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Least squares for programmers

— with color plates —

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Coin toss experiment

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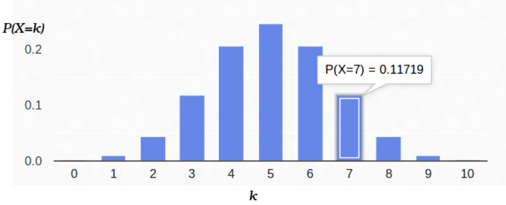

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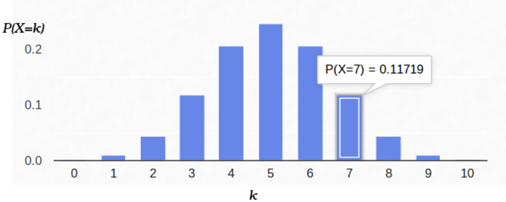

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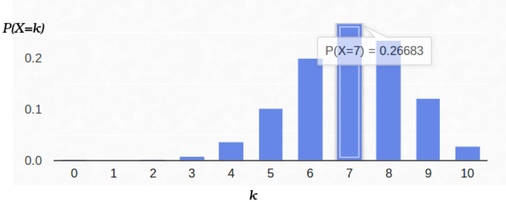

a biased coin ($p = 7/10$)

Coin toss: the likelihood function

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$$\mathcal{L}(p) = C_{10}^{7} p^7 (1 - p)^3$$

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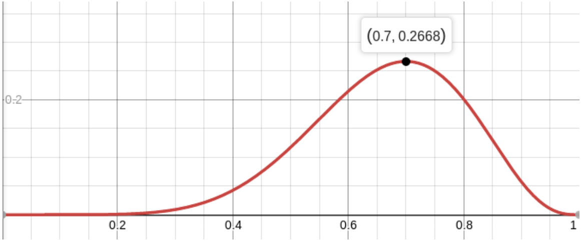

N.B. the function is continuous!

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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

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

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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

It is much harder for less trivial examples. Suppose we have N measurements $\{x_j, y_j\}_{j=1}^N$, and we want to fit a straight line onto it.

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$$= \underbrace{-N \left(\log\sqrt{2\pi} + \log\sigma \right)}_{\text{does not depend on } a,b} - \frac{1}{2\sigma^2} \underbrace{\sum_{j=1}^{N} (y_j - ax_j - b)^2}_{:=S(a,b)}$$

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As before, $\underset{a,b}{\arg\max} \log \mathcal{L} = \underset{a,b}{\arg\min}\, S(a, b)$.

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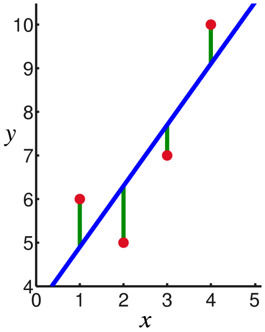

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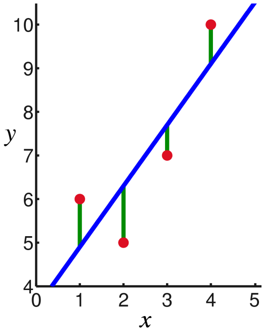

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$$a = \frac{N \sum\limits_{j=1}^{N} x_j y_j - \sum\limits_{j=1}^{N} x_j \sum\limits_{j=1}^{N} y_j}{N \sum\limits_{j=1}^{N} x_j^2 - \left(\sum\limits_{j=1}^{N} x_j\right)^2}$$

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

The takeaway message

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

The more we 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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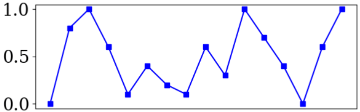

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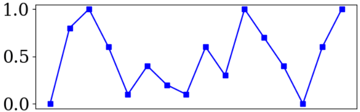

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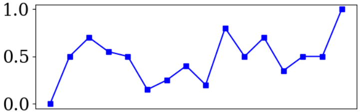

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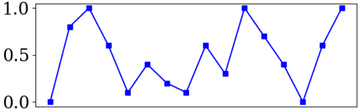

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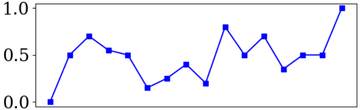

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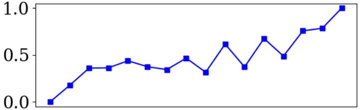

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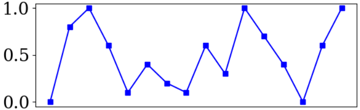

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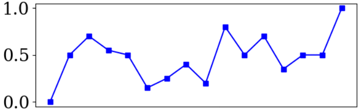

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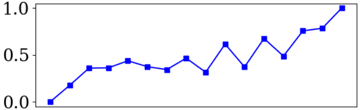

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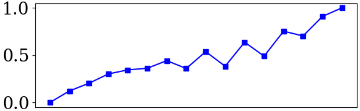

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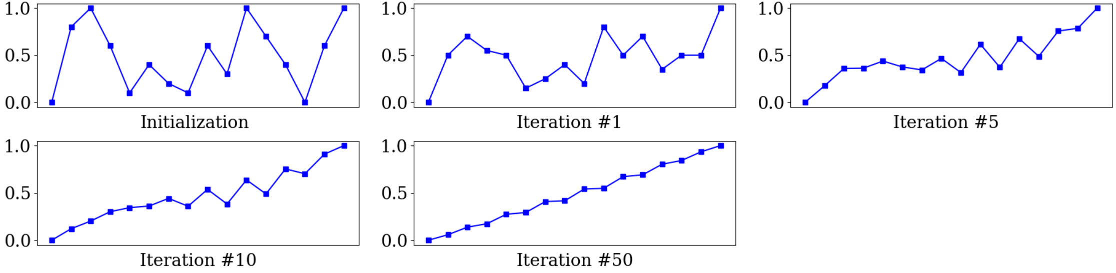

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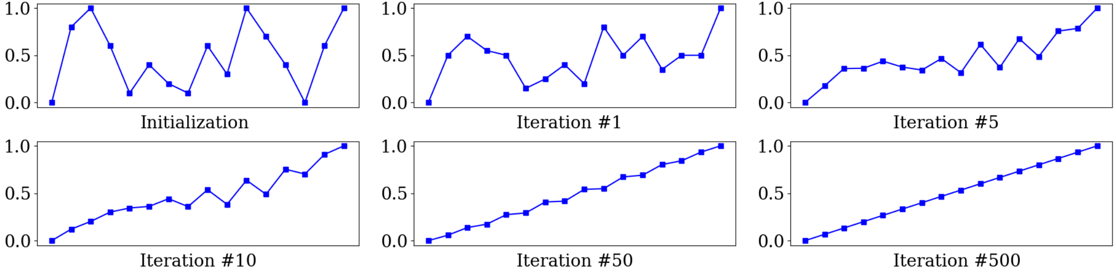

The Jacobi iterative method

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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x_1^{(1)} &= \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(0)} - a_{13}x_3^{(0)} - \cdots - a_{1n}x_n^{(0)}) \\
x_2^{(1)} &= \frac{1}{a_{22}}(b_2 - a_{21}x_1^{(0)} - a_{23}x_3^{(0)} - \cdots - a_{2n}x_n^{(0)}) \\
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\end{aligned}
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Repeating the process k times, the solution can be approximated by the vector
$\vec{x}^{(k)} = \left(x_1^{(k)}, x_2^{(k)}, \ldots, x_n^{(k)}\right)$.

Back to the array smoothing

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$$\Updownarrow$$

$$x_i - x_{i-1} = x_{i+1} - x_i$$

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$$x_i = \frac{x_{i-1} + x_{i+1}}{2}$$

$$\Updownarrow$$

$$x_i - x_{i-1} = x_{i+1} - x_i$$

$$\begin{cases} x_0 &= 0 \\ x_1 - x_0 &= x_2 - x_1 \\ x_2 - x_1 &= x_3 - x_1 \\ & \vdots \\ x_{13} - x_{12} &= x_{14} - x_{13} \\ x_{14} - x_{13} &= x_{15} - x_{14} \\ x_{15} &= 1 \end{cases}$$

The Gauß-Seidel iterative method

Jacobi:

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

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

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:

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

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```

Smooth an array : Gauß-Seidel

```
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for _ in range(512):
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```

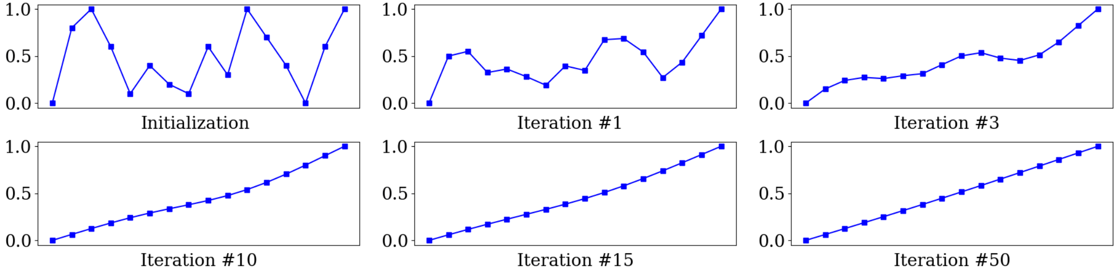

Equality of derivatives vs zero curvature

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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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```

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

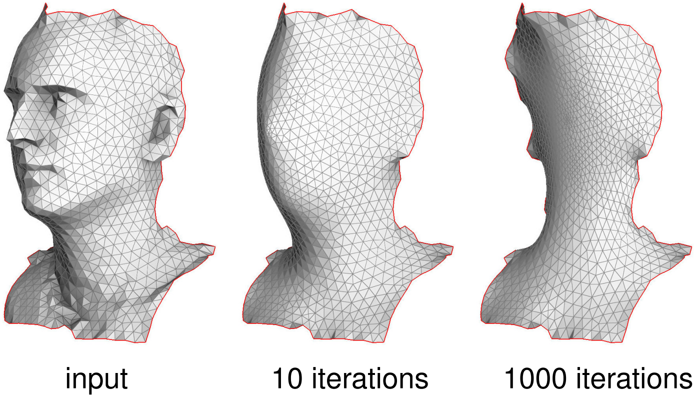
It also works for 3d surfaces

```
#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



Prescribe the right hand side

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

for _ in range(512):
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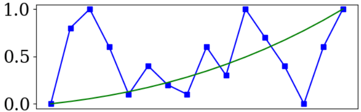
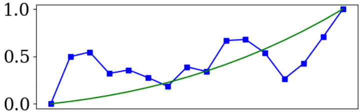
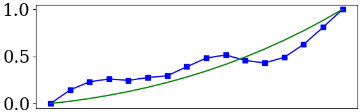


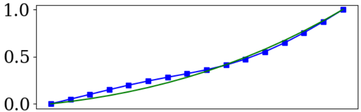
Initialization



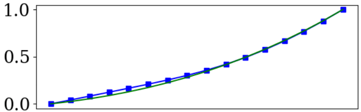
Iteration #1



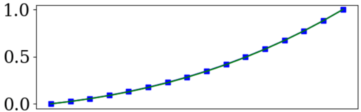
Iteration #3



Iteration #10



Iteration #15



Iteration #50

Well duh... Of course it is a cubic polynomial!

The takeaway message

We just saw that mere 3 lines of code can be sufficient to solve a linear system, effectively solving a differential equation.

While it is extremely cool, it raises questions:

- What are the practical consequences for a programmer?
- How do we build these systems?
- Where do we use them?

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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float f(float x) {
    return x*a*x;
}
```

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The same goes for matrices, what is a matrix $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$?

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

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}
```

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

```
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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Definition

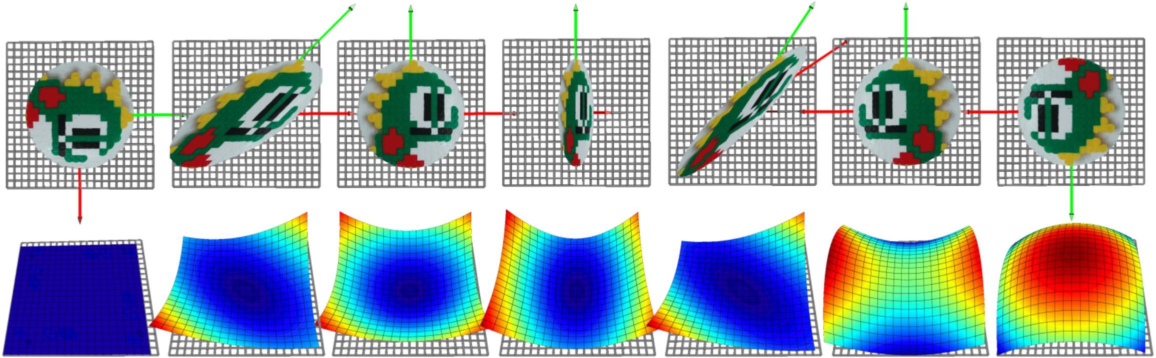
The real number a is positive if and only if for all non-zero real $x \in \mathbb{R},\ x \neq 0$ the condition $ax^2 > 0$ is satisfied.

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 $x^\top Ax > 0$ is met, i.e. the corresponding quadratic form is strictly positive everywhere except at the origin.

What is a positive number?



$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1/2 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

positive definite

symmetric

Minimizing a 1d quadratic function

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

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

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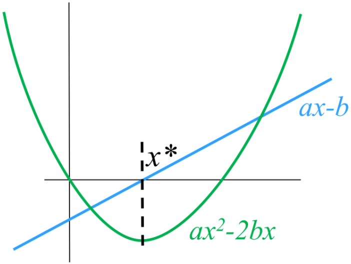

In 1d, the solution x^* of the equation $ax - b = 0$ solves the minimization problem $\arg\min_x (ax^2 - 2bx)$ as well.

Differentiating matrix expressions

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

Theorem

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

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

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

Differentiating matrix expressions

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Theorem

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

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

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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Differentiating matrix expressions

$$
\begin{aligned}
\frac{\partial(x^\top Ax)}{\partial x_i} &= \frac{\partial}{\partial x_i}\left(\sum_{k_1}\sum_{k_2} a_{k_1k_2}x_{k_1}x_{k_2}\right) = \\
&= \frac{\partial}{\partial x_i}\left(\underbrace{\sum_{k_1\neq i}\sum_{k_2\neq i} a_{k_1k_2}x_{k_1}x_{k_2}}_{k_1\neq i, k_2\neq i} + \underbrace{\sum_{k_2\neq i} a_{ik_2}x_ix_{k_2}}_{k_1=i,k_2\neq i} + \underbrace{\sum_{k_1\neq i} a_{k_1i}x_{k_1}x_i}_{k_1\neq i,k_2=i} + \underbrace{a_{ii}x_i^2}_{k_1=i,k_2=i}\right) = \\
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&= \sum_{k_2} a_{ik_2}x_{k_2} + \sum_{k_1} a_{k_1i}x_{k_1} = \\
&= \sum_j (a_{ij}+a_{ji})x_j \qquad\qquad \Rightarrow \nabla(x^\top Ax) = (A+A^\top)x
\end{aligned}
$$

Minimum of a quadratic form and the linear system

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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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Now add a **third** point (x_3, y_3):

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

Back to the linear regression

No biggie, let us rewrite the system:

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

Back to the linear regression

No biggie, let us rewrite the system:

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

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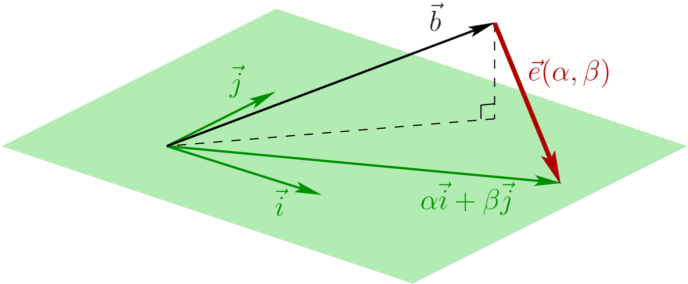
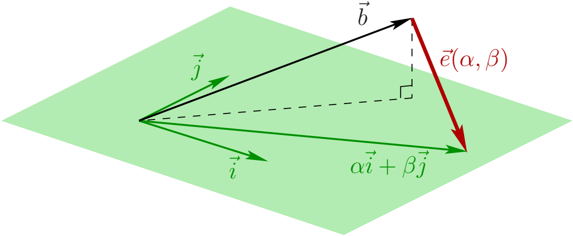
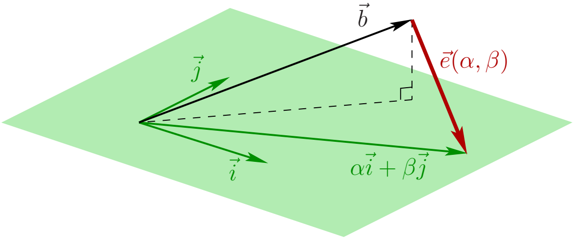
Solve for $\arg\min\limits_{\alpha,\beta} \|\vec{e}(\alpha,\beta)\|$, where $\vec{e}(\alpha,\beta) := \alpha\vec{i} + \beta\vec{j} - \vec{b}$:



Back to the linear regression



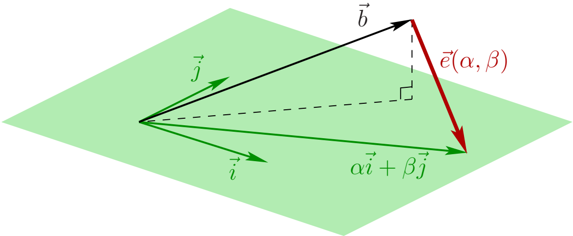
Back to the linear regression



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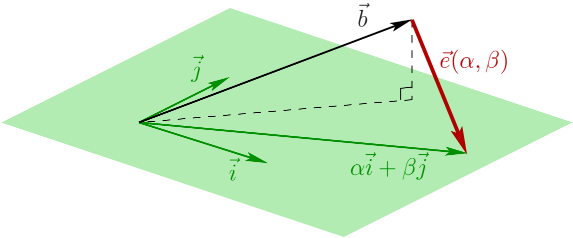
$$\begin{cases}\vec{i}^\top\vec{e}(\alpha,\beta)=0\\ \vec{j}^\top\vec{e}(\alpha,\beta)=0\end{cases}$$

$$\begin{bmatrix}x_1 & x_2 & x_3\\ 1 & 1 & 1\end{bmatrix}\left(\alpha\begin{bmatrix}x_1\\x_2\\x_3\end{bmatrix}+\beta\begin{bmatrix}1\\1\\1\end{bmatrix}-\begin{bmatrix}y_1\\y_2\\y_3\end{bmatrix}\right)=\begin{bmatrix}0\\0\end{bmatrix}$$

Back to the linear regression



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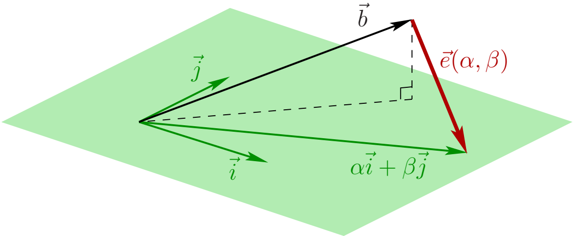
$$\begin{bmatrix} x_1 & x_2 & x_3 \\ 1 & 1 & 1 \end{bmatrix} \left(\alpha \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \beta \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$A^\top (Ax - b) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Back to the linear regression



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$$A^\top (Ax - b) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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

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

Some nice properties of $A^\top A$

Theorem

$A^\top A$ is symmetric.

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It is very easy to show:

$$(A^\top A)^\top = A^\top (A^\top)^\top = A^\top A.$$

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$A^\top A$ positive semidefinite: $\forall x \in \mathbb{R}^n \quad x^\top A^\top A x \geq 0.$

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Theorem

$A^\top A$ positive semidefinite: $\forall x \in \mathbb{R}^n \quad x^\top A^\top A x \geq 0.$

It follows from the fact that $x^\top A^\top A x = (Ax)^\top Ax > 0$. 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

The same reasoning applies, here is an algebraic way to show it:

$$\arg\min \|Ax - b\|^2$$

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$$\arg\min \|Ax-b\|^2 = \arg\min (Ax-b)^\top (Ax-b) = \arg\min (x^\top A^\top - b^\top)(Ax-b) =$$

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$$\begin{aligned}\arg\min \|Ax - b\|^2 &= \arg\min (Ax-b)^\top (Ax-b) = \arg\min (x^\top A^\top - b^\top)(Ax-b) = \\ &= \arg\min (x^\top A^\top A x - b^\top A x - x^\top A^\top b + \underbrace{b^\top b}_{\mathrm{const}}) = \\ &= \arg\min (x^\top A^\top A x - 2b^\top A x) = \end{aligned}$$

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The takeaway message

The least squares problem $\arg\min \|Ax-b\|^2$ is equivalent to minimizing the quadratic function $\arg\min \left(x^\top A' x - 2b'^\top x\right)$ 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

2. Introduction to systems of linear equations

3. Minimization of quadratic functions

4. **Least squares through examples**

Linear-quadratic regulator

Imagine a car going at $v_0 = 0.5$ m/s. The goal is to accelerate to $v_n = 2.3$ m/s in $n = 30$ s maximum. We can control the acceleration u_i via the gas pedal:

$$v_{i+1} = v_i + u_i$$

Linear-quadratic regulator

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So, we need to find $\{u_i\}_{i=0}^{n-1}$ that optimizes some quality criterion $J(\vec{v}, \vec{u})$:

$$\arg\min J(\vec{v}, \vec{u}) \quad s.t. \quad v_{i+1} = v_i + u_i = v_0 + \sum_{j=0}^{i-1} u_j \quad \forall i \in 0..n-1$$

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What happens if we ask for the car to reach the final speed as quickly as possible?
It can be written as follows:

$$J(\vec{v}, \vec{u}) := \sum_{i=1}^{n} (v_i - v_n)^2 = \sum_{i=1}^{n} \left(\sum_{j=0}^{i-1} u_j - v_n + v_0 \right)^2$$

Linear-quadratic regulator

$$J(\vec{v}, \vec{u}) := \sum_{i=1}^{n} \left(\sum_{j=0}^{i-1} u_j - v_n + v_0 \right)^2$$

Solve in the least squares sense:

$$\begin{cases} u_0 & & & & = v_n - v_0 \\ u_0 & +u_1 & & & = v_n - v_0 \\ \vdots & & \ddots & & \vdots \\ u_0 & +u_1 & \dots & +u_{n-1} & = v_n - v_0 \end{cases}$$

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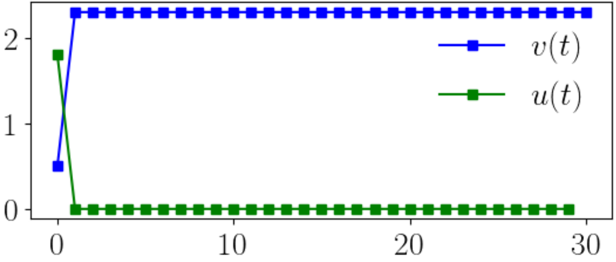
Ouch... Quite brutal accelerations: obvious solution $u_0 = v_n - v_0$, $u_i = 0\ \forall i > 0$.



Linear-quadratic regulator

Ok, no problem, let us penalize large accelerations:

$$J(\vec{v}, \vec{u}) := \sum_{i=0}^{n-1} {u_i}^2 + \left(\sum_{i=0}^{n-1} u_i - v_n\right)^2$$

Solve in the least squares sense:

$$\left\{\begin{array}{lllll} u_0 & & & & = 0 \\ & u_1 & & & = 0 \\ & & \ddots & & \vdots \\ & & & u_{n-1} & = 0 \\ u_0 & +u_1 & \dots & +u_{n-1} & = v_n - v_0 \end{array}\right.$$

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```
import numpy as np
n,v0,vn = 30,0.5,2.3
A = np.matrix(np.vstack((np.diag([1]*n), [1]*n)))
b = np.matrix([[0]]*n + [[vn-v0]])
u = np.linalg.inv(A.T*A)*A.T*b
v = [v0 + np.sum(u[:i]) for i in range(0,n+1)]
```

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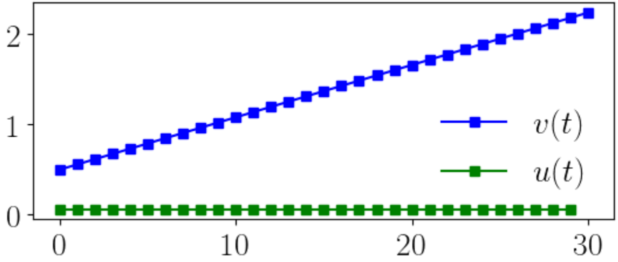

Low acceleration, however the transient time becomes unacceptable.

Linear-quadratic regulator

Optimize for competing goals:

$$J(\vec{v}, \vec{u}) := \sum_{i=1}^{n} (v_i - v_n)^2 + \boxed{4} \sum_{i=0}^{n-1} u_i^2$$

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$$\sum_{i=1}^{n}\left(\sum_{j=0}^{i-1} u_j - v_n + v_0\right)^2 + \boxed{4} \sum_{i=0}^{n-1} u_i^2$$

N.B. Note the tradeoff coefficients!

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$$\begin{cases} u_0 & & & & = v_n - v_0 \\ u_0 & +u_1 & & & = v_n - v_0 \\ \vdots & & \ddots & & \vdots \\ u_0 & +u_1 & \dots & +u_{n-1} & = v_n - v_0 \\ \boxed{2}\, u_0 & & & & = 0 \\ & \boxed{2}\, u_1 & & & = 0 \\ & & \ddots & & \vdots \\ & & & \boxed{2}\, u_{n-1} & = 0 \end{cases}$$

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```
import numpy as np
n,v0,vn = 30,0.5,2.3
A = np.matrix(np.vstack((np.tril(np.ones((n,n))), np.diag([2]*n))))
b = np.matrix([[vn-v0]]*n + [[0]]*n)
u = np.linalg.inv(A.T*A)*A.T*b
v = [v0 + np.sum(u[:i]) for i in range(0,n+1)]
```

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u_0 & & & & = v_n - v_0 \\
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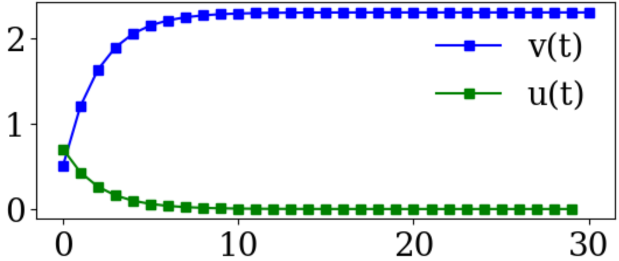
\boxed{2}\, u_0 & & & & = 0 \\
 & \boxed{2}\, u_1 & & & = 0 \\
 & & \ddots & & \vdots \\
 & & & \boxed{2}\, u_{n-1} & = 0
\end{cases}$$

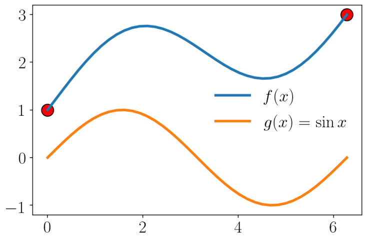


Poisson's equation

Problem: find $f(x)$ defined on $x \in [0, 2\pi]$ as close as possible to $g(x) := \sin x$, constrained to $f(0) = 1$ and $f(2\pi) = 3$.

Formulate it as the Poisson's equation with Dirichlet boundary conditions:

$\frac{d^2}{dx^2} f = \frac{d^2}{dx^2} g \quad \text{s.t. } f(0) = 1,\ f(2\pi) = 3$



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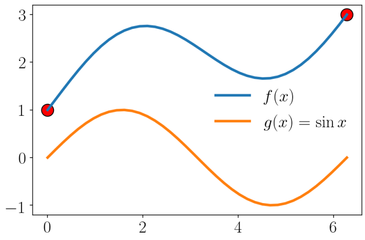

Neanderthal method:

```
import numpy as np
n,f0,fn = 32,1.,3.
g = [np.sin(x) for x in np.linspace(0, 2*np.pi, n+1)]
f = [f0] + [0]*(n-1) + [fn]
for _ in range(512):
    for i in range(1, n):
        f[i] = ( f[i-1] + f[i+1] + (2*g[i]-g[i-1]-g[i+1]) )/2.
```

N.B: extremely slow convergence for larger problems, very hard to build upon

Poisson's equation

Least squares formulation:

$$\arg\min_{f} \int_0^{2\pi} \| f' - g' \|^2$$

with $f(0) = 1,\ f(2\pi) = 3$

Poisson's equation

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Discretization:

$$\begin{cases} f_1 & & & & = g_1 - g_0 + f_0 \\ -f_1 & +f_2 & & & = g_2 - g_1 \\ & \ddots & \ddots & & \vdots \\ & & -f_{n-3} & +f_{n-2} & = g_{n-2} - g_{n-3} \\ & & & -f_{n-2} & = g_{n-1} - g_{n-2} - f_{n-1} \end{cases}$$

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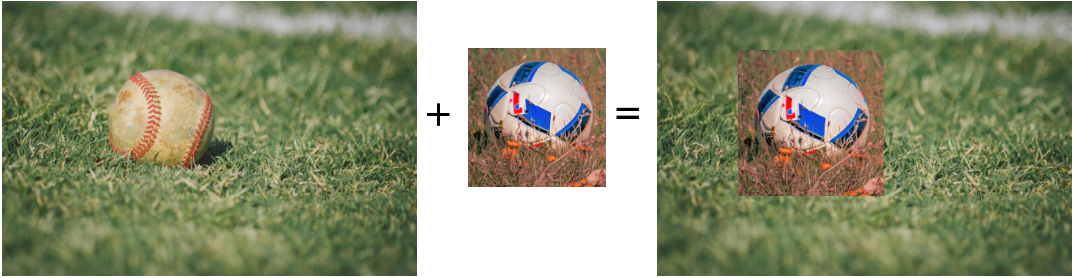
```python
import numpy as np
n,f0,fn = 32,1.,3.
g = [np.sin(x) for x in np.linspace(0, 2*np.pi, n+1)]
A = np.matrix(np.zeros((n-1,n-2)))
np.fill_diagonal(A,      1)
np.fill_diagonal(A[1:], -1)
b = np.matrix([[g[i]-g[i-1]] for i in range(1,n)])
b[ 0,0] = b[ 0,0] + f0
b[-1,0] = b[-1,0] - fn
f = [f0] + (np.linalg.inv(A.T*A)*A.T*b).T.tolist()[0] + [fn]
```

Poisson image editing



Poisson image editing

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We can do better: solve a linear system per color channel.

Poisson image editing

 $+$  $=$ 

We can do better: solve a linear system per color channel.

Let *a* be:

$a : \Omega \to \mathbb{R}$

Poisson image editing

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We can do better: solve a linear system per color channel.

Let a be:

$a : \Omega \to \mathbb{R}$

Let b be:

$b : \Omega \to \mathbb{R}$

Poisson image editing


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=


We can do better: solve a linear system per color channel.

Let a be:

$a : \Omega \to \mathbb{R}$

Let b be:

$b : \Omega \to \mathbb{R}$

Solve for f who takes its boundary conditions from a and the gradients from b:

$$\arg\min_{f} \int_{\Omega} \|\nabla f - \nabla b\|^2 \quad \text{with } f|_{\partial\Omega} = a|_{\partial\Omega}$$

Poisson image editing

Discretize the problem: having $w \times h$ pixels grayscale images a and b, we compute a $w \times h$ pixels image f, solve in the least squares sense:

$$\begin{cases} f_{i+1,j} - f_{i,j} &= b_{i+1,j} - b_{i,j} \quad \forall (i,j) \in [0 \dots w-2] \times [0 \dots h-2] \\ f_{i,j+1} - f_{i,j} &= b_{i,j+1} - b_{i,j} \quad \forall (i,j) \in [0 \dots w-2] \times [0 \dots h-2] \\ f_{i,j} &= a_{i,j} \quad \forall (i,j) \text{ s.t. } i=0 \text{ or } i=w-1 \text{ or } j=0 \text{ or } j=h-1 \end{cases}$$

N.B: sparse system solver!

Poisson image editing

Discretize the problem: having $w \times h$ pixels grayscale images a and b, we compute a $w \times h$ pixels image f, solve in the least squares sense:

$$\begin{cases} f_{i+1,j} - f_{i,j} &= b_{i+1,j} - b_{i,j} \quad \forall (i,j) \in [0 \dots w-2] \times [0 \dots h-2] \\ f_{i,j+1} - f_{i,j} &= b_{i,j+1} - b_{i,j} \quad \forall (i,j) \in [0 \dots w-2] \times [0 \dots h-2] \\ f_{i,j} &= a_{i,j} \qquad\qquad\quad \forall (i,j) \text{ s.t. } i=0 \text{ or } i=w-1 \text{ or } j=0 \text{ or } j=h-1 \end{cases}$$

+

=

Caricature

```
x = [100,100,97,93 ...  23,21,19] # 2d closed polyline
y = [0,25,27,28,30 ...  11,6,4,1]
n = len(x)                          # number of points
cx = [x[i] - (x[(i-1+n)%n]+x[(i+1)%n])/2 for i in range(n)] #precompute the
cy = [y[i] - (y[(i-1+n)%n]+y[(i+1)%n])/2 for i in range(n)] #discrete curvature
for _ in range(1000): # Gauss-Seidel iterations
    for i in range(n):
        x[i] = (x[(i-1+n)%n]+x[(i+1)%n])/2 + cx[i]*1.9
        y[i] = (y[(i-1+n)%n]+y[(i+1)%n])/2 + cy[i]*1.9
```

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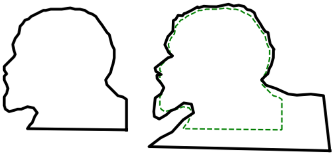
```



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```

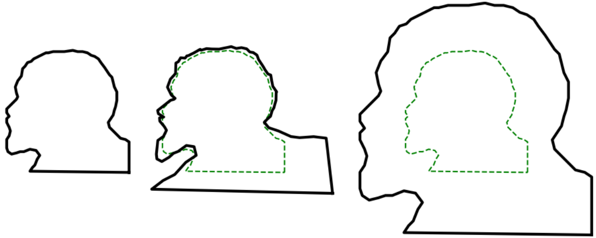

Almost, but no :(

Caricature

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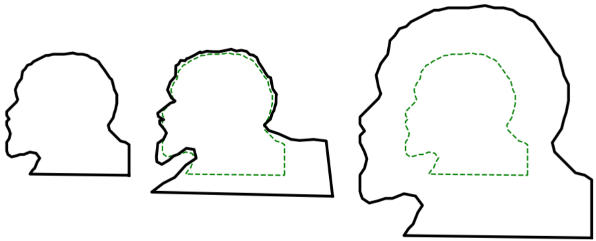

Almost, but no :(

Least squares equivalent:

$$\arg\min_{\{x'_i\}_{i=0}^{n-1}} \sum_{\forall \text{ edge } (i,j)} \left(x'_j - x'_i - c\cdot(x_j - x_i)\right)^2$$

x_i are the input coordinates and x'_i are the unknowns (separable in x and y)

Caricature

A quick fix:

$$\underset{\{x'_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } (i,j)} \left(x'_j - x'_i - c_0 \cdot (x_j - x_i) \right)^2$$

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$$\underset{\{x'_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } (i,j)} \left(x'_j - x'_i - c_0 \cdot (x_j - x_i) \right)^2 + \sum_{\forall \text{ vertex } i} c_1^2 \left(x'_i - x_i \right)^2$$

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$$\underset{\{x'_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } (i,j)} \left(x'_j - x'_i - c_0 \cdot (x_j - x_i) \right)^2 + \sum_{\forall \text{ vertex } i} c_1^2 \left(x'_i - x_i \right)^2$$

$$\left\{ \begin{array}{lllllll} -x'_0 & +x'_1 & & & & & = c_0 \cdot (x_1 - x_0) \\ & -x'_1 & +x'_2 & & & & = c_0 \cdot (x_2 - x_1) \\ & & \ddots & \ddots & & & \vdots \\ & & & -x'_{n-2} & +x'_{n-1} & & = c_0 \cdot (x_{n-2} - x_{n-1}) \\ x'_0 & & & & -x'_{n-1} & & = c_0 \cdot (x_{n-1} - x_0) \\ c_1 \cdot x'_0 & & & & & & = c_1 \cdot x_0 \\ & c_1 \cdot x'_1 & & & & & = c_1 \cdot x_1 \\ & & \ddots & & & & \vdots \\ & & & & c_1 \cdot x'_{n-1} & & = c_1 \cdot x_{n-1} \end{array} \right.$$

Caricature

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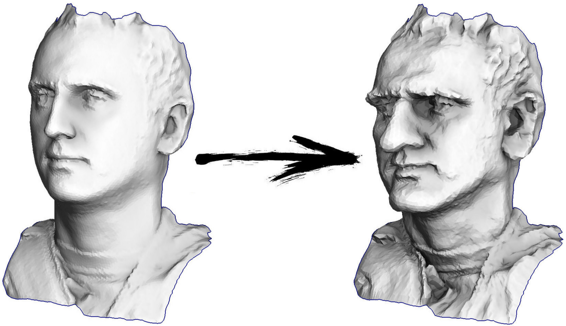
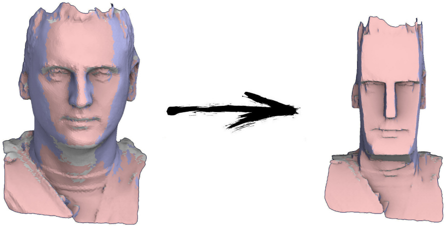


And it works out of the box for 3d surfaces as well!

Cubify it!

$$\vec{a}_{ijk} := \underset{\vec{a}\in\{(1,0,0),(0,1,0),(0,0,1)\}}{\arg\max} \left|\vec{a}\cdot\vec{N}_{ijk}\right|$$



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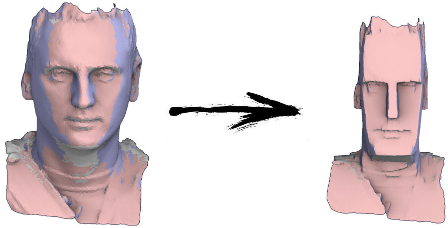

Let $\vec{e}_{ij} := \vec{x}_j - \vec{x}_i$ be the input geometry, and $\vec{e}'_{ij} := \vec{x}'_j - \vec{x}'_i$ the unknowns.

Quick test

What would be the result?

$$\mathop{\arg\min}_{\{\vec{x}'_i\}_{i=0}^{n-1}} \sum_{\forall \text{ edge } ij} \left\|\vec{e}'_{ij} - \vec{e}_{ij}\right\|^2$$

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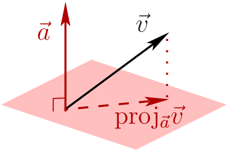


$$\mathrm{proj}_{\vec{a}}\vec{v} := \vec{v} - \frac{\vec{v}\cdot\vec{v}}{\vec{a}\cdot\vec{a}}\vec{a}$$

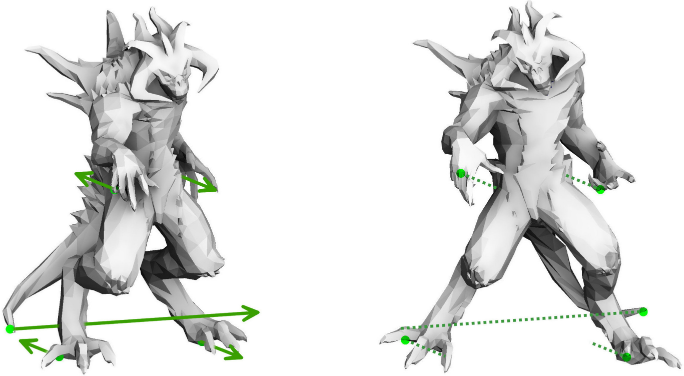
Let $\vec{e}_{ij} := \vec{x}_j - \vec{x}_i$ be the input geometry, and $\vec{e}'_{ij} := \vec{x}'_j - \vec{x}'_i$ the unknowns.

$$\underset{\{\vec{x}'_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } ij} \left\|\vec{e}'_{ij} - \vec{e}_{ij}\right\|^2 + \sum_{\forall \text{ triangle } ijk} \boxed{c} \cdot \left(\left\|\vec{e}'_{ij} - \mathrm{proj}_{\vec{a}_{ijk}}\vec{e}_{ij}\right\|^2 + \left\|\vec{e}'_{jk} - \mathrm{proj}_{\vec{a}_{ijk}}\vec{e}_{jk}\right\|^2 + \left\|\vec{e}'_{ki} - \mathrm{proj}_{\vec{a}_{ijk}}\vec{e}_{ki}\right\|^2 \right)$$

N.B: still a separable problem

As-rigid-as-possible deformation

Problem: compute a deformation of a mesh with several constrained vertex positions.



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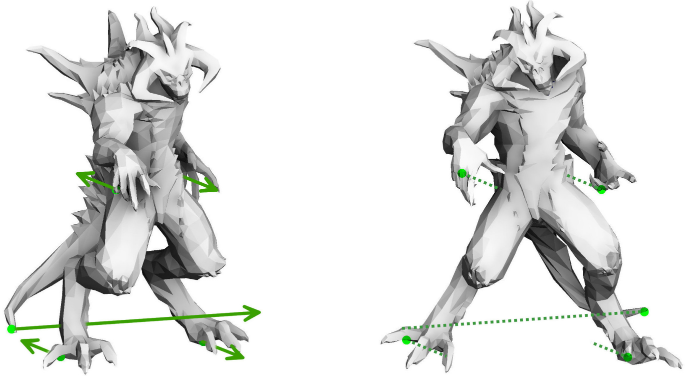

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Choose a subset of vertices $\mathcal{I} \subset [0 \dots n-1]$, to have final position $\{\vec{p}_k\}_{k\in\mathcal{I}}$

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Naive solution

$$\underset{\{\vec{x}'_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } ij} \left\| \vec{e}'_{ij} - \vec{e}_{ij} \right\|^2 \text{ subject to the constraints } \vec{x}'_k = p_k \ \ \forall k \in \mathcal{I}$$

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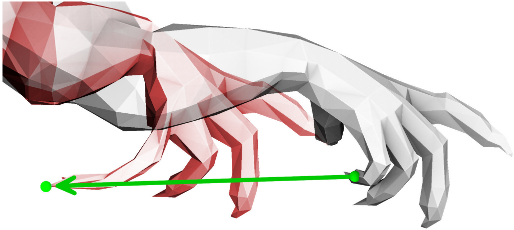
Problem: huge stretching near the constraints



As-rigid-as-possible deformation

Penalize stretching: make the deformation be a rotation locally

Introduce new variables: a rotation matrix R_i per vertex

$$\underset{\{\vec{x}_i', R_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } ij} \left\| \vec{e}_{ij}' - R_i \times \vec{e}_{ij} \right\|^2$$

As-rigid-as-possible deformation

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N.B: it is a non-linear problem!

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Solve alternatively for the vertex positions $\{\vec{x}'_i\}_{i=0}^{n-1}$ and rotations $\{R_i\}_{i=0}^{n-1}$:

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- Solving for $\{\vec{x}'_i\}_{i=0}^{n-1}$ having $\{R_i\}_{i=0}^{n-1}$ fixed is a **separable** linear problem: 3 conjugate gradients calls

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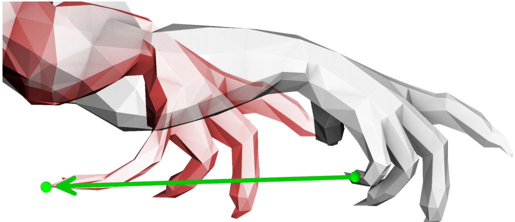
- Solving for $\{\vec{x}_i'\}_{i=0}^{n-1}$ having $\{R_i\}_{i=0}^{n-1}$ fixed is a **separable** linear problem: 3 conjugate gradients calls
- Solving for $\{R_i\}_{i=0}^{n-1}$ is the *orthogonal Procrustes problem* (closed form solution): let $U_i \Sigma_i V_i^\top$ be the s.v.d. of the 3×3 matrix $\sum_{j \text{ neighbor of } i} \vec{e}_{ij}' \vec{e}_{ij}^\top$, then $R_i \leftarrow U_i V_i^\top$

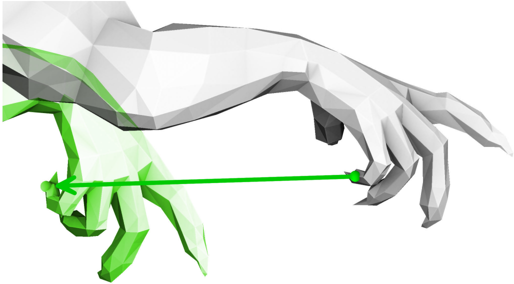
As-rigid-as-possible deformation

Penalize stretching: make the deformation be a rotation locally

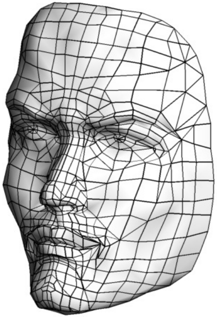
Introduce new variables: a rotation matrix R_i per vertex

$$\underset{\{\vec{x}'_i, R_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } ij} \left\| \vec{e}'_{ij} - R_i \times \vec{e}_{ij} \right\|^2$$

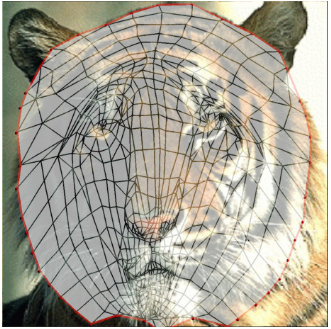




Mix the coordinates: least squares conformal maps

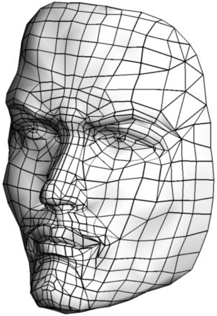


$$U(x, y, z) \longrightarrow = (u, v)$$



$$U^{-1}(u, v) \longrightarrow = (x, y, z)$$

Mix the coordinates: least squares conformal maps



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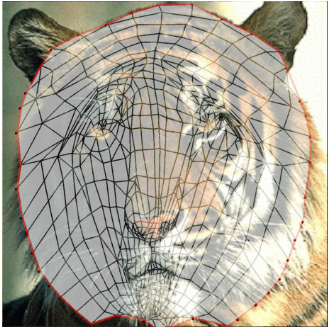
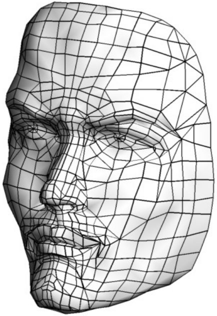


$$U^{-1}(u, v) \longrightarrow = (x, y, z)$$

How to create such a map?

Mix the coordinates: least squares conformal maps



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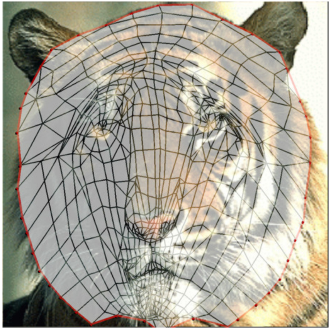


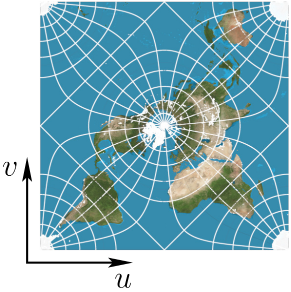
$$U^{-1}(u,v) \longrightarrow = (x,y,z)$$

How to create such a map?

Let us compute a conformal map!

Mix the coordinates: least squares conformal maps

Maps that preserve angles
(but not distances or areas):



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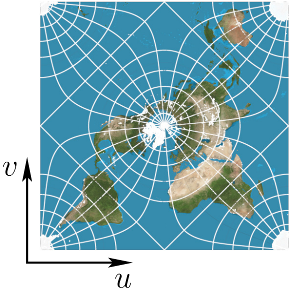
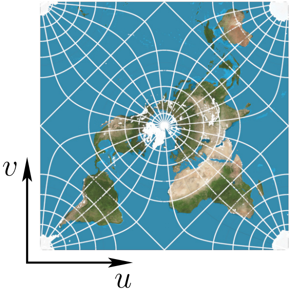


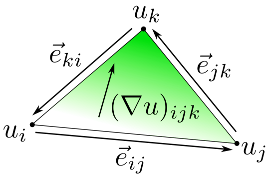
Cauchy–Riemann condition:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}$$
$$\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

Mix the coordinates: least squares conformal maps

Maps that preserve angles (but not distances or areas):





Sample tex coords at vertices: (u_i, v_i), interpolate linearly inside triangles.

$\Rightarrow$ The gradient is **constant** across each triangle

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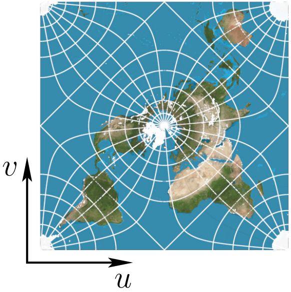

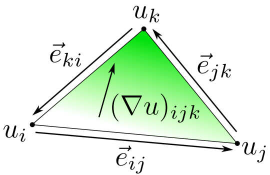

Sample tex coords at vertices: (u_i, v_i), interpolate linearly inside triangles.
$\Rightarrow$ The gradient is **constant** across each triangle

Very simple formula for a gradient over a triangle:

$$\vec{N}_{ijk} \times (\nabla u)_{ijk} = -\frac{1}{2A_{ijk}}(u_i\vec{e}_{jk} + u_j\vec{e}_{ki} + u_k\vec{e}_{ij})$$

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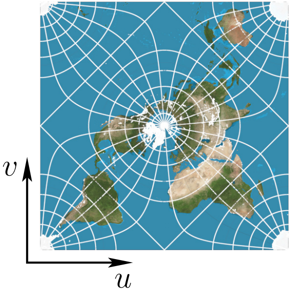

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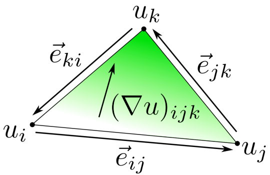

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$$\vec{N}_{ijk} \times (\nabla u)_{ijk} = -\frac{1}{2A_{ijk}}(u_i \vec{e}_{jk} + u_j \vec{e}_{ki} + u_k \vec{e}_{ij})$$

Sum failure of Cauchy–Riemann condition to hold:

$$\arg\min_{u,v} \sum_{\forall \text{ triangle } ijk} A_{ijk} \left((\nabla u)_{ijk} - \vec{N}_{ijk} \times (\nabla v)_{ijk} \right)^2$$

N.B: Beware of the zero solution!

Mix the coordinates: least squares conformal maps

Quick hack: pin two arbitrary vertices.

Dmitry Sokolov

Least squares for programmers

— with color plates —