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Least squares for programmers

— with color plates —

Dmitry Sokolov

November 16, 2020

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Coin toss experiment

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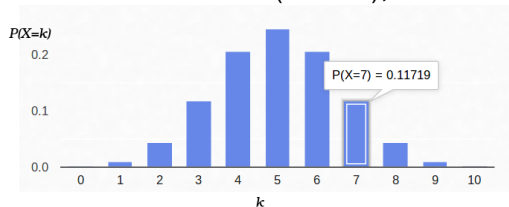
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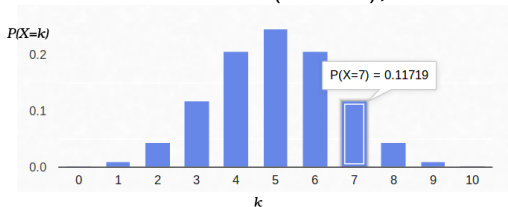
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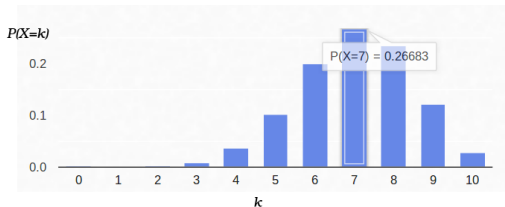
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a biased coin ($p = 7/10$)

Coin toss: the likelihood function

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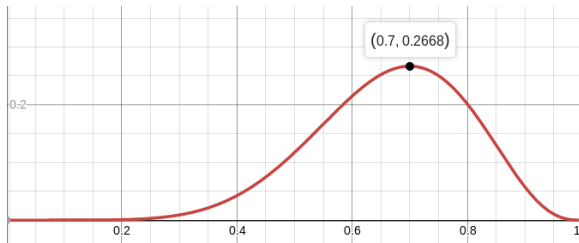
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N.B. the function is continuous!

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That is, the maximum likelihood (about 27%) is reached at the point $p = 7/10$. Just in case, let us check the second derivative:

$$\frac{d^2 \log \mathcal{L}}{dp^2} = -\frac{7}{p^2} - \frac{3}{(1 - p)^2}$$

At the point $p = 7/10$ it is negative, therefore this point is indeed a maximum of the function \mathcal{L} :

$$\frac{d^2 \log \mathcal{L}}{dp^2}(0.7) \approx -48 < 0$$

Least squares through maximum likelihood

Let us measure a constant value; all measurements are inherently noisy.

For example, if we measure the battery voltage N times, we get N different measurements:

$$\{U_j\}_{j=1}^N$$

Suppose that each measurement U_j is i.i.d. and subject to a Gaussian noise, e.g. it is equal to the real value plus the Gaussian noise. The probability density can be expressed as follows:

$$p(U_j) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(U_j - U)^2}{2\sigma^2}\right),$$

where U is the (unknown) value and σ is the noise amplitude (can be unknown).

Least squares through maximum likelihood

$$\log \mathcal{L}(U, \sigma) = \log \left(\prod_{j=1}^N \frac{1}{\sqrt{2\pi}\sigma} \exp \left(-\frac{(U_j - U)^2}{2\sigma^2} \right) \right)$$

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Under Gaussian noise

$$\arg \max_U \log \mathcal{L} = \arg \min_U \sum_{j=1}^N (U_j - U)^2$$

Least squares through maximum likelihood

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$$\frac{\partial \log \mathcal{L}}{\partial \sigma} = -\frac{N}{\sigma} + \frac{1}{\sigma^3} \sum_{j=1}^N (U_j - U)^2 = 0 \qquad \sigma = \sqrt{\frac{\sum_{j=1}^N (U_j - U)^2}{N}}$$

Such a convoluted way to obtain a simple average of all measurements. . .

Linear regression

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As before, $\arg \max_{a,b} \log \mathcal{L} = \arg \min_{a,b} S(a, b)$.

Linear regression

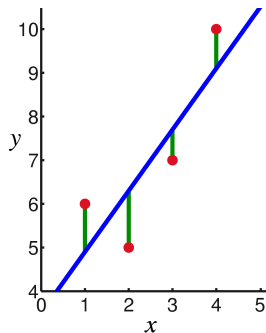
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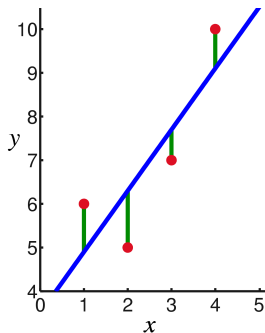
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$$a = \frac{N \sum_{j=1}^N x_j y_j - \sum_{j=1}^N x_j \sum_{j=1}^N y_j}{N \sum_{j=1}^N x_j^2 - \left(\sum_{j=1}^N x_j \right)^2}$$

$$b = \frac{1}{N} \left(\sum_{j=1}^N y_j - a \sum_{j=1}^N x_j \right)$$



The takeaway message

The least squares method is a particular case of maximizing likelihood in cases where the probability density is Gaussian.

The more parameters we have, the more cumbersome the analytical solutions are. Fortunately, we are not living in XVIII century anymore, we have computers!

Next we will try to build a geometric intuition on least squares, and see how can least squares problems be efficiently implemented.

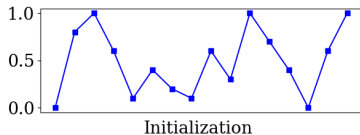
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Smooth an array

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x = [0, .8, 1, .6, .1, .4, .2, .1, .6, .3, 1, .7, .4, 0, .6, 1]
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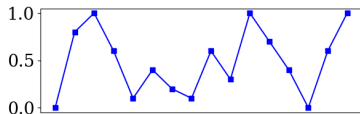
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for _ in range(512):  
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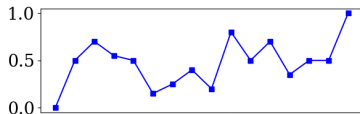
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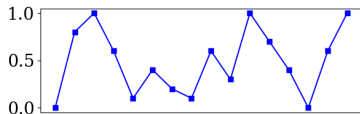


Iteration #1

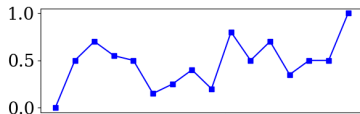
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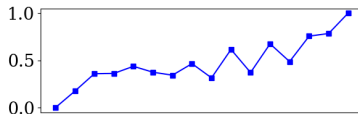
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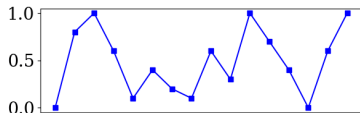


Iteration #5

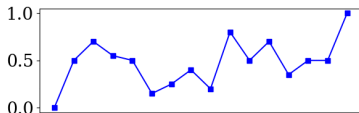
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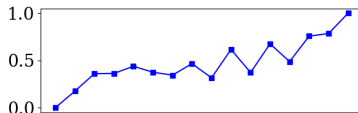
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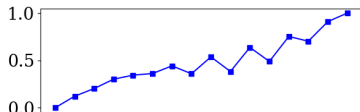
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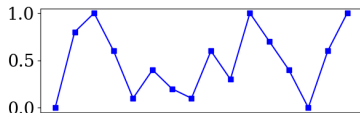


Iteration #10

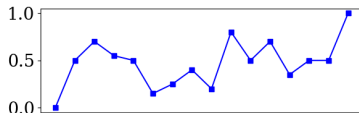
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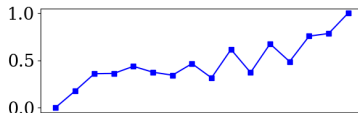
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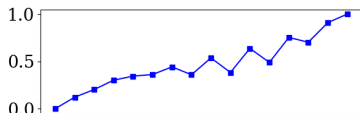
Initialization



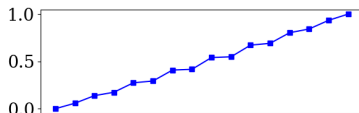
Iteration #1



Iteration #5



Iteration #10

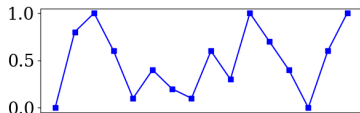


Iteration #50

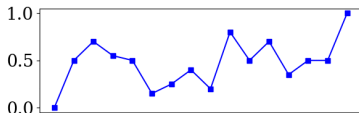
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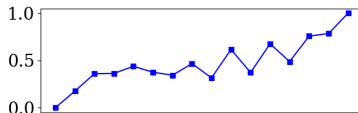
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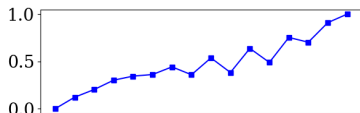
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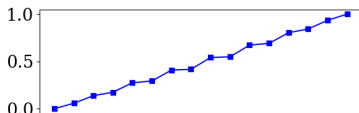
Iteration #1



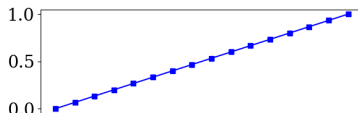
Iteration #5



Iteration #10



Iteration #50



Iteration #500

The Jacobi iterative method

Given an ordinary system of linear equations:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{cases}$$

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Let us rewrite it as follows:

$$\begin{aligned} x_1 &= \frac{1}{a_{11}}(b_1 - a_{12}x_2 - a_{13}x_3 - \cdots - a_{1n}x_n) \\ x_2 &= \frac{1}{a_{22}}(b_2 - a_{21}x_1 - a_{23}x_3 - \cdots - a_{2n}x_n) \\ &\vdots \\ x_n &= \frac{1}{a_{nn}}(b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1}) \end{aligned}$$

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Repeating the process k times, the solution can be approximated by the vector $\vec{x}^{(k)} = (x_1^{(k)}, x_2^{(k)}, \dots, x_n^{(k)})$.

Back to the array smoothing

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x = [0, .8, 1, .6, .1, .4, .2, .1, .6, .3, 1, .7, .4, 0, .6, 1]

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The Gauß-Seidel iterative method

Jacobi:

$$x_i^{(k)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1, j \neq i}^n a_{ij} x_j^{(k-1)} \right), \quad \text{for } i = 1, 2, \dots, n$$

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The Gauß-Seidel iterative method

Jacobi:

```
x = [0, .8, 1, .6, .1, .4, .2, .1, .6, .3, 1, .7, .4, 0, .6, 1]

for _ in range(512):
    x = [ x[0] ] + \
        [ (x[i-1]+x[i+1])/2. for i in range(1, len(x)-1) ] + \
        [ x[-1] ]
```

Gauß-Seidel:

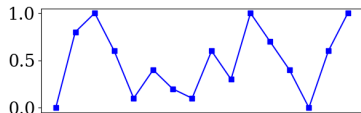
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```

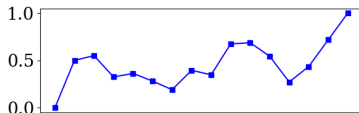
Smooth an array : Gauß-Seidel

```
x = [0, .8, 1, .6, .1, .4, .2, .1, .6, .3, 1, .7, .4, 0, .6, 1]
```

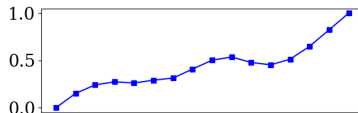
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for _ in range(512):  
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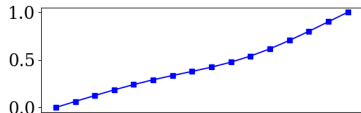
Initialization



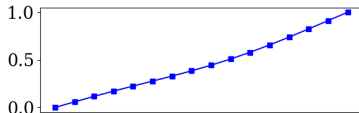
Iteration #1



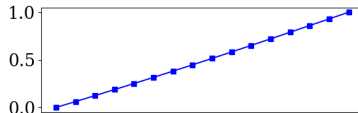
Iteration #3



Iteration #10



Iteration #15



Iteration #50

Equality of derivatives vs zero curvature

```
x = [0, .8, 1, .6, .1, .4, .2, .1, .6, .3, 1, .7, .4, 0, .6, 1]
```

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for _ in range(512):  
    for i in range(1, len(x)-1):  
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```

$$\left\{ \begin{array}{llllll} x_0 & & & & & & = 0 \\ -x_0 & +2x_1 & -x_2 & & & & = 0 \\ & & -x_2 & +2x_3 & -x_4 & & = 0 \\ & & & & \ddots & & \vdots \\ & & & & & -x_{12} & +2x_{13} & -x_{14} & = 0 \\ & & & & & & -x_{13} & +2x_{14} & -x_{15} & = 0 \\ & & & & & & & & x_{15} & = 1 \end{array} \right.$$

It also works for 3d surfaces

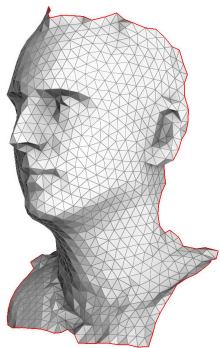
```
#include "model.h"

int main(void) {
    Model m("../input.obj"); // parse the input mesh

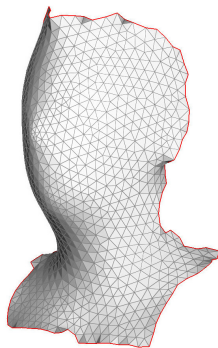
    // smooth the surface through Gauss-Seidel iterations
    for (int it=0; it<1000; it++)
        for (int v=0; v<m.nverts(); v++) // for all vertices
            if (!m.is_boundary_vert(v)) // fix the boundary
                m.point(v) = m.one_ring_barycenter(v);

    std::cout << m; // drop the result
    return 0;
}
```

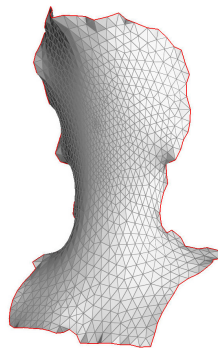
It also works for 3d surfaces



input



10 iterations



1000 iterations

Prescribe the right hand side

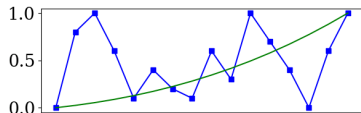
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```

```
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        x[i] = ( x[i-1] + x[i+1] - (i+15)/15**3 )/2.
```

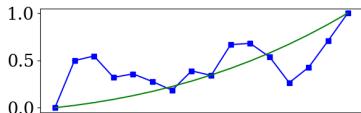
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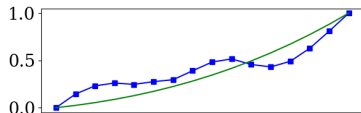
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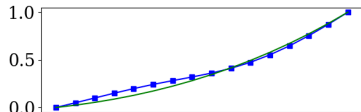
Initialization



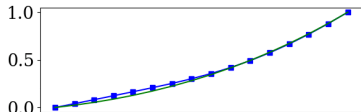
Iteration #1



Iteration #3



Iteration #10



Iteration #15



Iteration #50

Table of Contents

- 1 Maximum likelihood through examples
- 2 Introduction to systems of linear equations
- 3 Minimization of quadratic functions**
- 4 Least squares through examples

Matrices and numbers

What is a number a ?

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float a;
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vector<float> f(vector<float> x) {  
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```

Or $f(x) = x^T Ax = \sum_i \sum_j a_{ij} x_i x_j : \mathbb{R}^2 \rightarrow \mathbb{R}$?

```
float f(vector<float> x) {  
    return x[0]*a11*x[0] + x[0]*a12*x[1] +  
           x[1]*a21*x[0] + x[1]*a22*x[1];  
}
```

What is a positive number?

We have a great tool called the predicate “greater than” $>$.

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Definition

The real number a is positive if and only if for all non-zero real $x \in \mathbb{R}$, $x \neq 0$ the condition $ax^2 > 0$ is satisfied.

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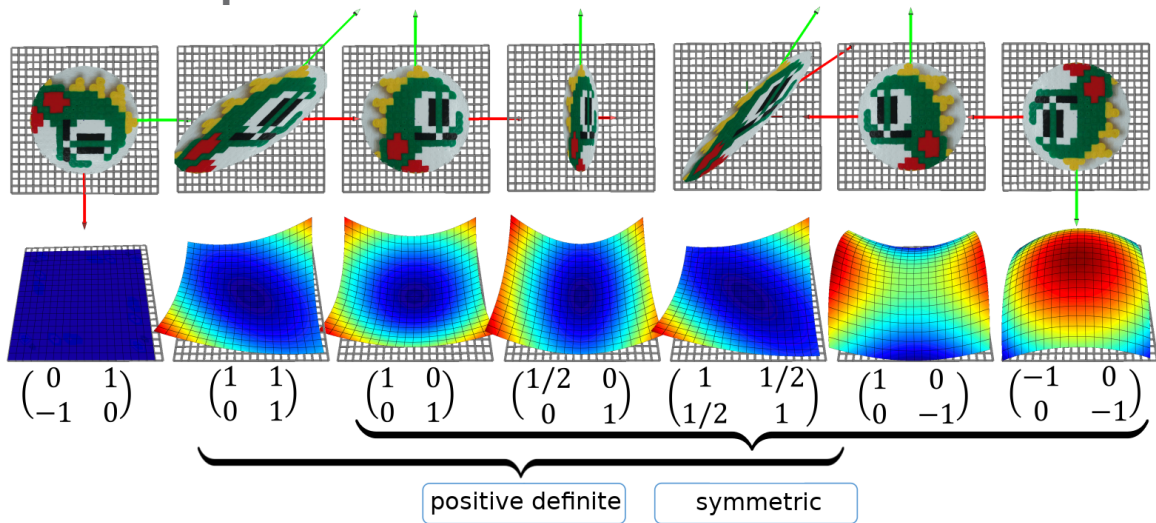
The real number a is positive if and only if for all non-zero real $x \in \mathbb{R}$, $x \neq 0$ the condition $ax^2 > 0$ is satisfied.

This definition looks pretty awkward, but it applies perfectly to matrices:

Definition

The square matrix A is called positive definite if for any non-zero x the condition $x^T A x > 0$ is met, i.e. the corresponding quadratic form is strictly positive everywhere except at the origin.

What is a positive number?



Minimizing a 1d quadratic function

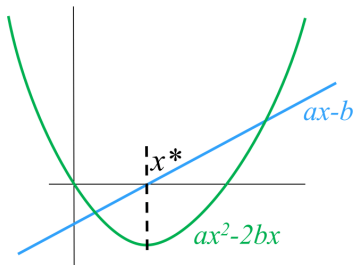
Let us find the minimum of the function $f(x) = ax^2 - 2bx$ (with a positive).

$$\frac{d}{dx}f(x) = 2ax - 2b = 0$$

Minimizing a 1d quadratic function

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In 1d, the solution x^* of the equation $ax - b = 0$ solves the minimization problem $\arg \min_x (ax^2 - 2bx)$ as well.

Differentiating matrix expressions

The first theorem states that 1×1 matrices are invariant w.r.t the transposition:

Theorem

$$x \in \mathbb{R} \Rightarrow x^T = x$$

The proof is left as an exercise.

Differentiating matrix expressions

For a 1d function bx we know that $\frac{d}{dx}(bx) = b$, but what happens in the case of a real function of n variables?

Theorem

$$\nabla b^\top x = \nabla x^\top b = b$$

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$$\nabla b^\top x = \nabla x^\top b = b$$

$$\nabla(b^\top x) = \begin{bmatrix} \frac{\partial(b^\top x)}{\partial x_1} \\ \vdots \\ \frac{\partial(b^\top x)}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial(b_1 x_1 + \dots + b_n x_n)}{\partial x_1} \\ \vdots \\ \frac{\partial(b_1 x_1 + \dots + b_n x_n)}{\partial x_n} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix} = b$$

Differentiating matrix expressions

For a 1d function ax^2 we know that $\frac{d}{dx}(ax^2) = 2ax$, but what about quadratic forms?

Theorem

$$\nabla(x^\top Ax) = (A + A^\top)x$$

Note that if A is symmetric, then $\nabla(x^\top Ax) = 2Ax$.

The proof is straightforward, let us express the quadratic form as a double sum:

$$x^\top Ax = \sum_i \sum_j a_{ij} x_i x_j$$

Differentiating matrix expressions

$$\frac{\partial(x^\top Ax)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\sum_{k_1} \sum_{k_2} a_{k_1 k_2} x_{k_1} x_{k_2} \right) =$$

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 &= \sum_{k_2 \neq i} a_{ik_2} x_{k_2} + \sum_{k_1 \neq i} a_{k_1 i} x_{k_1} + 2a_{ii} x_i = \\
 &= \sum_{k_2} a_{ik_2} x_{k_2} + \sum_{k_1} a_{k_1 i} x_{k_1} = \\
 &= \sum_j (a_{ij} + a_{ji}) x_j \qquad \Rightarrow \nabla(x^\top Ax) = (A + A^\top)x
 \end{aligned}$$

Minimum of a quadratic form and the linear system

Recall that for $a > 0$ solving the equation $ax = b$ is equivalent to the quadratic function $\arg \min_x (ax^2 - 2bx)$ minimization.

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Recall that A is symmetric: $Ax = b$.

Back to the linear regression

Given two points (x_1, y_1) and (x_2, y_2) , find the line that passes through: $y = \alpha x + \beta$.

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$$\begin{cases} \alpha x_1 + \beta = y_1 \\ \alpha x_2 + \beta = y_2 \end{cases} \quad \underbrace{\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \end{bmatrix}}_{:=A} \underbrace{\begin{bmatrix} \alpha \\ \beta \end{bmatrix}}_{:=x} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}}_{:=b} \quad \Rightarrow x^* = A^{-1}b$$

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$$\underbrace{\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \end{bmatrix}}_{:=A(3 \times 2)} \underbrace{\begin{bmatrix} \alpha \\ \beta \end{bmatrix}}_{:=x(2 \times 1)} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}}_{:=b(3 \times 1)}$$

A is rectangular, and thus it is not invertible. Oops!

Back to the linear regression

No biggie, let us rewrite the system:

$$\alpha \underbrace{[x_1 \ x_2 \ x_3]^T}_{:=\vec{i}} + \beta \underbrace{[1 \ 1 \ 1]^T}_{:=\vec{j}} = [y_1 \ y_2 \ y_3]^T$$

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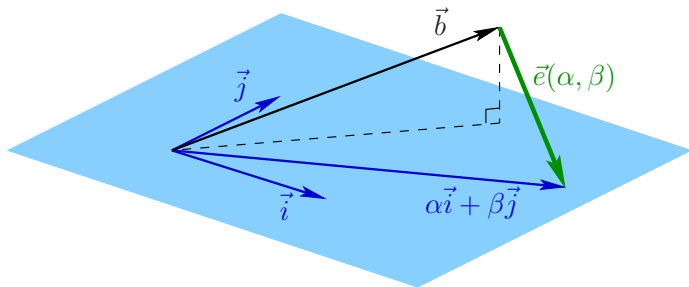
$$\alpha \vec{i} + \beta \vec{j} = \vec{b}.$$

Back to the linear regression

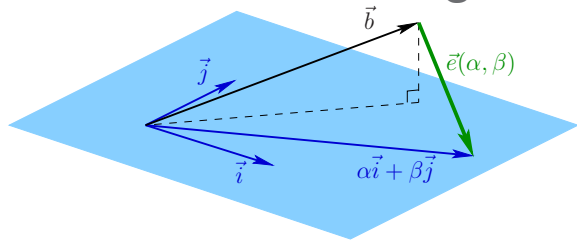
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$$\alpha \underbrace{\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^\top}_{:=\vec{i}} + \beta \underbrace{\begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^\top}_{:=\vec{j}} = \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix}^\top \quad \alpha\vec{i} + \beta\vec{j} = \vec{b}.$$

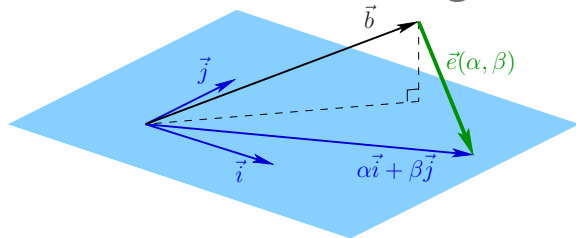
Solve for $\arg \min_{\alpha, \beta} \|\vec{e}(\alpha, \beta)\|$, where $\vec{e}(\alpha, \beta) := \alpha\vec{i} + \beta\vec{j} - \vec{b}$:



Back to the linear regression



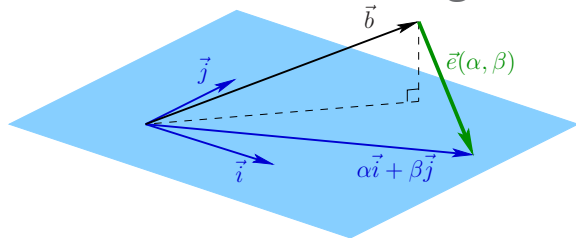
Back to the linear regression



The $\|\vec{e}(\alpha, \beta)\|$ is minimized when $\vec{e}(\alpha, \beta) \perp \text{span}\{\vec{i}, \vec{j}\}$:

$$\begin{cases} \vec{i}^\top \vec{e}(\alpha, \beta) = 0 \\ \vec{j}^\top \vec{e}(\alpha, \beta) = 0 \end{cases}$$

Back to the linear regression

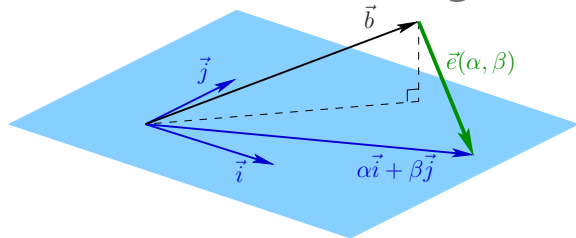


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Back to the linear regression



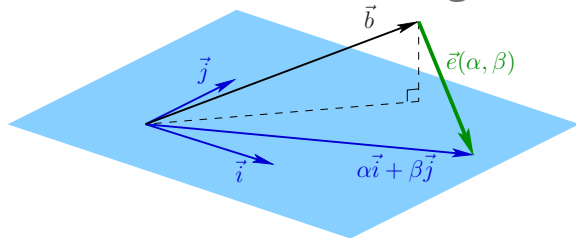
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In a general case the matrix $A^\top A$ can be invertible!

$$A^\top Ax = A^\top b.$$

Some nice properties of $A^\top A$

Theorem

$A^\top A$ is symmetric.

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It follows from the fact that $x^\top A^\top A x = (Ax)^\top Ax \geq 0$. Moreover, $A^\top A$ is positive definite in the case where A has linearly independent columns (rank A is equal to the number of the variables in the system).

Least squares in more than two dimensions

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The takeaway message

The least squares problem $\arg \min \|Ax - b\|^2$ is equivalent to minimizing the quadratic function $\arg \min (x^\top A' x - 2b'^\top x)$ with (in general) a symmetric positive definite matrix A' . This can be done by solving a linear system $A'x = b'$.

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- 1 Maximum likelihood through examples
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Linear-quadratic regulator

Imagine that we have a car going at 0.5m/s. The goal is to accelerate to 2.3m/s. We can not control the speed directly, but we can act on the acceleration via the gas pedal:

$$v_{k+1} = v_k + u_k,$$

where the signals are sampled every 1 second, v_k is the car speed and u_k is the acceleration of the car.

We have half a minute maximum to reach the goal, i.e, $v_0 = 0.5\text{m/s}$, $v_n = 2.3\text{m/s}$, $n = 30\text{s}$. So, we need to find $\{u_i\}_{i=0}^{n-1}$ that optimizes some quality criterion $J(\vec{v}, \vec{u})$:

$$\min J(\vec{v}, \vec{u}) \quad \text{s.t.} \quad v_{i+1} = v_i + u_i \quad \forall i \in 0..n-1$$



Dmitry Sokolov

Least squares for programmers
— with color plates —