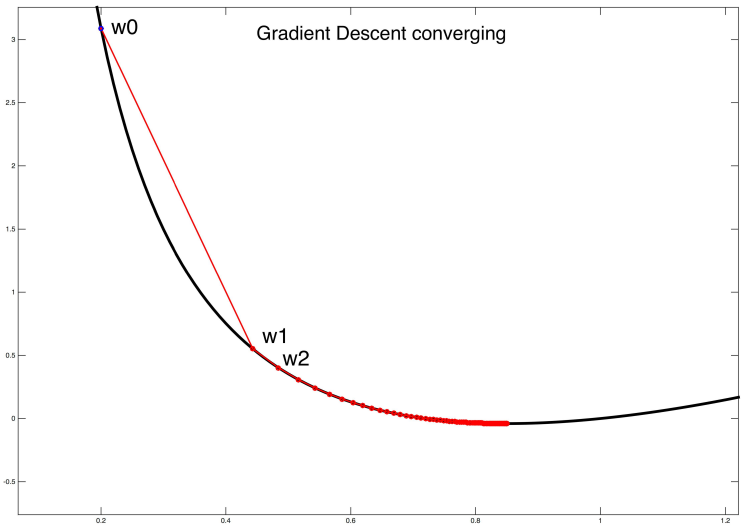
Local minima

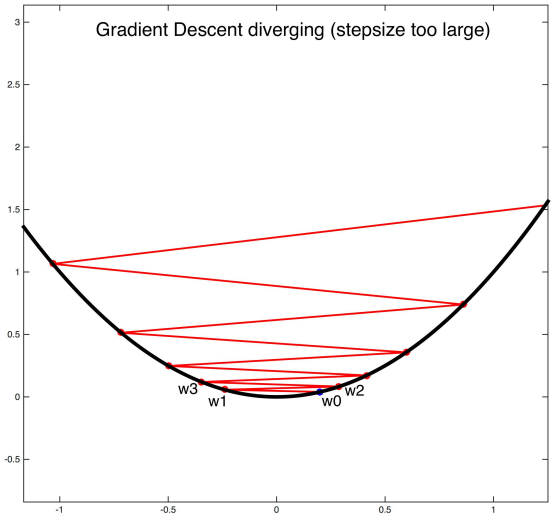
- The result depends on the initial approximation
- Multi-start



Size of step

- Choosing of the stepsize η is art





Size of step

- Small step - more chance of convergence, but required more iterations
- Big step - there is a risk of lack of convergence
- Steepest gradient descent:

$$\eta_t = arg\min_{\eta} Q(w^{t-1} - \eta \nabla Q(w^{t-1})$$

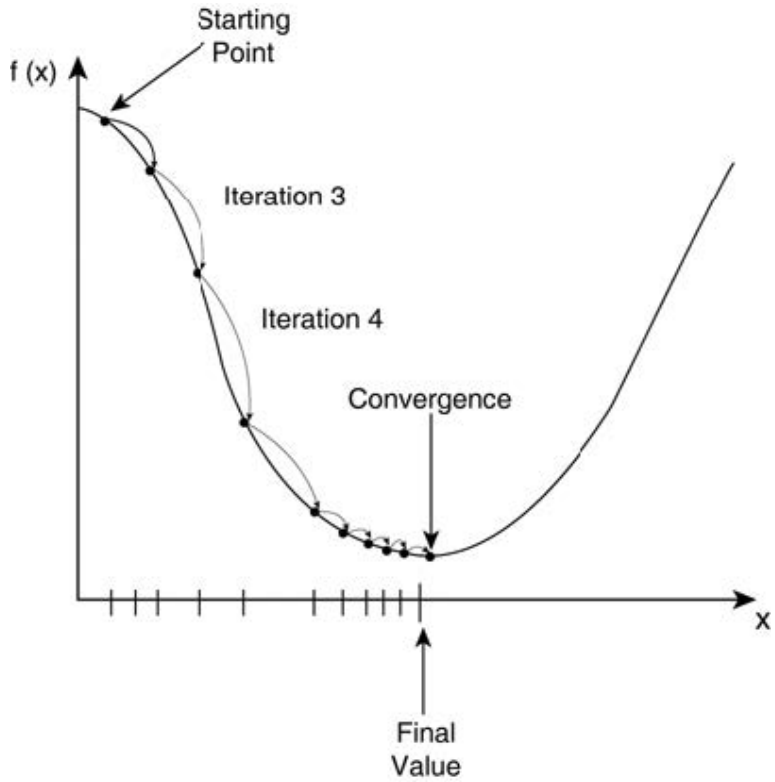
- It is necessary to do a one-dimensional search at each iteration

Size of step

- Usually use heuristics
- The closer to a minimum, the less it is necessary to tread
- Works well

$$\eta_t = \frac{1}{t}$$

- Even better: $\eta_t = \lambda \left(\frac{s}{s+t}\right)^p$



Other optimization methods

- First-order methods - use first derivatives
  - Gradient descent
  - Stochastic gradient descent
  - Quasi-Newtonian methods, BFGS
  - Stochastic Average Gradient, Nesterov momentum, ...
- Second-order methods - use second derivatives
  - The Newton method
- Zero-order methods - without derivatives
  - Coordinate descent
  - Stochastic optimization

Nuances in learning linear regressors

- Selecting the step length η - we try different values
- The sample must be scaled
- Features should not be correlated

An example

$$X = \begin{pmatrix} 1 & 1000 & 5 & 3 & 4 \\ 9 & 9000 & 10 & 5 & 7.5 \\ 5 & 5000 & 1 & 3 & 2 \end{pmatrix}$$

- The task of predicting the profit of the store in the next month
- Consider vectors of the matrix (features) as vectors

An example

$$X = \begin{pmatrix} 1 & 1000 & 5 & 3 & 4 \\ 9 & 9000 & 10 & 5 & 7.5 \\ 5 & 5000 & 1 & 3 & 2 \end{pmatrix}$$

- The first and second signs:$x_2 = 1000x_1$
- First - the total weight of goods in tonnes, the second - in kilograms
- $x_5 = 0.5x_3 + 0.5x_4$
- Fifth - average profit for the last two months
- Third and fourth - profit in the past and the year before last

Linear dependence

Linear dependence - one of the vectors is equal to the sum of the weights of the remaining vectors

- Redundant information
- Extra storage costs
- Damages some machine learning methods

Linear dependence

- Suppose we found a solution w^*
- Modify: $w_1 = w^* + t\alpha$, where t - a number such that:

$$\alpha_1 x_1 + \cdots + \alpha_d x_d = \langle \alpha, x \rangle = 0$$

- The worst case is linearly dependent features
- The answer of the new algorithm on any object:

$$\langle w_1, x \rangle = \langle w^* + t\alpha, x \rangle = \langle w^*, x \rangle + t\langle \alpha, x \rangle = \langle w^*, x \rangle$$

- w_1 is also s solution!

Correlating features

- Also bad!

$$\rho(\xi\eta) = \frac{\mathbb{E}(\xi - \xi)(\eta - \mathbb{E}\eta)}{\sqrt{\mathbb{D}\xi\mathbb{D}\eta}}$$

$$\rho(x, z) = \frac{\sum_{i=1}^{l}(x_i - \bar{x})(z_i - \bar{z})}{\sqrt{\sum_{i=1}^{l}(x_i - \bar{x})^2 \sum_{i=1}^{l}(z_i - \bar{z})^2}}$$

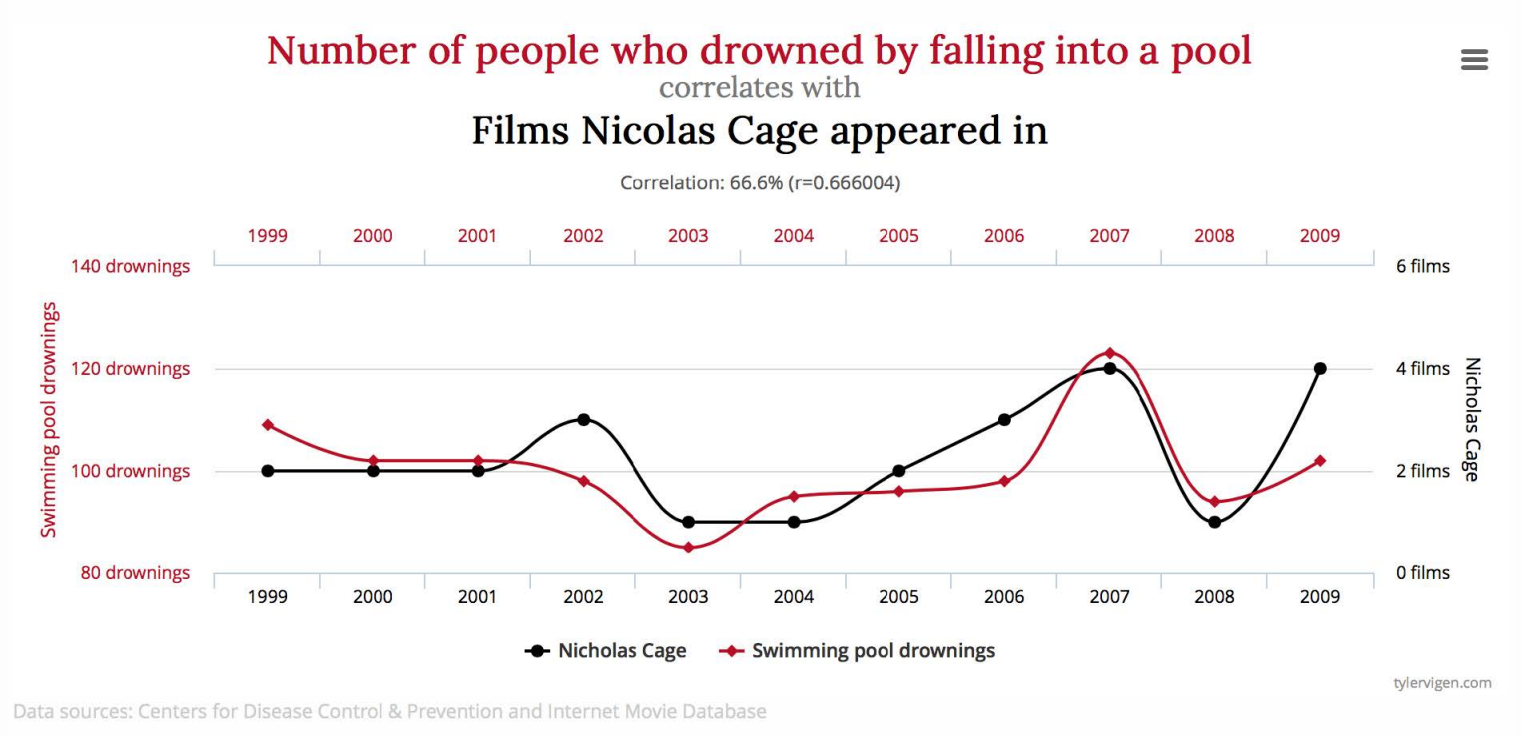
$$\bar{x} = \frac{1}{l}\sum_{j=1}^{l} x_j, \bar{z} = \frac{1}{l}\sum_{j=1}^{l} z_j$$

- $\rho(x, z) \in [-1, +1]$
- Very roughly: the closer to $+1$ or -1, the more accurately equation

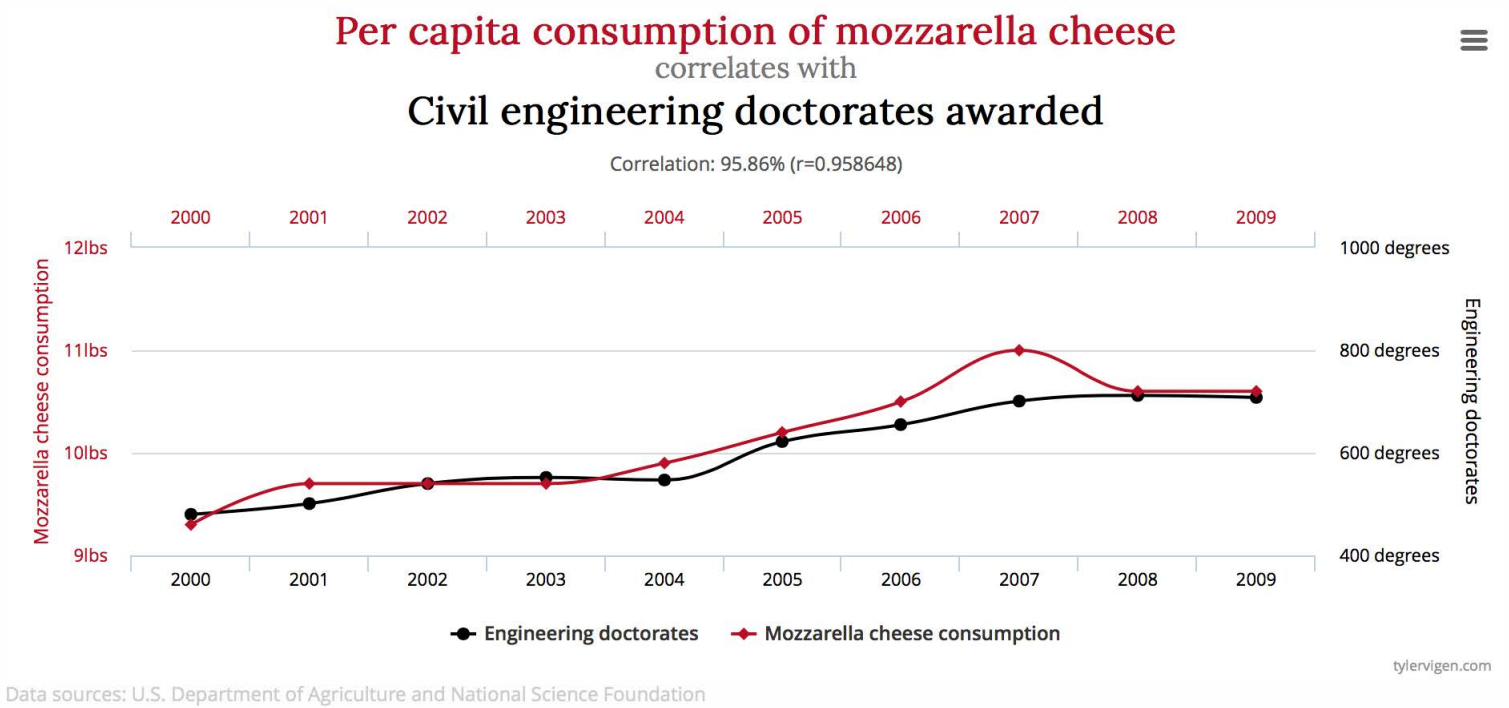
$$z = az + b$$

- The measure of linear dependence

Examples


Number of people who drowned by falling into a pool
correlates with
Films Nicolas Cage appeared in
Correlation: 66.6% (r=0.666004)
1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009
140 drownings
120 drownings
100 drownings
80 drownings
Swimming pool drownings
6 films
4 films
2 films
0 films
Nicholas Cage
Nicholas Cage
Swimming pool drownings
tylervigen.com
Data sources: Centers for Disease Control & Prevention and Internet Movie Database

Examples

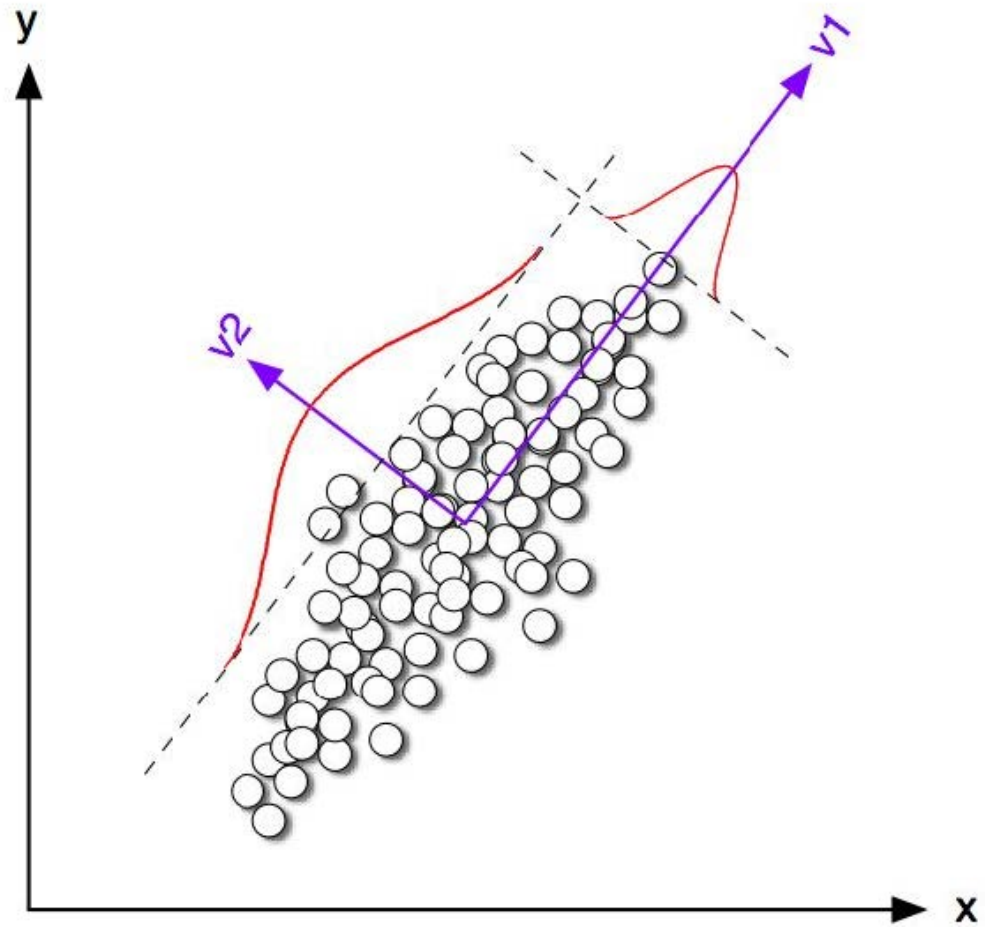

Per capita consumption of mozzarella cheese
correlates with
Civil engineering doctorates awarded
Correlation: 95.86% (r=0.958648)
2000 2001 2002 2003 2004 2005 2006 2007 2008 2009
12lbs
11lbs
10lbs
9lbs
Mozzarella cheese consumption
1000 degrees
800 degrees
600 degrees
400 degrees
Engineering doctorates
Engineering doctorates
Mozzarella cheese consumption
tylervigen.com
Data sources: U.S. Department of Agriculture and National Science Foundation

A common misconception

- It may seem that correlation follows a causal relationship
- This is not true!
- Correlation means that events often occur together
- But they do not follow each other in any way
- More examples: `http://tylervigen.com/spurious-correlations`

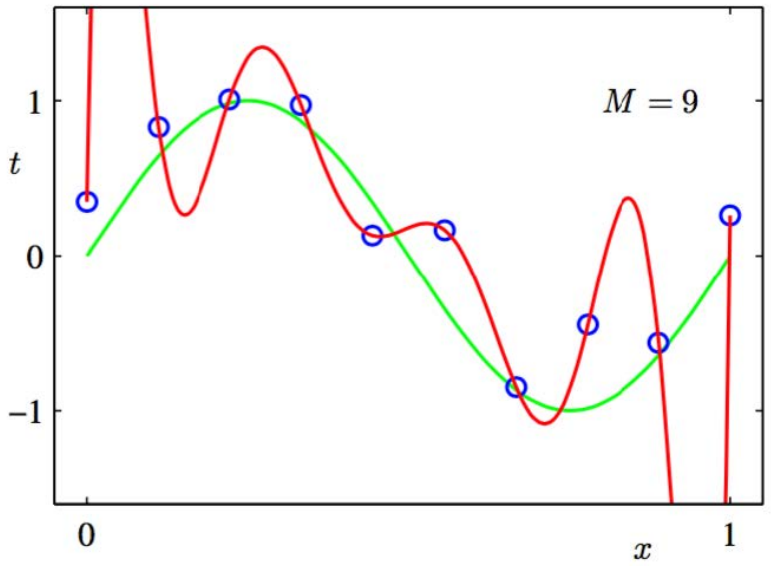
Correlating features

- It is bad if there are correlating signs
- Solution: selection of features or decorrelation



Correlating features

- One feature x
- $a(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w9x^9$



- Coefficients:

$$a(x) = 0.5 + 13458922x - 43983740x^2 + \cdots + 2740x^9$$

- Large coefficients - a symptom of retraining (empirical observation)

Regularization

- We will fine for the big weights!
- Functionality:

$$Q(w, x) = \frac{1}{l} \sum_{i=1}^{l} (\langle w, x_i \rangle - y_i)^2 \to \min_w$$

- Regularizer:

$$\|w\|^2 = \sum_{j=1}^{d} w_j^2$$

- The regularized error functional:

$$\frac{1}{l} \sum_{i=1}^{l} (\langle w, x_i \rangle - y_i)^2 + \lambda \|w\|^2 \to \min_w$$

- Still smooth and convex

Regularization

- λ - new parameter, it is necessary to select
- High λ - simple models
- Low λ - risk of retraining
- It is necessary to balance
- Selection of λ - using cross-validation

The meaning of regularization

- Minimization of a regularized functional is equivalent to solving a conditional problem:

$$\begin{cases} \frac{1}{l}\sum_{i=1}^{l}(\langle w, x_i\rangle - y_i)^2 + \lambda\|w\|^2 \to \min_w \\ \|w\|^2 \leq C \end{cases}$$

L_1 regularization

- L_1 regularizer:

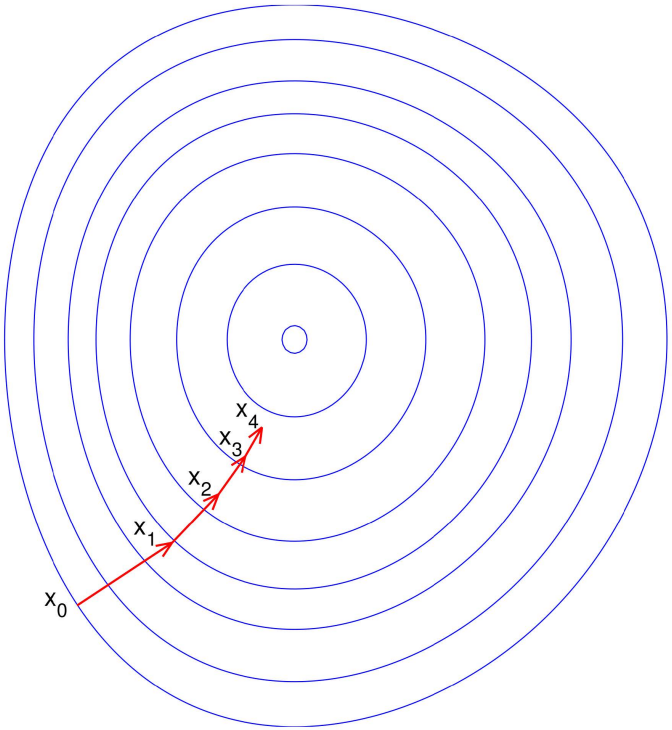
$$\|w\|_1 = \sum_{j=1}^{d} |w_j|$$

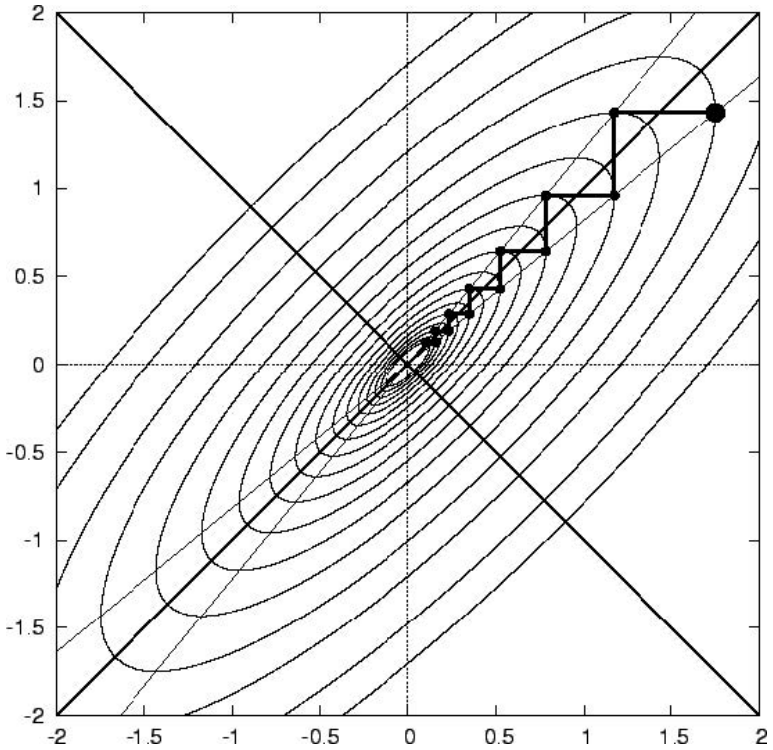
- The regularized error functional:

$$\frac{1}{l}\sum_{i=1}^{l}(\langle w, x_i\rangle - y_i)^2 + \lambda\|w\|_1 \to \min_w$$

- Functionality becomes non-smooth
- It is more difficult to optimize
- But the selection of characteristics
- Some of the weights in the solution will be zero

Scaling the sample





Scaling the sample

- Task: Will the grant application be approved?
- 1st feature: how many successful applications did the applicant have before
- 2nd feature: the year of birth of the applicant
- Scale: units and thousands
- All features must have the same scale

Scaling the sample

- We scale the j-th feature
- Calculate the mean and standard deviation of the trait on the training sample:

$$\mu_j = \frac{1}{l}\sum_{i=1}^{l} x_j^j$$

$$\sigma_j = \sqrt{\frac{1}{l}\sum_{i=1}^{l}(x_j^j - \mu_j)^2}$$

- We scale the j-th feature
- Subtract from each characteristic value the average and divide by the standard deviation:

$$x_i^j := \frac{x_i^j - \mu_j}{\sigma_j}$$