Numerical features

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- Throughout this lecture we assume that all features are numerical, i.e., feature vectors belong to $\mathbb{R}^n$.
- Most non-numerical features can be conveniently transformed to numerical ones.

  For example:

  - Colors $\{blue, red, yellow\}$ can be represented by

    $$\{(1,0,0),(0,1,0),(0,0,1)\}$$

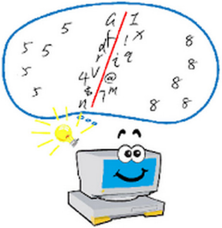
    (one-hot encoding)
  - Words can be embedded into vector spaces by various means (word2vec etc.)
  - A black-and-white picture of $x \times y$ pixels can be encoded as a vector of xy numbers that capture the shades of gray of the pixels.
    (Even though this is not the best way of representing images.)

Basic Problems

We consider two basic problems:

- (Binary) classification

  Our goal: Classify inputs into two categories.



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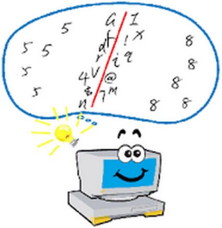

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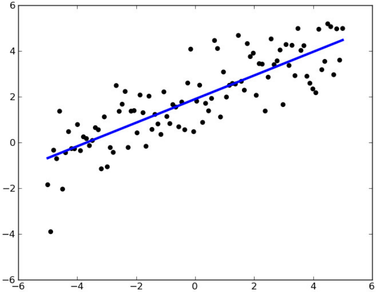

- Regressin

  Our goal: Find a (hypothesized) functional dependency in data.

Binary classification in $\mathbb{R}^n$

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- Given a set D of training examples of the form $(\vec{x}, c)$ where $\vec{x} \in \mathbb{R}^n$ and $c \in \{0, 1\}$,

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Comments:

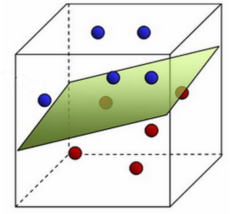
- In practice, we often do not strictly demand $h(\vec{x}) = c$ for all training examples $(\vec{x}, c) \in D$ (often it is impossible)
- We are more interested in good **generalization**, that is how well h classifies new instances that do not belong to D.

  (Recall that we usually evaluate accuracy of the resulting hypothesized function h on a test set.)

Hypothesis Spaces

We consider two kinds of hypothesis spaces:

- Linear (affine) classifiers (this lecture)



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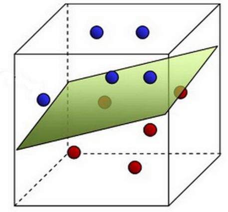
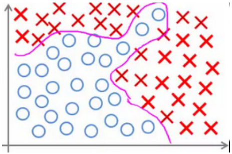
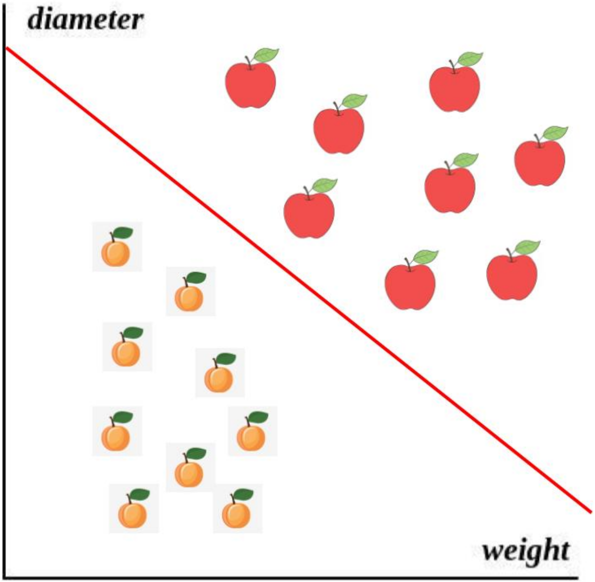


- Non-linear classifiers (kernel SVM, neural networks) (later lectures)



Linear Classifier – Example



Length and Scalar Product of Vectors

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- Euclidean metric on vectors: $||\vec{x}|| = \sqrt{\sum_{i=1}^{n} x_i^2}$
  The distance between two vectors (points) $\vec{x}, \vec{y}$ is $||\vec{x} - \vec{y}||$.

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  The distance between two vectors (points) $\vec{x}, \vec{y}$ is $||\vec{x} - \vec{y}||$.
- *Scalar product* $\vec{x} \cdot \vec{y}$ of vectors $\vec{x} = (x_1, \ldots, x_n)$ and $\vec{y} = (y_1, \ldots, y_n)$ defined by

$$\vec{x} \cdot \vec{y} = \sum_{i=1}^{n} x_i y_i$$

  - Recall that $\vec{x} \cdot \vec{y} = ||\vec{x}|| \, ||\vec{y}|| \cos\theta$ where θ is the angle between $\vec{x}$ and $\vec{y}$. That is $\vec{x} \cdot \vec{y}$ is the length of the projection of $\vec{y}$ on $\vec{x}$ multiplied by $||\vec{x}||$.
  - Note that $\vec{x} \cdot \vec{x} = ||\vec{x}||^2$

Linear Classifier

A *linear classifier* $h[\vec{w}]$ is determined by a vector of *weights* $\vec{w} = (w_0, w_1, \ldots, w_n) \in \mathbb{R}^{n+1}$ as follows:

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Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$,

$$h[\vec{w}](\vec{x}) := \begin{cases} 1 & w_0 + \sum_{i=1}^{n} w_i \cdot x_i \geq 0 \\ 0 & w_0 + \sum_{i=1}^{n} w_i \cdot x_i < 0 \end{cases}$$

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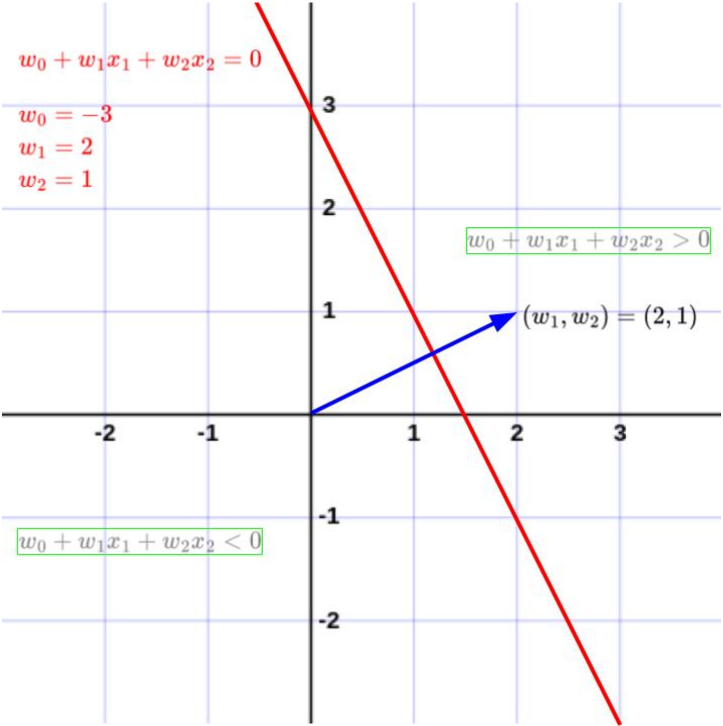
More succinctly:

$$h(\vec{x}) = sgn\left(w_0 + \sum_{i=1}^{n} w_i \cdot x_i\right) \qquad \text{where} \qquad sgn(y) = \begin{cases} 1 & y \geq 0 \\ 0 & y < 0 \end{cases}$$

We define separating hyperplane determined by $\vec{w}$ as the set of all $\vec{x} \in \mathbb{R}^n$ satisfying $w_0 + \sum_{i=1}^{n} w_i \cdot x_i = 0$.



$w_0 + w_1x_1 + w_2x_2 = 0$
$w_0 = -3$
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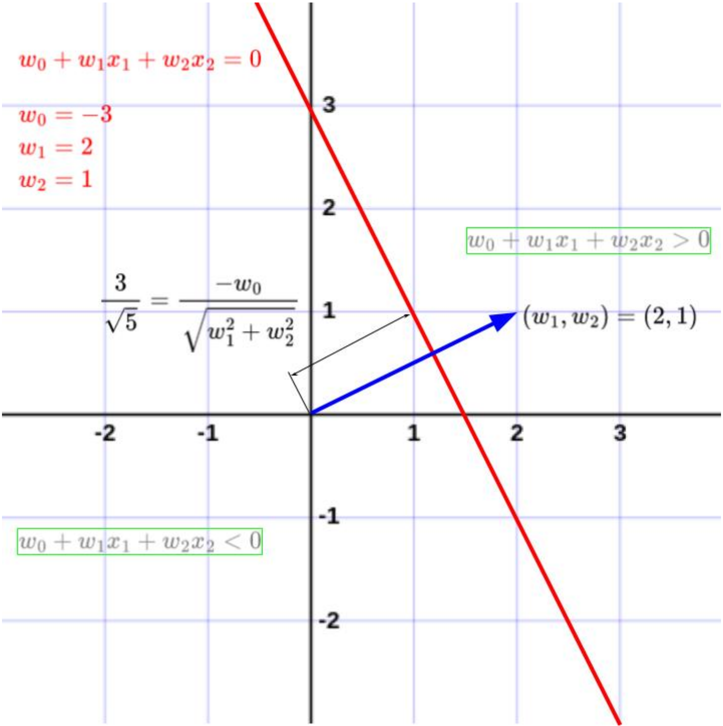
$w_2 = 1$
$w_0 + w_1x_1 + w_2x_2 > 0$
$(w_1, w_2) = (2, 1)$
$w_0 + w_1x_1 + w_2x_2 < 0$
3
2
1
-1
-2
-2
-1
1
2
3



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$\frac{3}{\sqrt{5}} = \frac{-w_0}{\sqrt{w_1^2 + w_2^2}}$
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2
1
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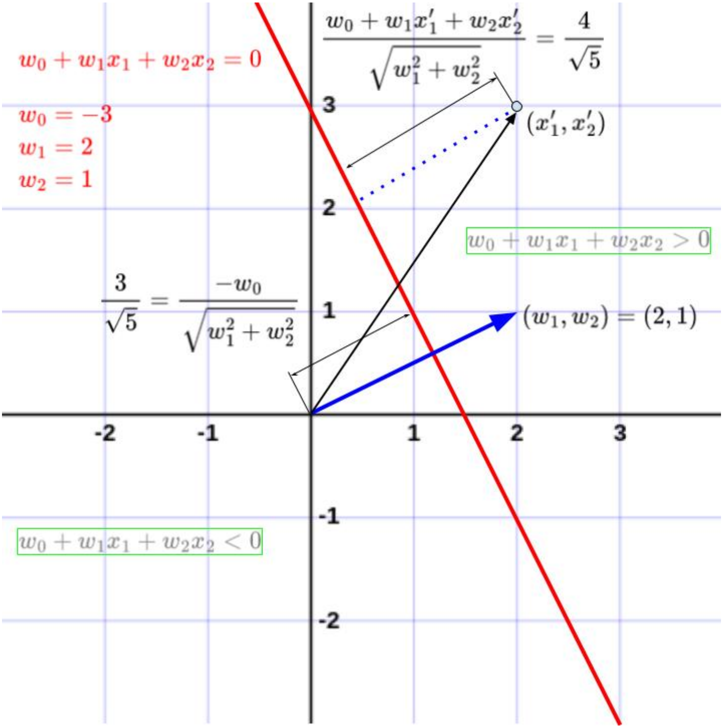

$w_0 + w_1 x_1 + w_2 x_2 = 0$
$w_0 = -3$
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$\frac{w_0 + w_1 x_1' + w_2 x_2'}{\sqrt{w_1^2 + w_2^2}} = \frac{4}{\sqrt{5}}$
(x_1', x_2')
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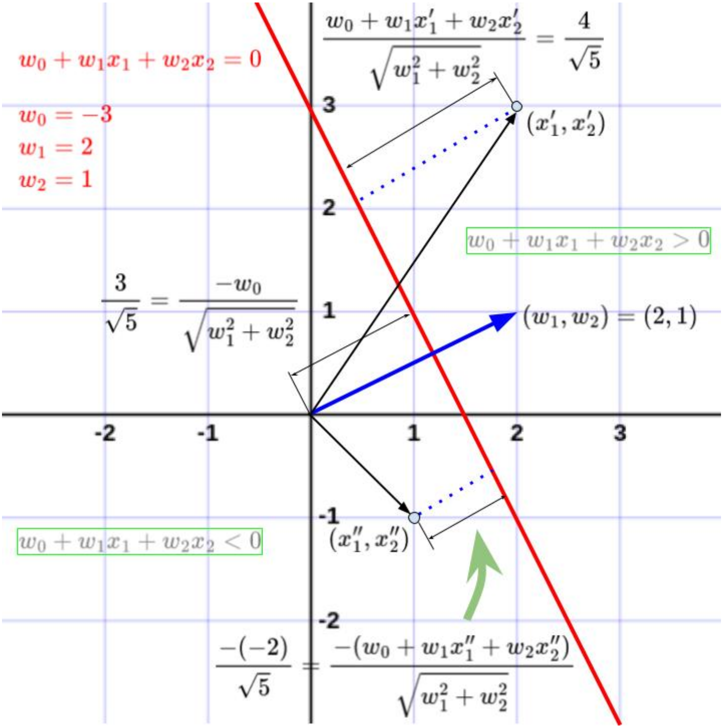

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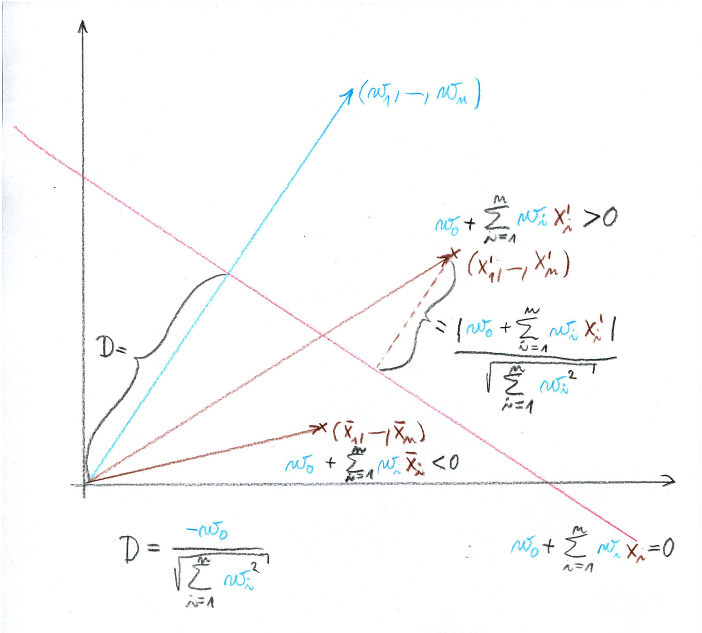
-2
-1
1
2
3

Linear Classifier – Geometry



Linear Classifier – Notation

Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ we define an *augmented feature vector*

$$\tilde{x} = (x_0, x_1, \ldots, x_n) \quad \text{where } x_0 = 1$$

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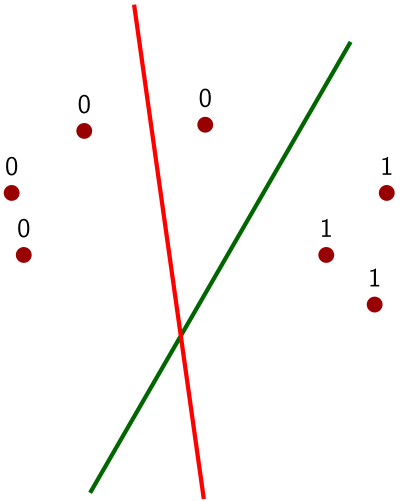
Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ we define an *augmented feature vector*

$$\tilde{\mathrm{x}} = (x_0, x_1, \ldots, x_n) \quad \text{where } x_0 = 1$$

This makes the notation for the linear classifier more succinct:

$$h[\vec{w}](\vec{x}) = sgn(\vec{w} \cdot \tilde{\mathrm{x}})$$

Linear Classifier – Learning



- classification in the plane using a linear classifier
- if a point is incorrectly classified, the learning algorithm turns the line (hyperplane) to improve the classification

Perceptron Learning

- Given a training set

$$D = \{(\vec{x}_1, c_1), (\vec{x}_2, c_2)), \ldots, (\vec{x}_p, c_p))\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in \mathbb{R}^n$ and $c_k \in \{0, 1\}$.

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- A weight vector $\vec{w} \in \mathbb{R}^{n+1}$ is **consistent with** D if

$$h[\vec{w}](\vec{x}_k) = sgn(\vec{w} \cdot \tilde{\mathrm{x}}_k) = c_k \qquad \text{for all } k = 1, \ldots, p$$

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D is **linearly separable** if there is a vector $\vec{w} \in \mathbb{R}^{n+1}$ which is consistent with D.

- Our goal is to find a consistent $\vec{w}$ assuming that D is linearly separable.

Perceptron – Learning Algorithm

Online learning algorithm:

Idea: Cyclically go through the training examples in D and adapt weights. Whenever an example is incorrectly classified, turn the hyperplane so that the example becomes closer to it's correct half-space.

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- In $(t+1)$-th step, $\vec{w}^{(t+1)}$ is computed as follows:

$$\vec{w}^{(t+1)} \;=\; \vec{w}^{(t)} - \varepsilon \cdot \left(h[\vec{w}^{(t)}](\vec{x}_k) - c_k \right) \cdot \tilde{\mathrm{x}}_k$$

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  Here $k = (t \mod p) + 1$, i.e., the examples are considered cyclically, and $0 < \varepsilon \leq 1$ is a **learning rate**.

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Theorem (Rosenblatt)

If D is linearly separable, then there is t^* such that $\vec{w}^{(t^*)}$ is consistent with D.

Example

Training set:

$$D = \{((2,-1),1),((2,1),1),((1,3),0)\}$$

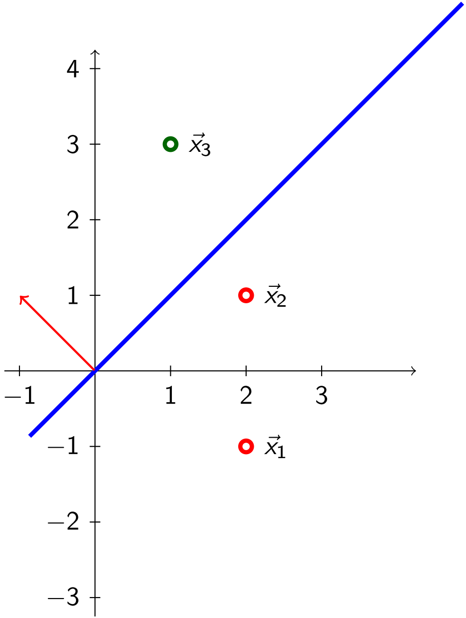
That is

$$\vec{x}_1 = (2,-1) \qquad \tilde{x}_1 = (1,2,-1)$$
$$\vec{x}_2 = (2,1) \qquad \tilde{x}_2 = (1,2,1)$$
$$\vec{x}_3 = (1,3) \qquad \tilde{x}_3 = (1,1,3)$$

$$c_1 = 1$$
$$c_2 = 1$$
$$c_3 = 0$$

Assume that the initial vector $\vec{w}^{(0)}$ is $\vec{w}^{(0)} = (0,-1,1)$.
Consider $\varepsilon = 1$.

Example: Separating by $\vec{w}^{(0)}$



Denoting $\vec{w}^{(0)} = (w_0, w_1, w_2) = (0, -1, 1)$ the blue separating line is given by $w_0 + w_1 x_1 + w_2 x_2 = 0$.

The red vector normal to the blue line is (w_1, w_2).

The points on the side of (w_1, w_2) are assigned 1 by the classifier, the others zero. (In this case $\vec{x}_3$ is assigned one and $\vec{x}_1, \vec{x}_2$ are assigned zero, all of this is inconsistent with $c_1 = 1, c_2 = 1, c_3 = 0$.)

Example: Computing $\vec{w}^{(1)}$

We have

$$\vec{w}^{(0)} \cdot \tilde{\mathrm{x}}_1 = (0, -1, 1) \cdot (1, 2, -1) = 0 - 2 - 1 = -3$$

thus

$$sgn\left(\vec{w}^{(0)} \cdot \tilde{\mathrm{x}}_1\right) = 0$$

and thus

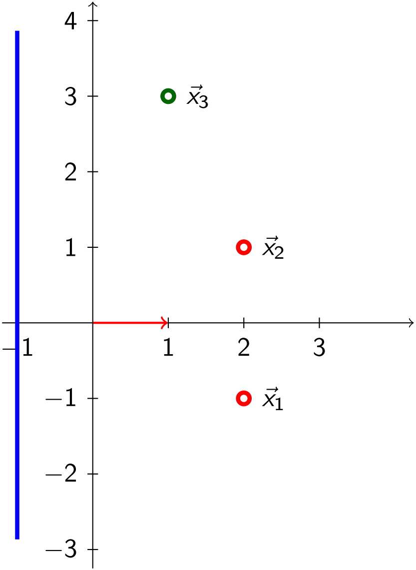
$$sgn\left(\vec{w}^{(0)} \cdot \tilde{\mathrm{x}}_1\right) - c_1 = 0 - 1 = -1$$

(I.e., $\vec{x}_1$ is not correctly classified, and $\vec{w}^{(0)}$ is not consistent with D.)

Hence,

$$\begin{aligned} \vec{w}^{(1)} &= \vec{w}^{(0)} - \left(sgn\left(\vec{w}^{(0)} \cdot \tilde{\mathrm{x}}_1\right) - c_1\right) \cdot \tilde{\mathrm{x}}_1 \\ &= \vec{w}^{(0)} + \tilde{\mathrm{x}}_1 \\ &= (0, -1, 1) + (1, 2, -1) \\ &= (1, 1, 0) \end{aligned}$$

Example: Separating by $\vec{w}^{(1)}$



Example: Computing $\vec{w}^{(2)}$

We have

$$\vec{w}^{(1)} \cdot \tilde{\mathrm{x}}_2 = (1,1,0) \cdot (1,2,1) = 1 + 2 = 3$$

thus

$$sgn\left(\vec{w}^{(1)} \cdot \tilde{\mathrm{x}}_2\right) = 1$$

and thus

$$sgn\left(\vec{w}^{(1)} \cdot \tilde{\mathrm{x}}_2\right) - c_2 = 1 - 1 = 0$$

(I.e., $\vec{x}_2$ *is* currently correctly classified by $\vec{w}^{(1)}$. However, as we will see, $\vec{x}_3$ is not well classified.)

Hence,

$$\vec{w}^{(2)} = \vec{w}^{(1)} = (1,1,0)$$

Example: Computing $\vec{w}^{(3)}$

We have

$$\vec{w}^{(2)} \cdot \tilde{x}_3 = (1,1,0) \cdot (1,1,3) = 1 + 1 = 2$$

thus

$$sgn\left(\vec{w}^{(2)} \cdot \tilde{x}_3\right) = 1$$

and thus

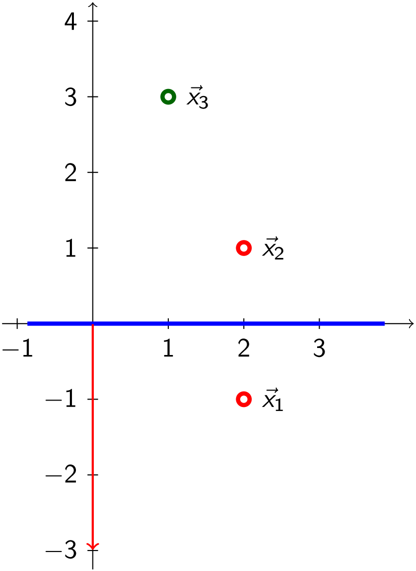
$$sgn\left(\vec{w}^{(2)} \cdot \tilde{x}_3\right) - c_3 = 1 - 0 = 1$$

(This means that $\vec{x}_3$ is not well classified, and $\vec{w}^{(2)}$ is not consistent with D.)

Hence,

$$\begin{aligned}
\vec{w}^{(3)} &= \vec{w}^{(2)} - \left(sgn\left(\vec{w}^{(2)} \cdot \tilde{x}_3\right) - c_3\right) \cdot \tilde{x}_3 \\
&= \vec{w}^{(2)} - \tilde{x}_3 \\
&= (1,1,0) - (1,1,3) \\
&= (0,0,-3)
\end{aligned}$$

Example: Separating by $\vec{w}^{(3)}$



Example: Computing $\vec{w}^{(4)}$

We have

$$\vec{w}^{(3)} \cdot \tilde{x}_1 = (0, 0, -3) \cdot (1, 2, -1) = 3$$

thus

$$sgn\left(\vec{w}^{(3)} \cdot \tilde{x}_1\right) = 1$$

and thus

$$sgn\left(\vec{w}^{(3)} \cdot \tilde{x}_1\right) - c_1 = 1 - 1 = 0$$

(I.e., $\vec{x}_1$ *is* currently correctly classified by $\vec{w}^{(3)}$. However, we shall see that $\vec{x}_2$ is not.)

Hence,

$$\vec{w}^{(4)} = \vec{w}^{(3)} = (0, 0, -3)$$

Example: Computing $\vec{w}^{(5)}$

We have

$$\vec{w}^{(4)} \cdot \tilde{x}_2 = (0, 0, -3) \cdot (1, 2, 1) = -3$$

thus

$$sgn\left(\vec{w}^{(4)} \cdot \tilde{x}_2\right) = 0$$

and thus

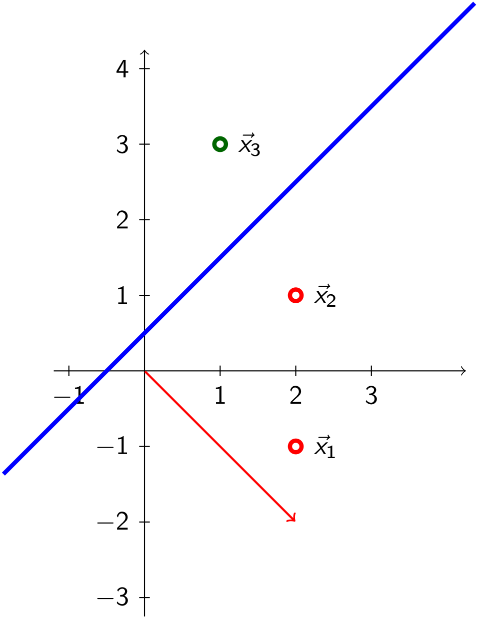
$$sgn\left(\vec{w}^{(4)} \cdot \tilde{x}_2\right) - c_2 = 0 - 1 = -1$$

(I.e., $\vec{x}_2$ is not correctly classified, and $\vec{w}^{(4)}$ is not consistent with D.)

Hence,

$$\begin{aligned}
\vec{w}^{(5)} &= \vec{w}^{(4)} - \left(sgn\left(\vec{w}^{(4)} \cdot \tilde{x}_2\right) - c_2\right) \cdot \tilde{x}_2 \\
&= \vec{w}^{(4)} + \tilde{x}_2 \\
&= (0, 0, -3) + (1, 2, 1) \\
&= (1, 2, -2)
\end{aligned}$$

Example: Separating by $\vec{w}^{(5)}$



Example: The result

The vector $\vec{w}^{(5)}$ is consistent with D:

$$sgn\left(\vec{w}^{(5)} \cdot \tilde{\mathrm{x}}_1\right) = sgn\left((1, 2, -2) \cdot (1, 2, -1)\right) = sgn(7) = 1 = c_1$$

$$sgn\left(\vec{w}^{(5)} \cdot \tilde{\mathrm{x}}_2\right) = sgn\left((1, 2, -2) \cdot (1, 2, 1)\right) = sgn(3) = 1 = c_2$$

$$sgn\left(\vec{w}^{(5)} \cdot \tilde{\mathrm{x}}_3\right) = sgn\left((1, 2, -2) \cdot (1, 1, 3)\right) = sgn(-3) = 0 = c_3$$

Perceptron – Learning Algorithm

Batch learning algorithm:

Compute a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

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Here $0 < \varepsilon \leq 1$ is a **learning rate**.

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Linear Regression – Oaks in Wisconsin

This example is from *How to Lie with Statistics* by Darrell Huff (1954)

Age (years)	*DBH* (inch)
97	12.5
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15	1.5
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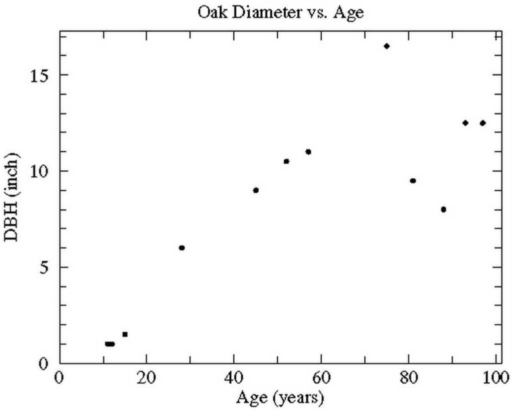

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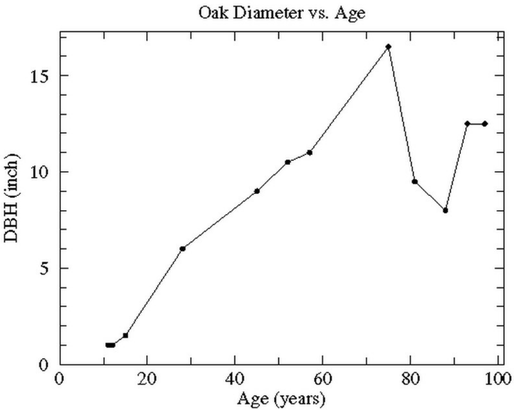

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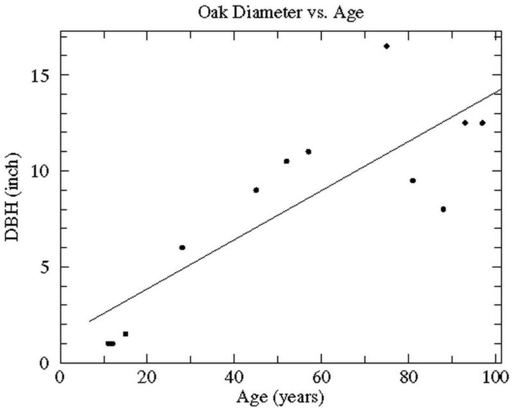

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In what follows we use the *squared error* defined by

$$E = \frac{1}{2} \sum_{(\vec{x},f) \in D} \left(h(\vec{x}) - f\right)^2$$

Our goal is to minimize E.

The main reason is that this function has nice mathematical properties (as opposed, e.g., to $\sum_{(\vec{x},f) \in D} |h(\vec{x}) - f|$).

Linear Function Approximation

- Given a set D of training examples:

$$D = \{(\vec{x}_1, f_1), (\vec{x}_2, f_2), \ldots, (\vec{x}_p, f_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in \mathbb{R}^n$ and $f_k \in \mathbb{R}$.

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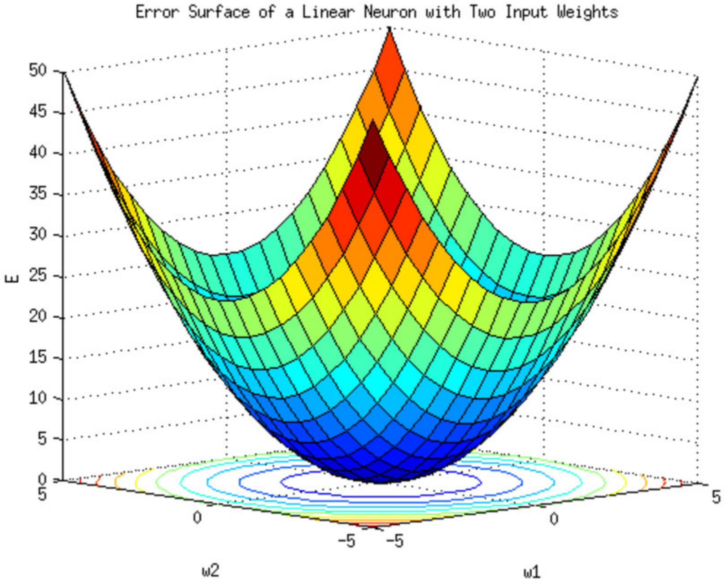
- **Squared Error Function:**

$$E(\vec{w}) = \frac{1}{2} \sum_{k=1}^{p} (\vec{w} \cdot \tilde{\mathrm{x}}_k - f_k)^2 = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=0}^{n} w_i x_{ki} - f_k \right)^2$$

Error function



Gradient of the Error Function

Consider the **gradient** of the error function:

$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w}) \right) = \sum_{k=1}^{p} (\vec{w} \cdot \tilde{\mathrm{x}}_k - f_k) \cdot \tilde{\mathrm{x}}_k$$

What is the gradient $\nabla E(\vec{w})$? It is a vector in $\mathbb{R}^{n+1}$ which points in the direction of the steepest *ascent* of E (it's length corresponds to the steepness). Note that here the vectors $\tilde{\mathrm{x}}_k$ are *fixed* parameters of E!

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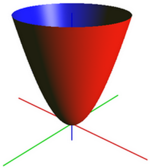
Fakt

If $\nabla E(\vec{w}) = \vec{0} = (0, \ldots, 0)$*, then* $\vec{w}$ *is a global minimum of* E*.*

This follows from the fact that E is a convex paraboloid that has a unique extreme which is a minimum.



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Consider $n = 1$, which means that $\vec{w} = (w_0, w_1)$ and we write x instead of $\vec{x}$ since $\vec{x} \in \mathbb{R}^n = \mathbb{R}^1 = \mathbb{R}$.

Then the model is $h[\vec{w}](x) = w_0 + w_1 \cdot x$.

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$$\begin{aligned} \mathcal{T} &= \{(2, 1), (3, 2), (4, 5)\} \\ &= \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} \end{aligned}$$

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Here $0 < \varepsilon \leq 1$ is a learning rate.

Note that the algorithm is almost similar to the batch perceptron algorithm!

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Tvrzení

For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (component-wisely) to the global minimum of E.

Training set:

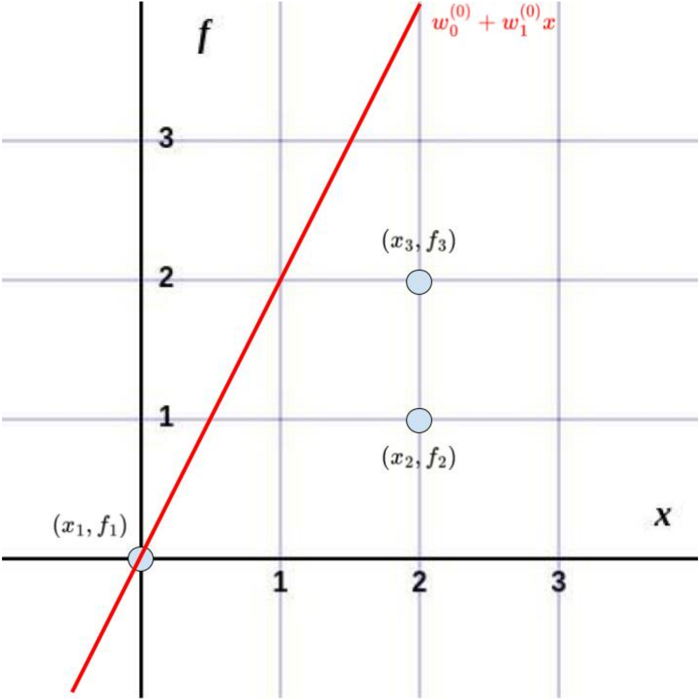
$$D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0,0), (2,1), (2,2)\}$$

Note that input vectors are one dimensional, so we write them as numbers.
That is

$$x_1 = 0 \qquad \tilde{x}_1 = (1, 0)$$
$$x_2 = 2 \qquad \tilde{x}_2 = (1, 2)$$
$$x_3 = 2 \qquad \tilde{x}_3 = (1, 2)$$

$$f_1 = 0$$
$$f_2 = 1$$
$$f_3 = 2$$

Assume that the initial vector $\vec{w}^{(0)}$ is $\vec{w}^{(0)} = (w_0^{(0)}, w_1^{(0)}) = (0, 2)$.
Consider $\varepsilon = \frac{1}{10}$.



$w_0^{(0)} + w_1^{(0)} x$
f
3
2
1
(x_3, f_3)
(x_2, f_2)
(x_1, f_1)
x
1
2
3

Training set: $D = \{(x_1, f_1), (x_2, f_2), (x_3, f_3)\} = \{(0,0), (2,1), (2,2)\}$
Augmented input vectors: $\tilde{\mathrm{x}}_1 = (1,0)$, $\tilde{\mathrm{x}}_2 = (1,2)$, $\tilde{\mathrm{x}}_1 = (1,2)$

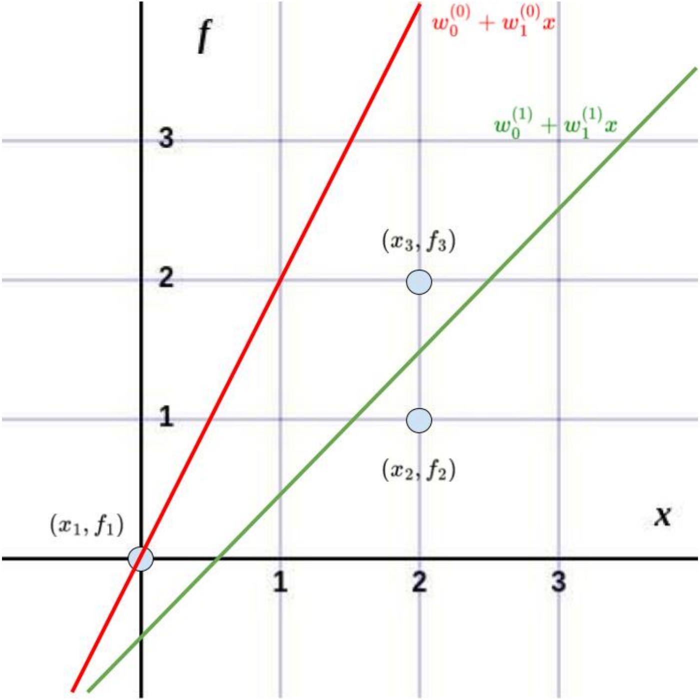
$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \frac{\partial E}{\partial w_1}(\vec{w})\right) = (w_0 + w_1 \cdot x_1 - f_1) \cdot \tilde{\mathrm{x}}_1 + (w_0 + w_1 \cdot x_2 - f_2) \cdot \tilde{\mathrm{x}}_2 + (w_0 + w_1 \cdot x_3 - f_3) \cdot \tilde{\mathrm{x}}_3$$

For $\vec{w}^{(0)} = (0,2)$ we have

$$\nabla E(\vec{w}^{(0)}) = (0 + 2 \cdot 0 - 0) \cdot (1,0) + (0 + 2 \cdot 2 - 1) \cdot (1,2) + (0 + 2 \cdot 2 - 2) \cdot (1,2) = (3,6) + (2,4) = (5,10)$$

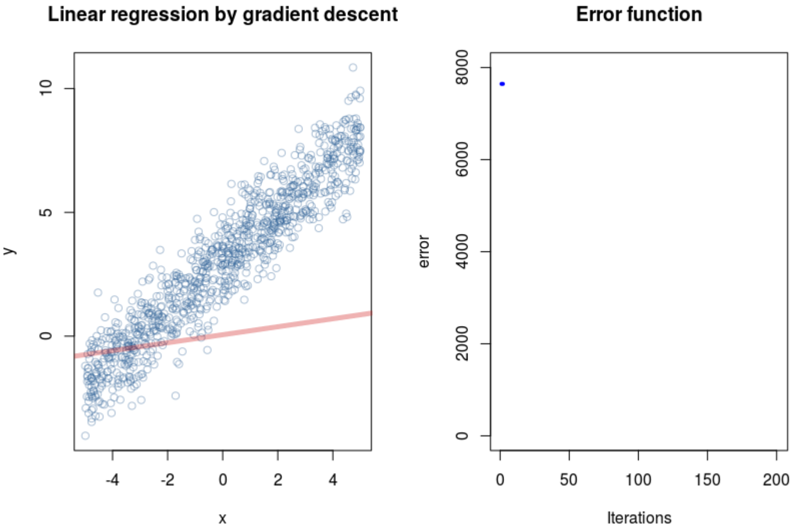
Finally, $\vec{w}^{(1)}$ is computed by

$$\vec{w}^{(1)} = \vec{w}^{(0)} - \varepsilon \cdot \nabla E(\vec{w}^{(0)}) = (0,2) - \frac{1}{10} \cdot (5,10) = (-1/2, 1)$$

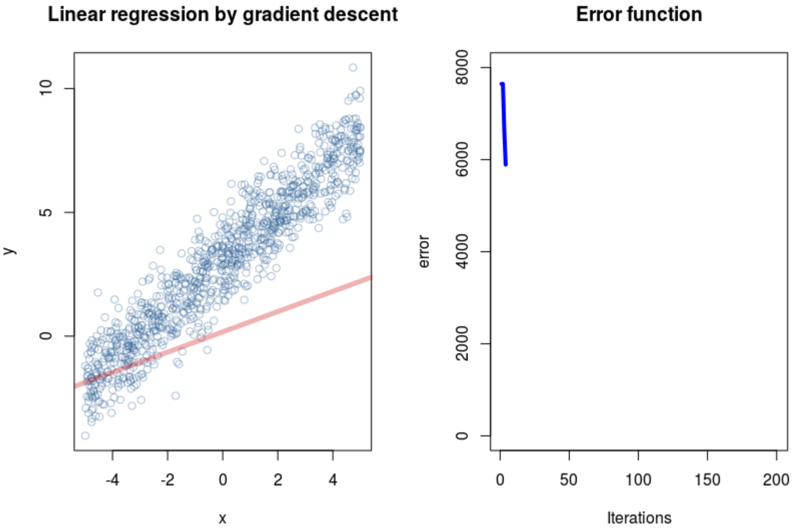


f
$w_0^{(0)} + w_1^{(0)}x$
$w_0^{(1)} + w_1^{(1)}x$
3
2
1
(x_3, f_3)
(x_2, f_2)
(x_1, f_1)
x
1
2
3

Linear Regression - Animation



Linear Regression - Animation



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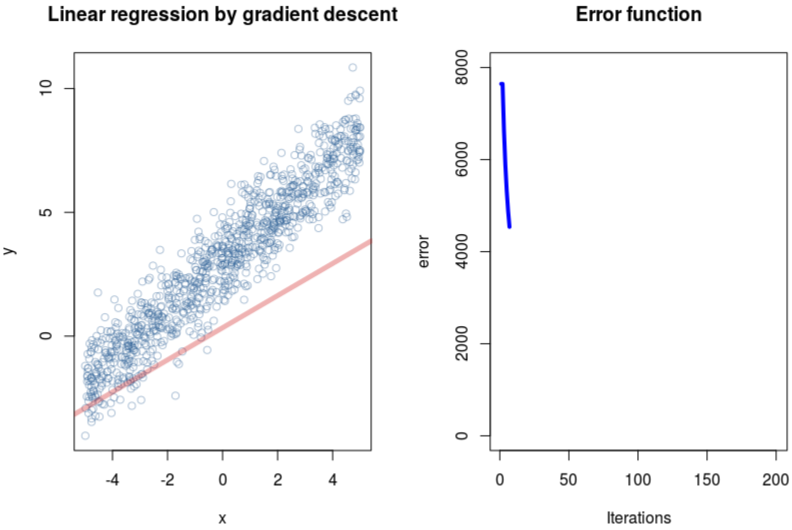
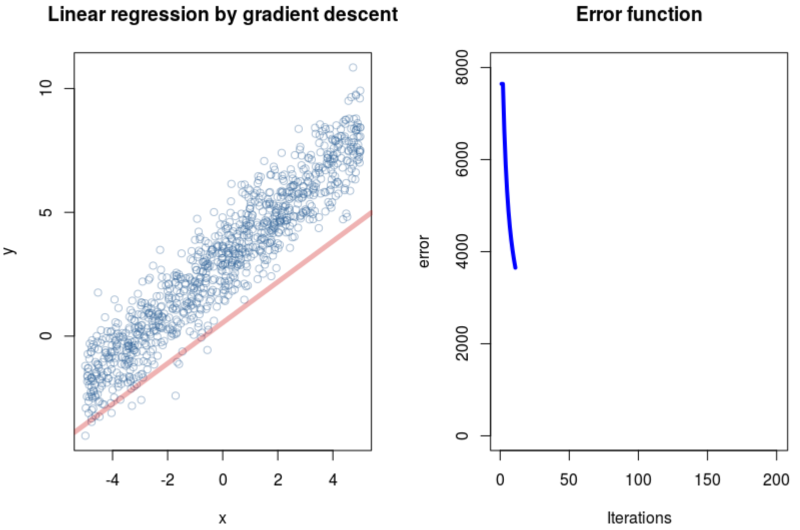


Linear Regression - Animation



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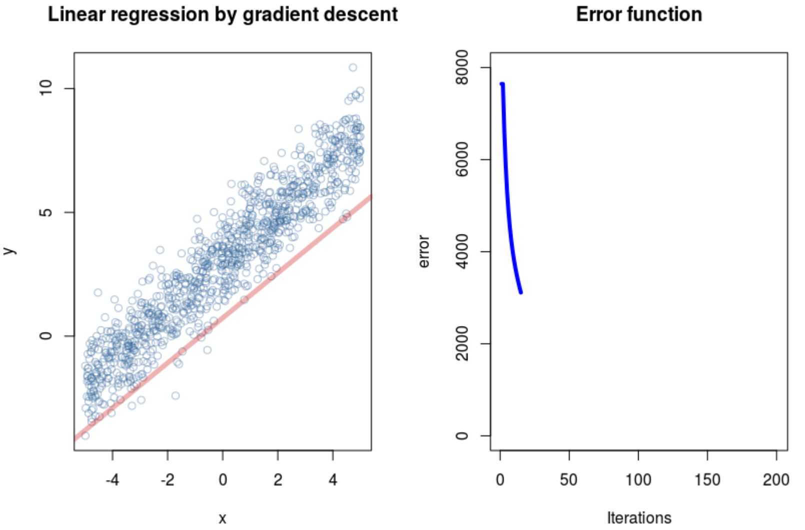

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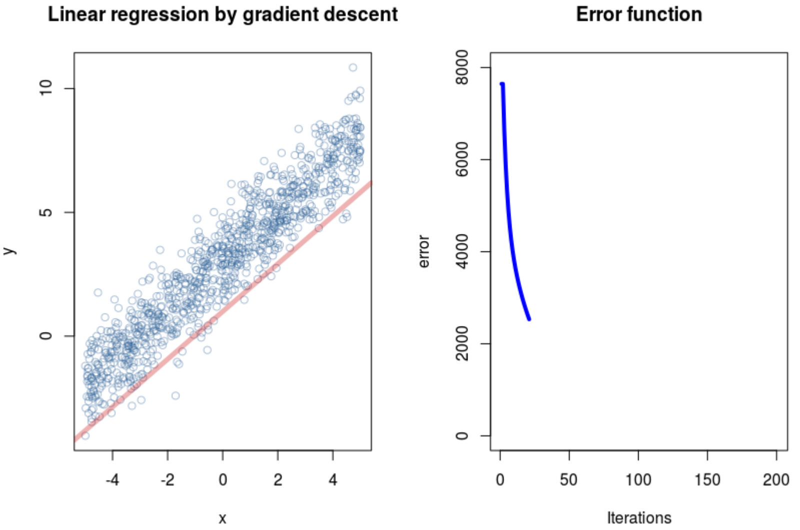

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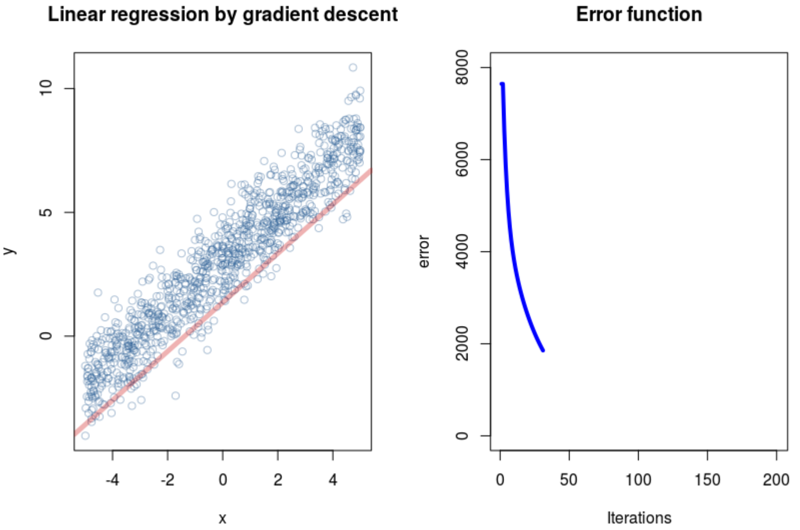

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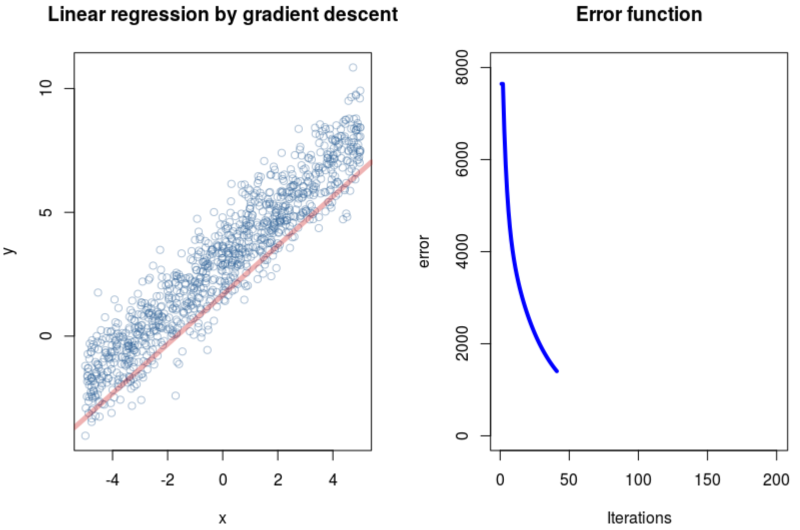

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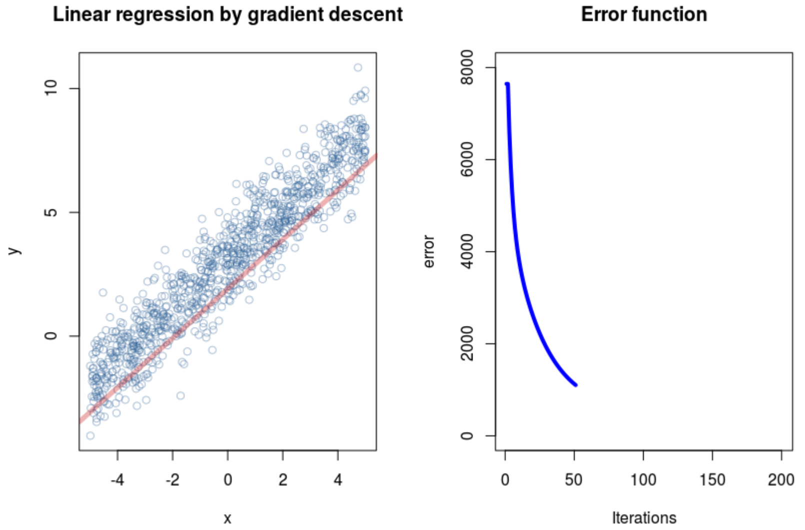

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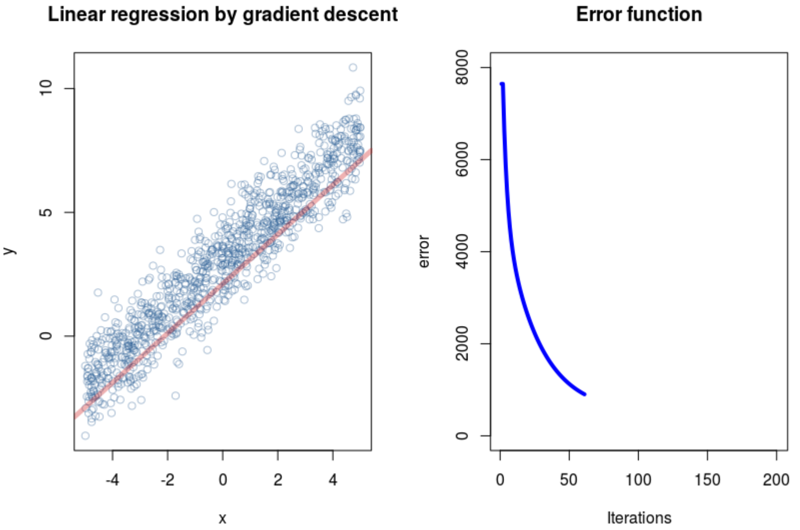

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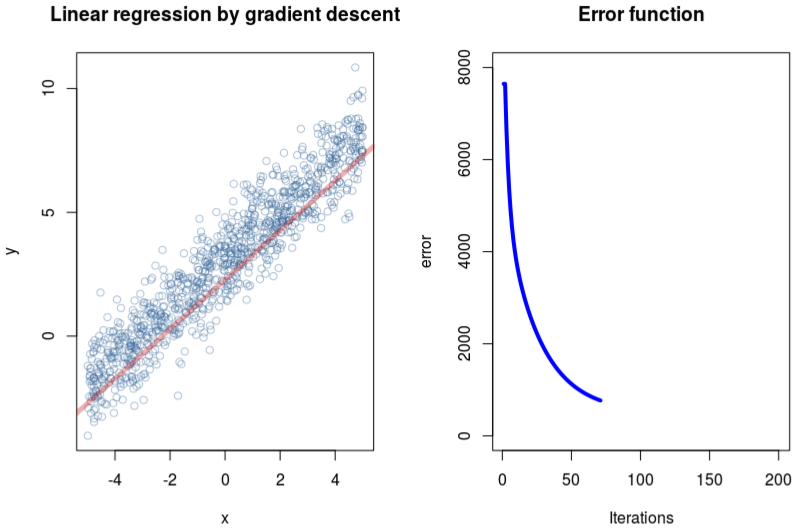

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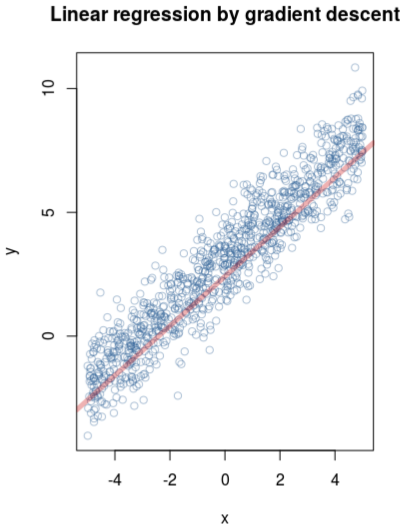

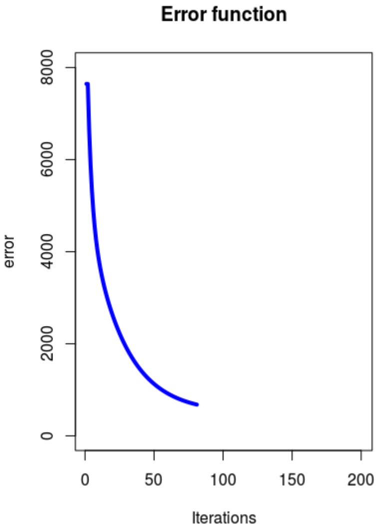

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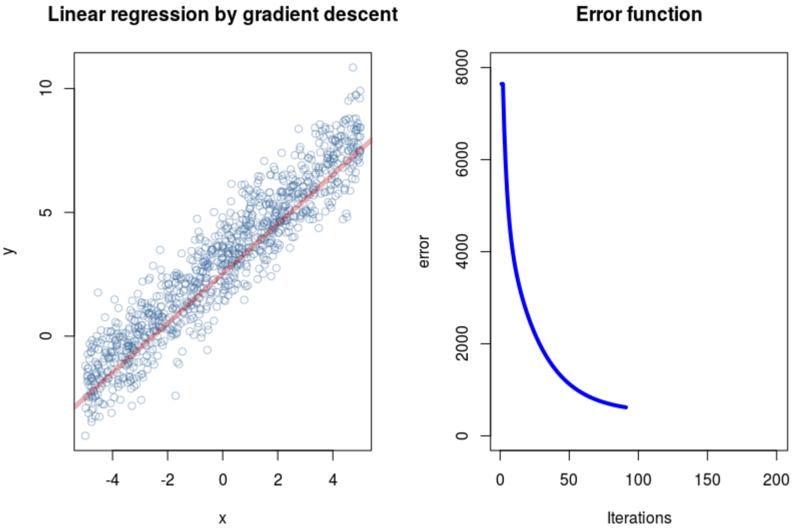

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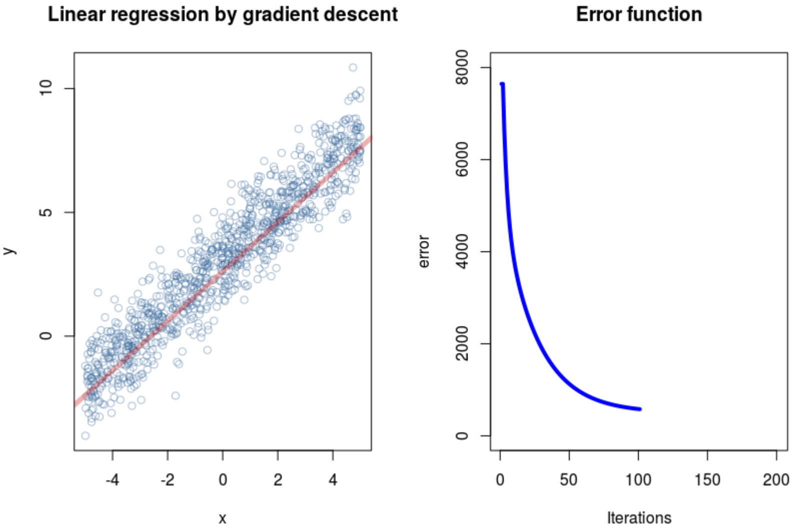

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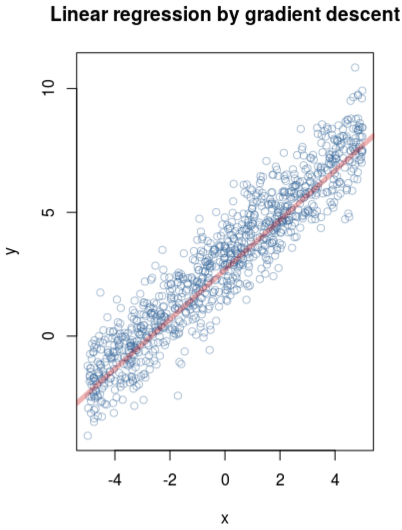

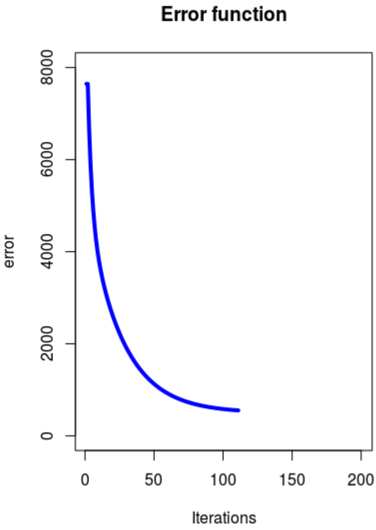

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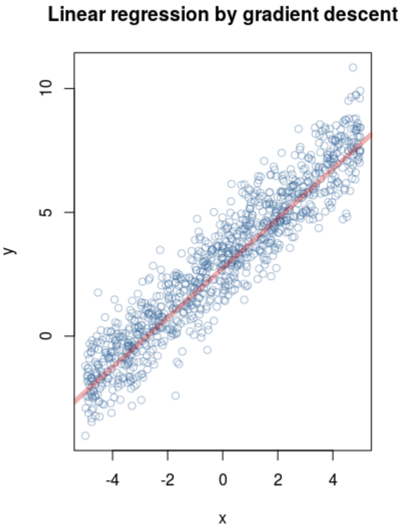

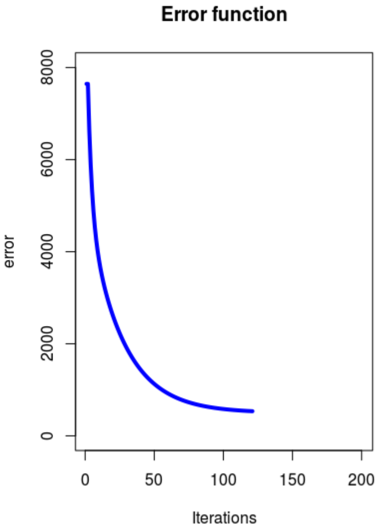

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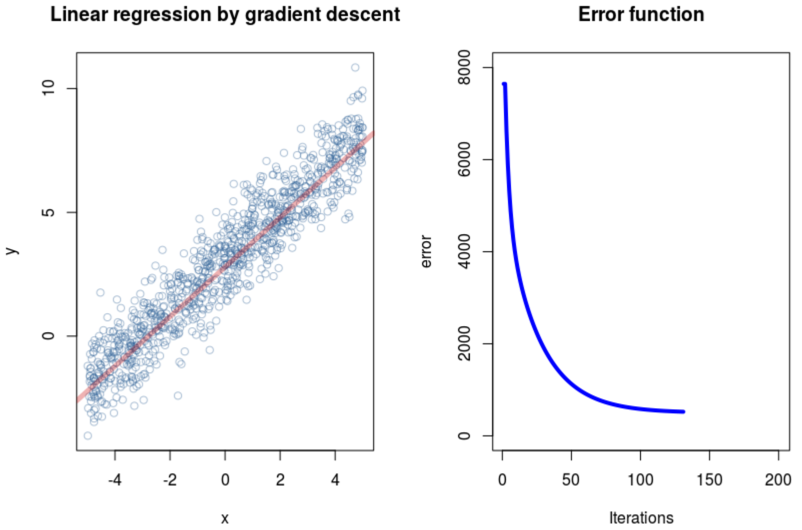

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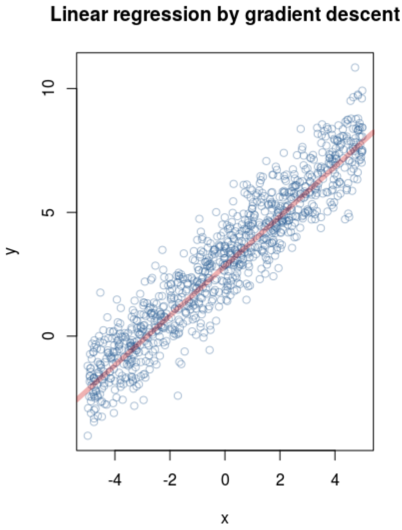

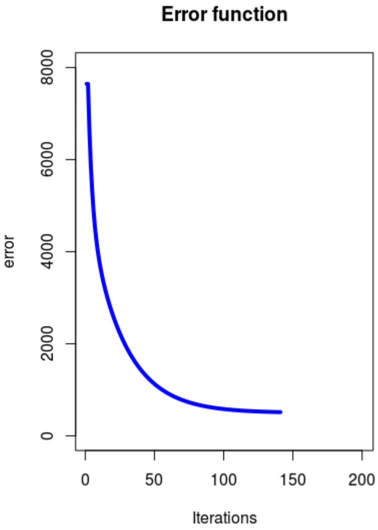

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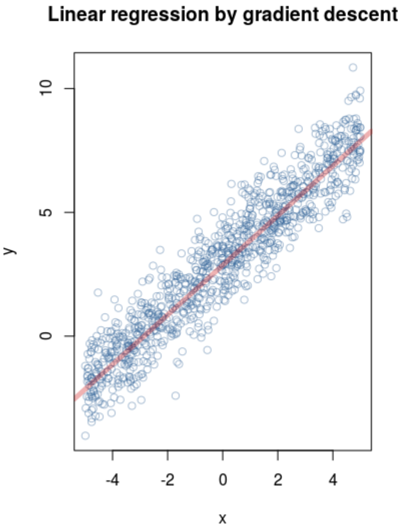

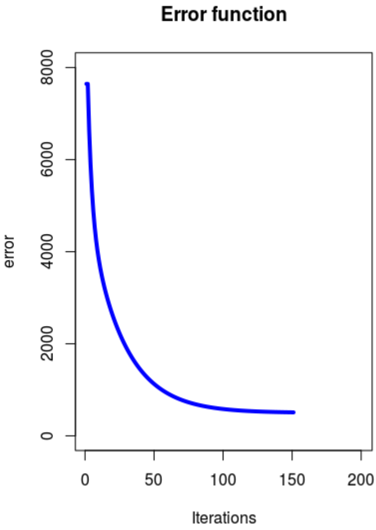

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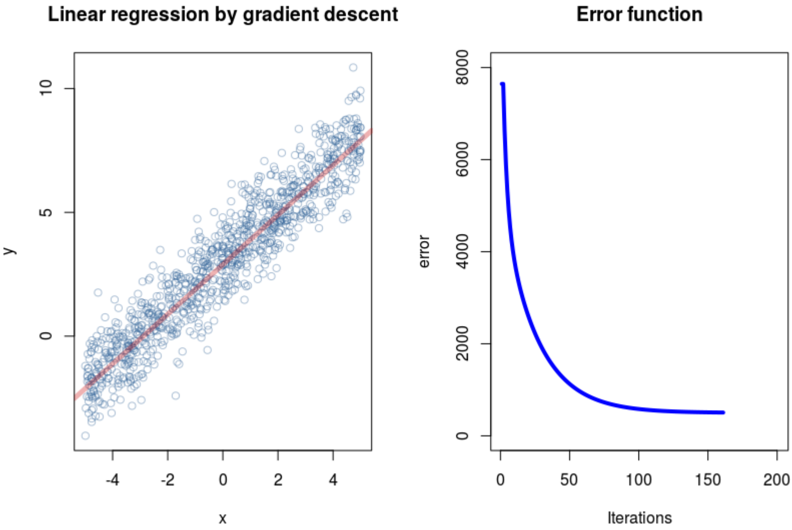

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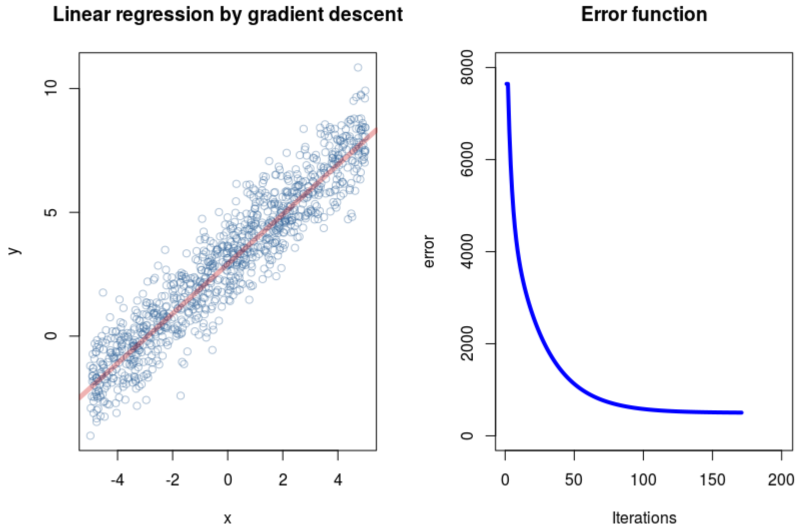

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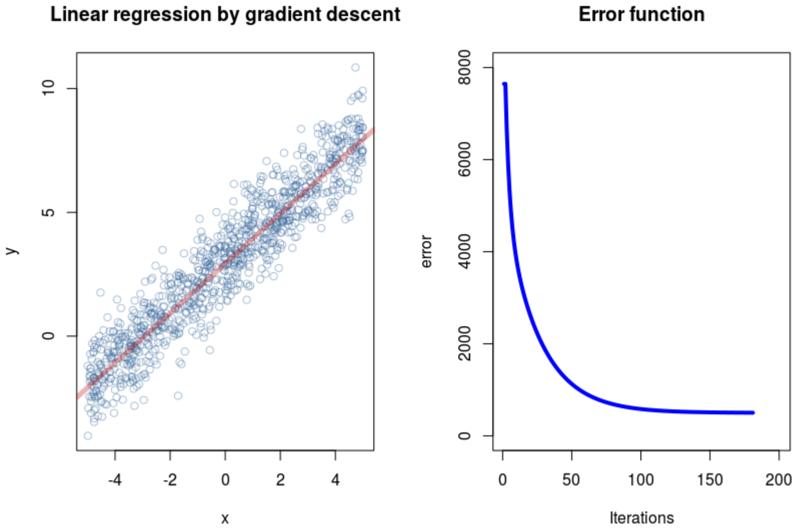

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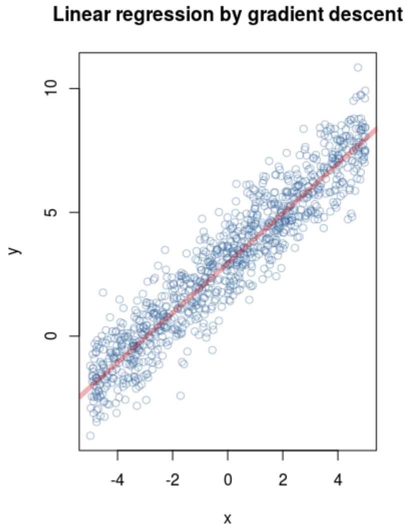

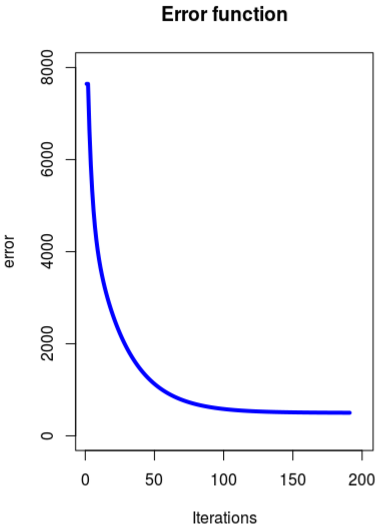

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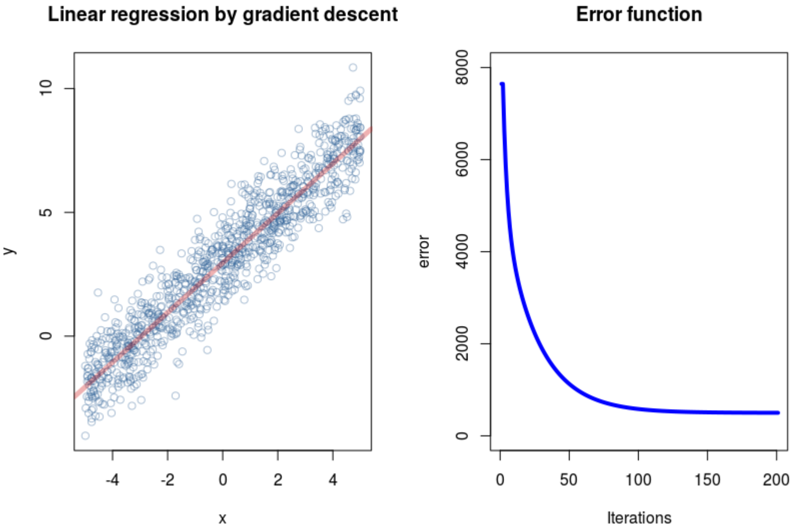

Finding the Minimum in Dimension One

Assume $n = 1$. Then the error function E is

$$E(w_0, w_1) = \frac{1}{2}\sum_{k=1}^{p}(w_0 + w_1 x_k - f_k)^2$$

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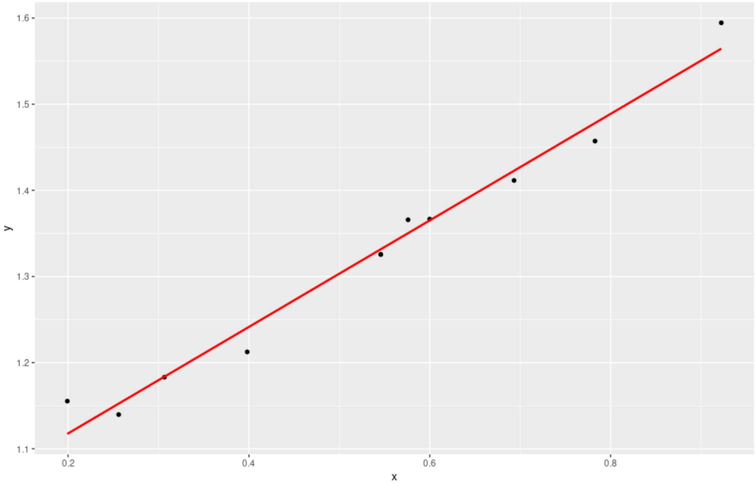
$$\frac{\partial E}{\partial w_1} = 0 \quad \Leftrightarrow \quad w_1 = \frac{\frac{1}{p}\sum_{k=1}^{p}(f_k - \bar{f})(x_k - \bar{x})}{\frac{1}{p}\sum_{k=1}^{p}(x_k - \bar{x})^2}$$

i.e. $w_1 = cov(f, x)/var(x)$

Effect of Outliers



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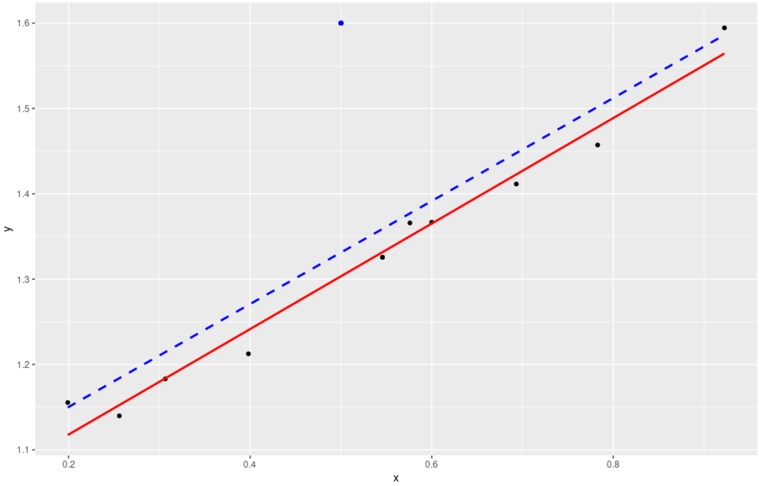

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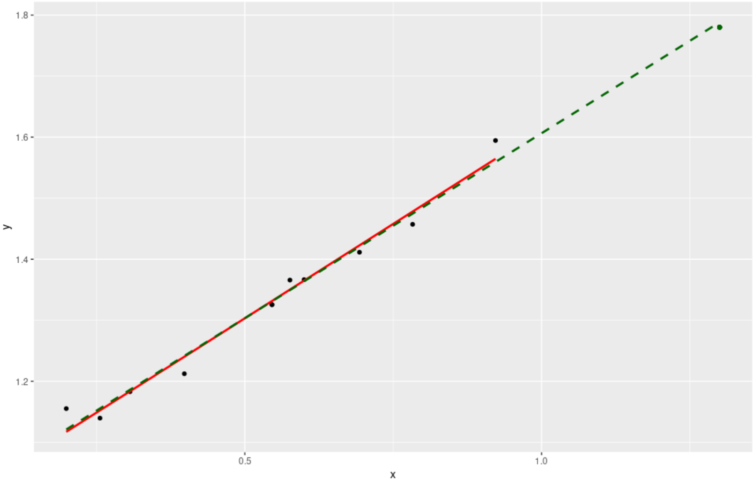

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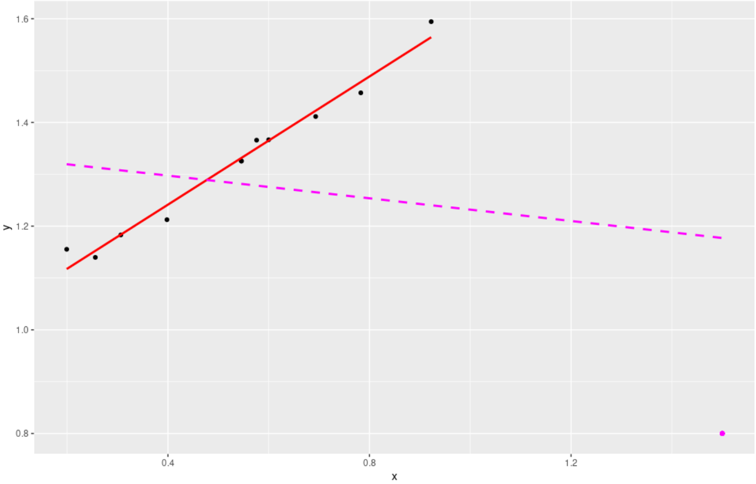

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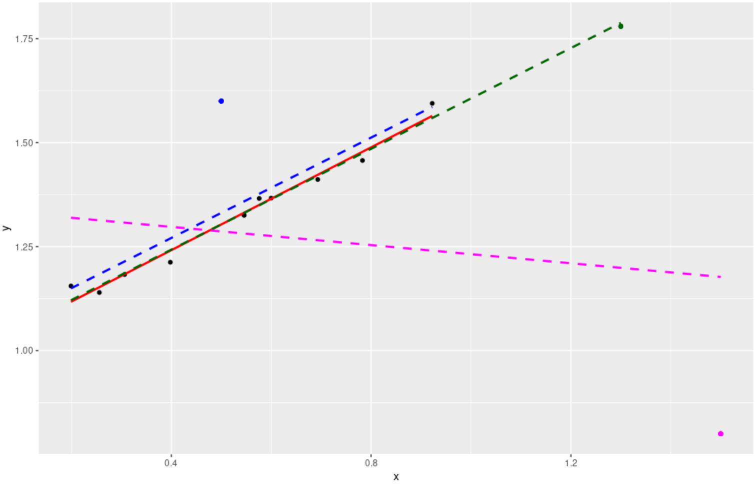
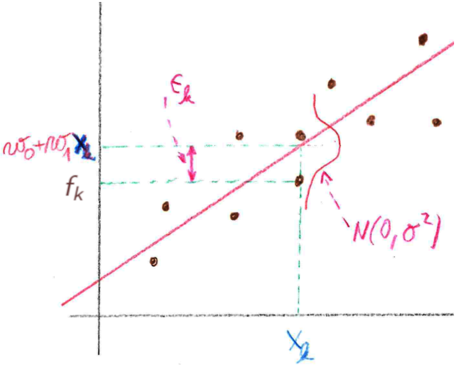


Maximum Likelihood vs Least Squares (Dim 1)

Fix a training set $D = \{(x_1, f_1), (x_2, f_2), \ldots, (x_p, f_p)\}$
Assume that each f_k has been generated randomly by

$$f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$$

where w_0, w_1 are **unknown weights**, and ϵ_k are independent, normally distributed noise values with mean 0 and some variance σ^2



How "probable" is it to generate the correct $f_1, \ldots, f_p$?

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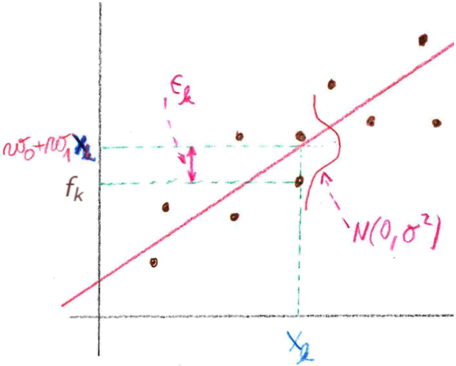

How "probable" is it to generate the correct $f_1, \ldots, f_p$?

The following conditions are equivalent:

- w_0, w_1 minimize the squared error E
- w_0, w_1 maximize the likelihood (i.e., the "probability") of generating the correct values $f_1, \ldots, f_p$ using $f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$

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