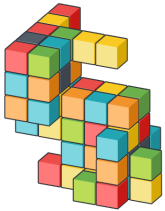

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Least squares for programmers

— with color plates —

Dmitry Sokolov, Nicolas Ray, Étienne Corman

June 3, 2021

The goal

This course is intended for students/engineers/researchers who know how to program in the traditional way: by breaking down complex tasks into a sequence of elementary operations over data structures.

An alternative

We can describe what a good result looks like, and let numerical optimization algorithms find it for us.

This course does not require an advanced mathematical background: basic calculus knowledge suffices. A solid programming basis would be of a great aid.

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Coin toss experiment

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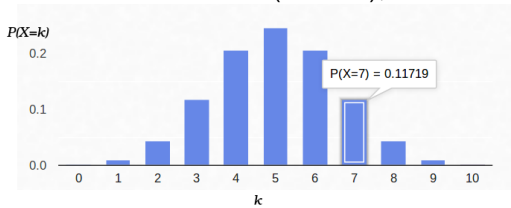

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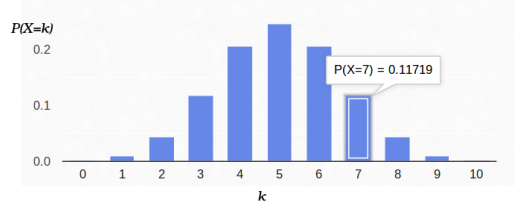

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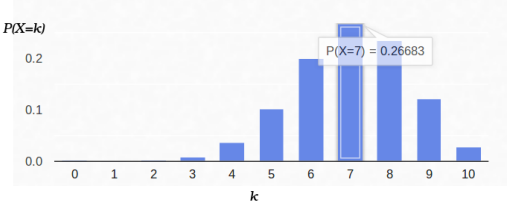

a biased coin ($p = 7/10$)

Coin toss: the likelihood function

Suppose we have a real coin, but we do not know p. However, we can toss it ten times. For example, we have counted seven tails. Would it help us to evaluate p?

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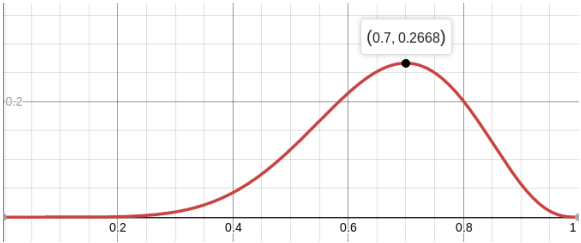

N.B. the function is continuous!

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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).

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

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$$= \underbrace{-N \left(\log \sqrt{2\pi} + \log \sigma \right)}_{\text{does not depend on } \{U_j\}_{j=1}^{N}} - \frac{1}{2\sigma^2} \sum_{j=1}^{N} (U_j - U)^2$$

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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$$U = \frac{\sum_{j=1}^{N} U_j}{N}$$

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$$\sigma = \sqrt{\frac{\sum_{j=1}^{N} (U_j - U)^2}{N}}$$

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

Linear regression

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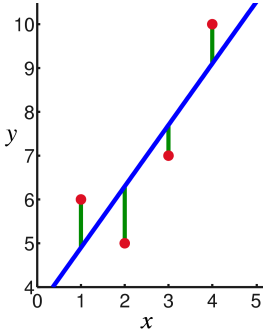

Linear regression

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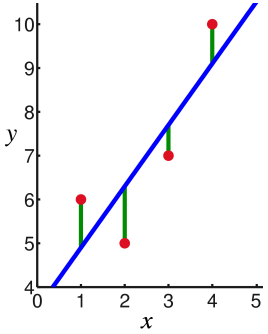
$$a = \frac{N \sum_{j=1}^{N} x_j y_j - \sum_{j=1}^{N} x_j \sum_{j=1}^{N} y_j}{N \sum_{j=1}^{N} x_j^2 - \left(\sum_{j=1}^{N} x_j \right)^2}$$



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

The takeaway message

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

The more 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.

Table of Contents

Smooth an array

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

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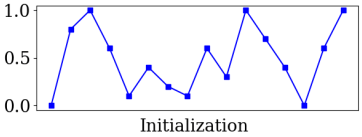

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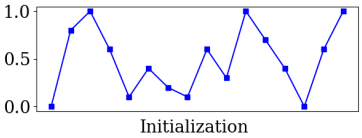
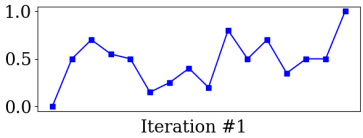


Initialization



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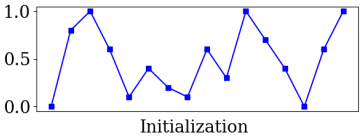

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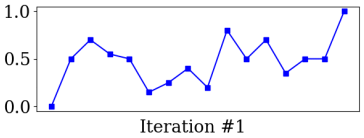

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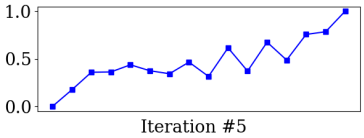

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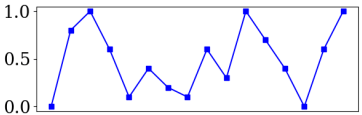

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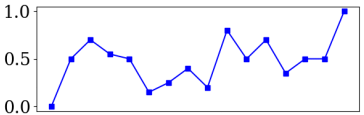

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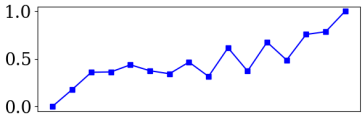
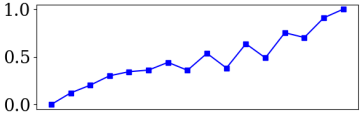


Iteration #5



Iteration #10

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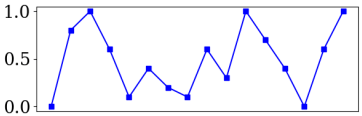

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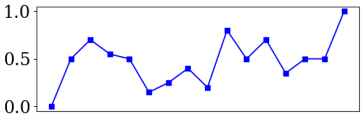

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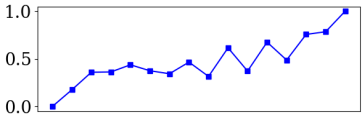
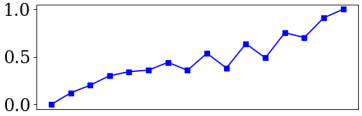
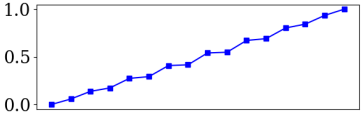


Iteration #5



Iteration #10



Iteration #50

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for _ in range(512):
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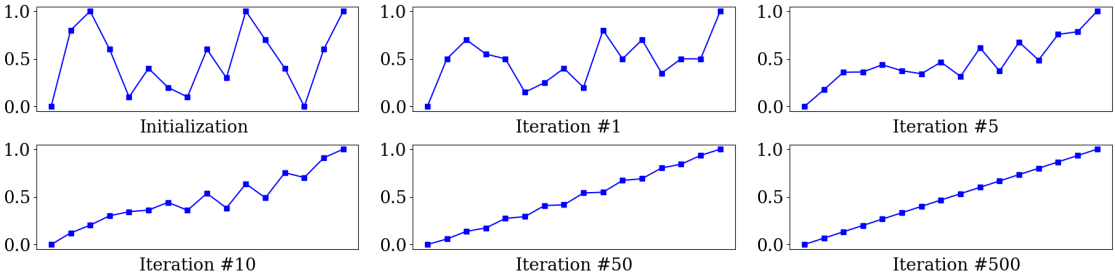

The Jacobi iterative method

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)}) \\
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\end{aligned}
$$

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

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

Jacobi vs Gauß–Seidel

$$x_1^{(1)} = \frac{1}{a_{11}}(b_1 - a_{12}x_2^{(0)} - a_{13}x_3^{(0)} - \cdots - a_{1n}x_n^{(0)})$$

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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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Gauß-Seidel:

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

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Jacobi:

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

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```

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]

for _ in range(512):
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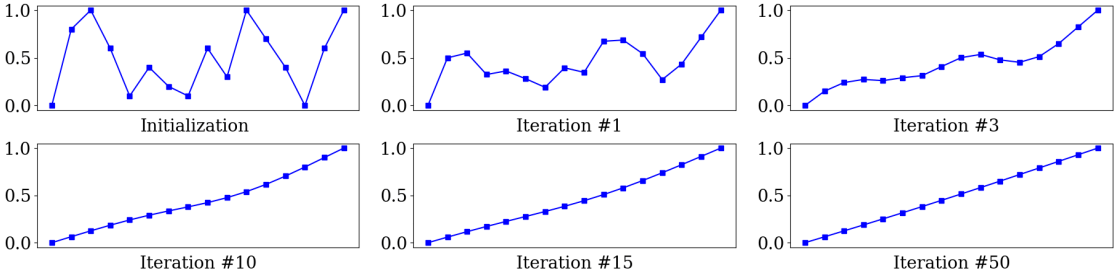
```



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

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```

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

It also works for 3d surfaces

```
from mesh import Mesh
import scipy.sparse

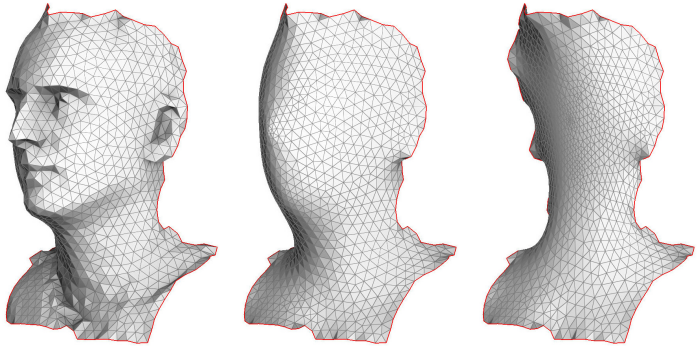
m = Mesh("input-face.obj") # load mesh

A = scipy.sparse.lil_matrix((m.nverts, m.nverts))
for v in range(m.nverts): # build a smoothing operator as a sparse matrix
    if m.on_border(v):
        A[v,v] = 1 # fix boundary verts
    else:
        neigh_list = m.neighbors(v)
        for neigh in neigh_list:
            A[v, neigh] = 1/len(neigh_list) # 1-ring barycenter for interior
A = A.tocsr() # sparse row matrix for fast matrix-vector multiplication

for _ in range(8192): # smooth the surface through Gauss-Seidel iterations
    m.V = A.dot(m.V)

print(m) # output smoothed mesh
```

It also works for 3d surfaces



input 10 iterations 1000 iterations

Prescribe the right hand side

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

for _ in range(512):
    for i in range(1, len(x)-1):
        x[i] = ( x[i-1] + x[i+1] - (i+15)/15**3 )/2.
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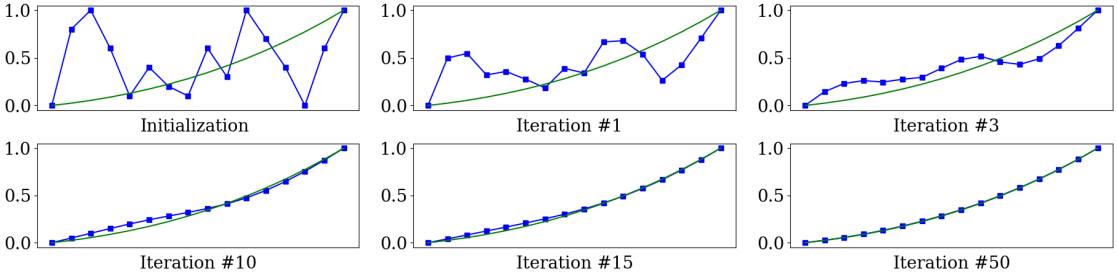

Well duh... Of course it is a cubic polynomial!

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

Matrices and numbers

What is a number a?

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float a = 2.7;
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float y(float x) {
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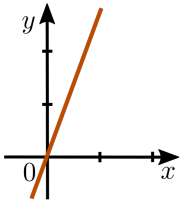

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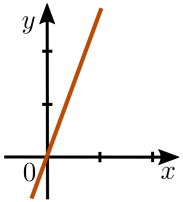

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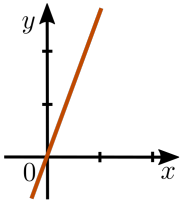

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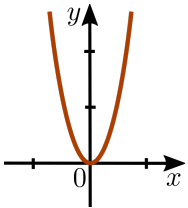

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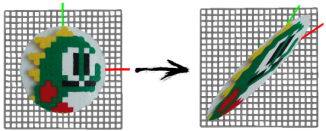

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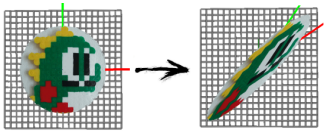

Or $f(x) = x^\top Ax = \sum_i \sum_j a_{ij} x_i x_j : \mathbb{R}^2 \to \mathbb{R}$?

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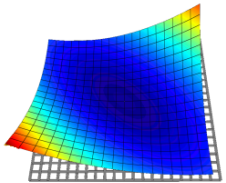

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Definition

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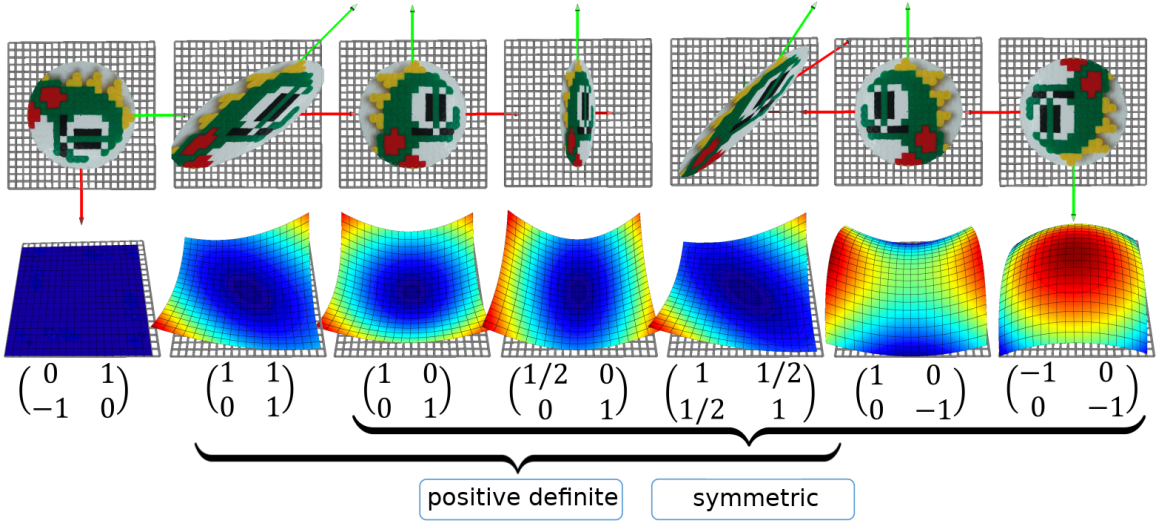
This definition looks pretty awkward, but it applies perfectly to matrices:

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?



Minimizing a 1d quadratic function

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

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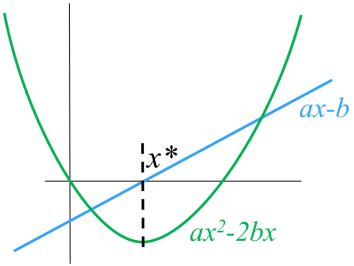

In 1d, the solution x^* of the equation $ax - b = 0$ solves the minimization problem $\arg\min_x (ax^2 - 2bx)$ as well.

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

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

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

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

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

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$$= \frac{\partial}{\partial x_i} \left(\underbrace{\sum_{k_1 \neq i} \sum_{k_2 \neq i} a_{k_1 k_2} x_{k_1} x_{k_2}}_{k_1 \neq i, k_2 \neq i} + \underbrace{\sum_{k_2 \neq i} a_{i k_2} x_i x_{k_2}}_{k_1 = i, k_2 \neq i} + \underbrace{\sum_{k_1 \neq i} a_{k_1 i} x_{k_1} x_i}_{k_1 \neq i, k_2 = i} + \underbrace{a_{ii} x_i^2}_{k_1 = i, k_2 = i} \right) =$$

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$$= \frac{\partial}{\partial x_i}\left(\underbrace{\sum_{k_1 \neq i}\sum_{k_2 \neq i} a_{k_1 k_2} x_{k_1} x_{k_2}}_{k_1 \neq i, k_2 \neq i} + \underbrace{\sum_{k_2 \neq i} a_{i k_2} x_i x_{k_2}}_{k_1 = i, k_2 \neq i} + \underbrace{\sum_{k_1 \neq i} a_{k_1 i} x_{k_1} x_i}_{k_1 \neq i, k_2 = i} + \underbrace{a_{ii} x_i^2}_{k_1 = i, k_2 = i}\right) =$$

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$$= \sum_j (a_{ij} + a_{ji}) x_j \qquad \Rightarrow \nabla (x^\top A x) = (A + A^\top) x$$

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

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

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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:

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

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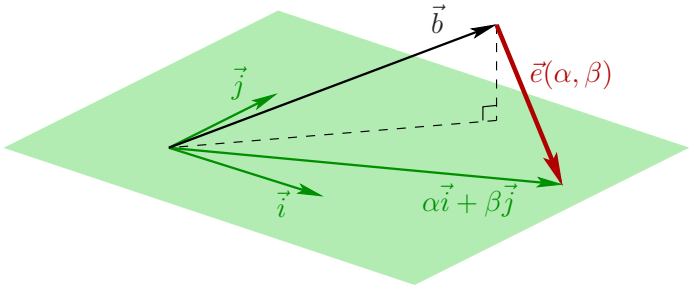
Solve for $\arg\min_{\alpha,\beta} \|\vec{e}(\alpha,\beta)\|$, where $\vec{e}(\alpha,\beta) := \alpha\vec{i} + \beta\vec{j} - \vec{b}$:



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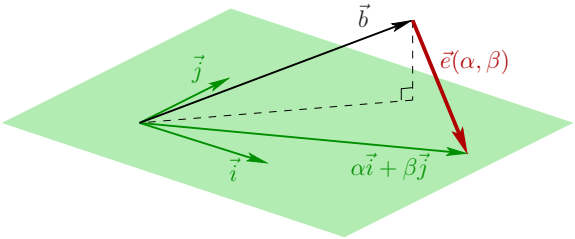

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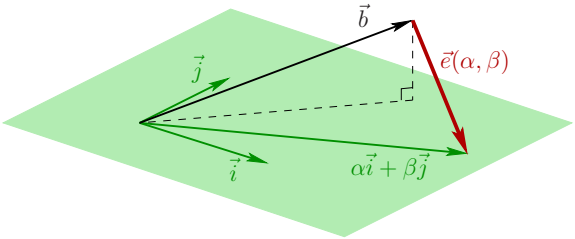

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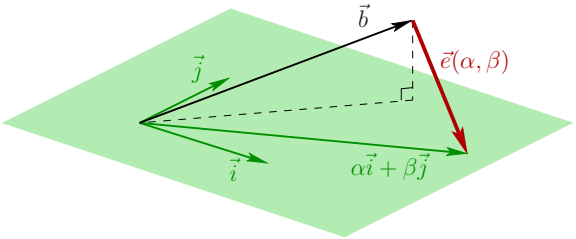

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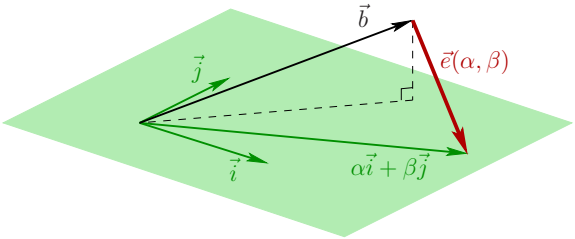

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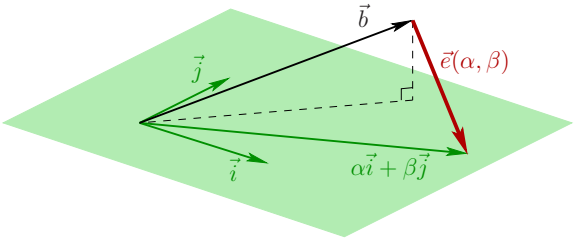

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$$A^\top (Ax - b) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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

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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:

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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 $A'x = b'$.

Table of Contents

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:

$$v_{i+1} = v_i + u_i = v_0 + \sum_{j=0}^{i} u_j$$

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

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

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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:

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

Linear-quadratic regulator

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

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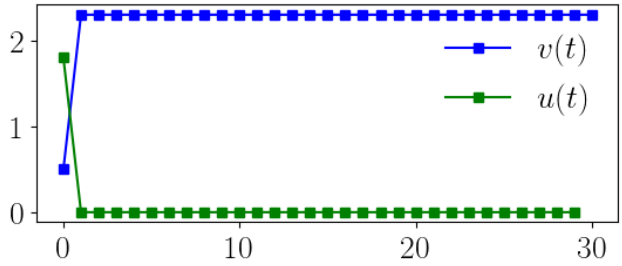
Ouch... Quite brutal accelerations: obvious solution $u_0 = v_n - v_0$, $u_i = 0 \; \forall i > 0$.



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Ok, no problem, let us penalize large accelerations:

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

Solve in the least squares sense:

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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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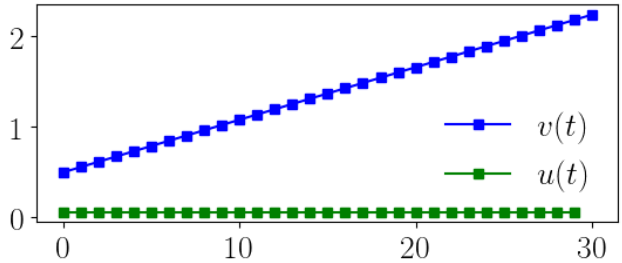

Low acceleration, however the transient time becomes unacceptable.

Linear-quadratic regulator

Optimize for competing goals:

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

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N.B. Note the tradeoff coefficients!

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

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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)]
```

Linear-quadratic regulator

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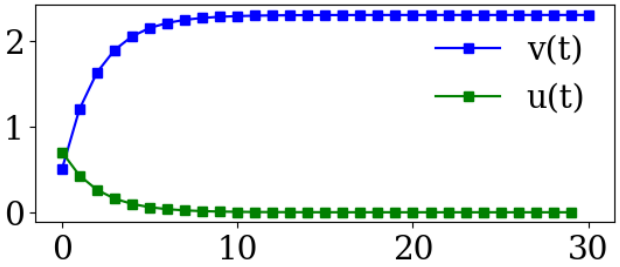


Linear-quadratic regulator

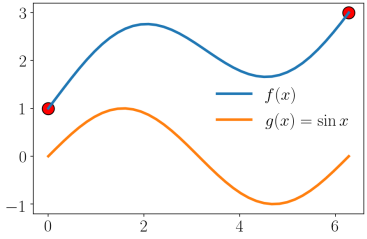
The takeaway message

For the same problem, the same choice of variables, tweaking the objective function produces very different results. Use it!

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



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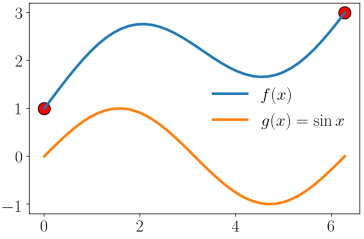

Neanderthal method:

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

Least squares formulation:

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

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Discretization:

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

Poisson's equation

Least squares formulation:

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

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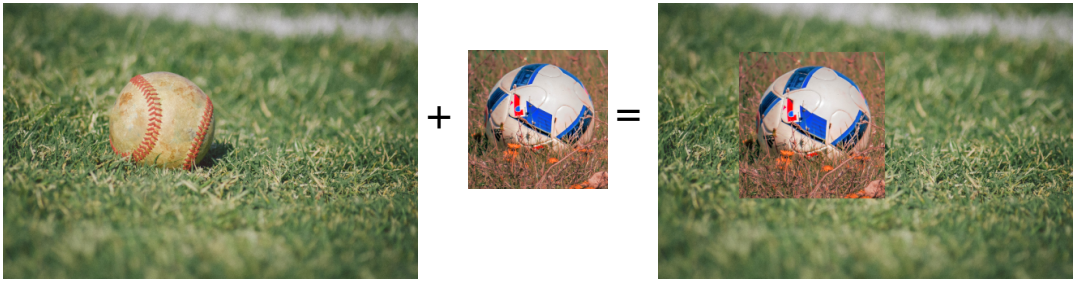
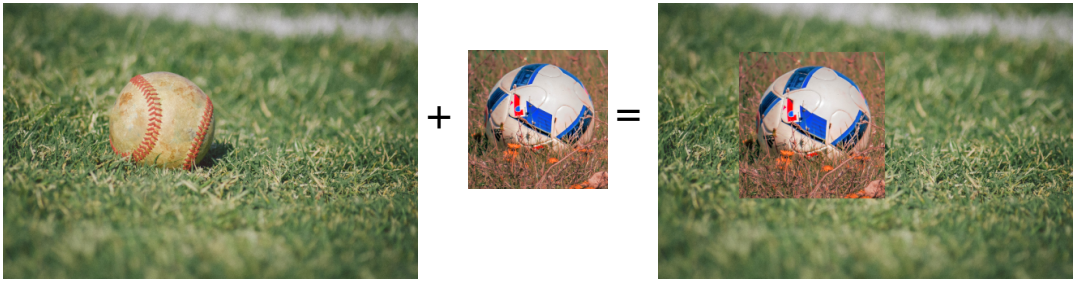
```
import numpy as np
n,f0,fn = 32,1.,3.
g = [np.sin(x) for x in np.linspace(0, 2*np.pi, n)]
A = np.matrix(np.zeros((n-1,n-2)))
np.fill_diagonal(A,      1)
np.fill_diagonal(A[1:], -1)
b = np.matrix([[g[i]-g[i-1]] for i in range(1,n)])
b[ 0,0] = b[ 0,0] + f0
b[-1,0] = b[-1,0] - fn
f = [f0] + (np.linalg.inv(A.T*A)*A.T*b).T.tolist()[0]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

Poisson image editing

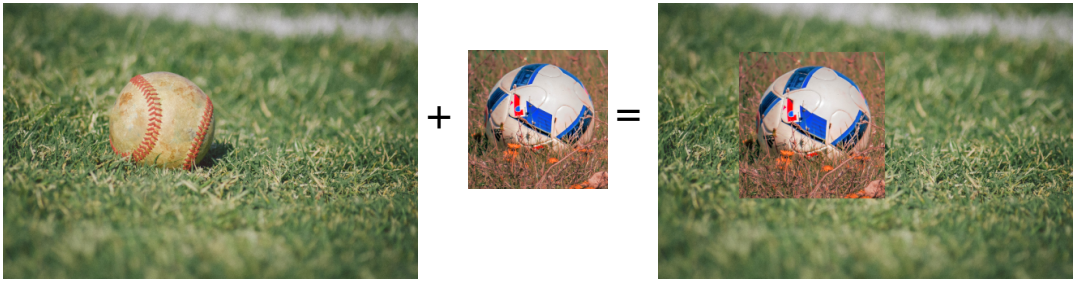


Poisson image editing



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

Poisson image editing

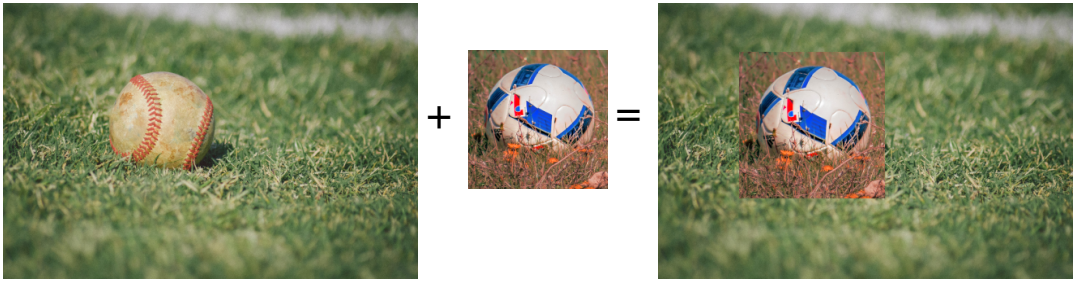


We can do better: solve a linear system per color channel.

Let a be:

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

Poisson image editing



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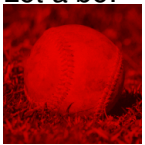

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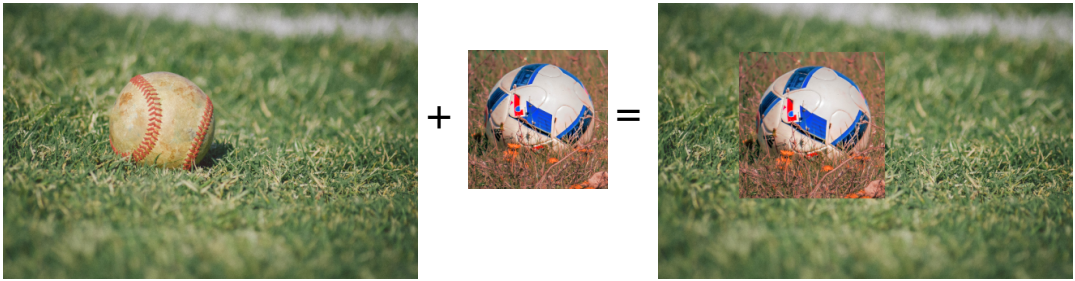
Let b be:

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

Poisson image editing



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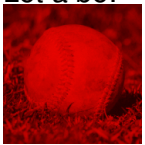

$a : \Omega \to \mathbb{R}$

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:

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

N.B: sparse system solver!

Poisson image editing

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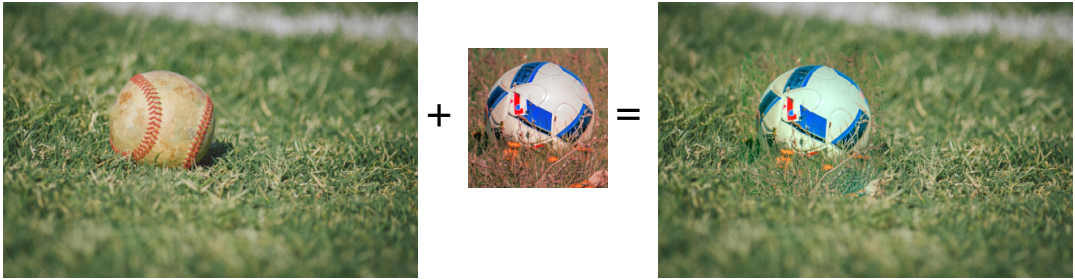

```
import matplotlib.image as mpimg
import scipy.sparse
from scipy.sparse.linalg import lsmr
base = mpimg.imread('baseball.png')
foot = mpimg.imread('football.png')
ox,oy, w,h = 100,60, len(foot[0]),len(foot) # working rectangle

A = scipy.sparse.lil_matrix((2*w+2*h + 2*(w-1)*(h-1), w*h))
for i in range(0,w):
    A[  i, i         ] = 1 #    top data fitting
    A[w+i, i+(h-1)*w] = 1 # bottom data fitting
for j in range(0,h):
    A[2*w  +j,     j*w] = 1 #  left data fitting
    A[2*w+h+j, w-1+j*w] = 1 # right data fitting
cnt = 2*w+2*h
for j in range(0,h-1): # gradient matrix
    for i in range(0,w-1):
        A[cnt,   i   + j*w] = -1
        A[cnt,   i+1 + j*w] =  1
        A[cnt+1, i +   j   *w] = -1
        A[cnt+1, i + (j+1)*w] =  1
        cnt += 2
A = A.tocsc() # sparse row matrix for fast matrix-vector multiplication

for channel in range(3):
    b = A.dot(foot[:,:,channel].flatten()) # fill the gradient part of the r.h.s.
    b[0:w]     = base[oy,ox:ox+w,channel]   # top data fitting
    b[w:2*w]   = base[oy+h,ox:ox+w,channel] # bottom data fitting
    b[2*w  :2*w+h]   = base[oy:oy+h, ox, channel]   # left data fitting
    b[2*w+h:2*w+2*h] = base[oy:oy+h, ox+w, channel] # right data fitting

    x = lsmr(A, b)[0] # call the least squares solver
    base[oy:oy+h,ox:ox+h, channel] = x.reshape((h, w)) # glue the football
mpimg.imsave('result.png', base)
```

Poisson's equation

The takeaway message

Poisson's problem is one of the most used tools in geometry processing.
Know your friends!

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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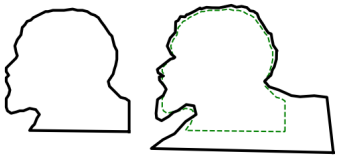

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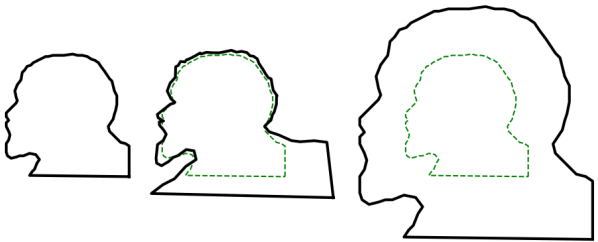
```

Almost, but no :(



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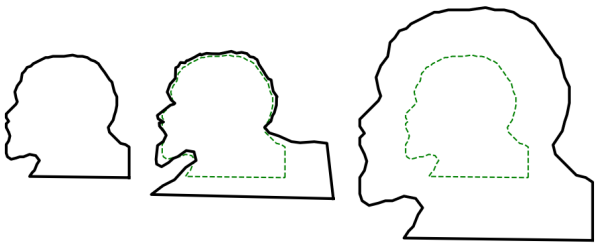
```



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:

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

Caricature

A quick fix:

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

Caricature

A quick fix:

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

$$\begin{cases}
-x'_0 + x'_1 = c_0 \cdot (x_1 - x_0) \\
-x'_1 + x'_2 = c_0 \cdot (x_2 - x_1) \\
\ddots \quad \ddots \quad \vdots \\
-x'_{n-2} + x'_{n-1} = c_0 \cdot (x_{n-2} - x_{n-1}) \\
x'_0 - x'_{n-1} = c_0 \cdot (x_{n-1} - x_0) \\
c_1 \cdot x'_0 = c_1 \cdot x_0 \\
c_1 \cdot x'_1 = c_1 \cdot x_1 \\
\ddots \quad \vdots \\
c_1 \cdot x'_{n-1} = c_1 \cdot x_{n-1}
\end{cases}$$

Caricature

A quick fix:

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

```
import numpy as np

def amplify(x):
    n = len(x)
    A = np.matrix(np.zeros((2*n,n)))
    b = np.matrix(np.zeros((2*n,1)))
    for i in range(n):
        A[i, i] = 1. # amplify the curvature
        A[i, (i+1)%n] = -1.
        b[i, 0] = (x[i] - x[(i+1)%n])*1.9

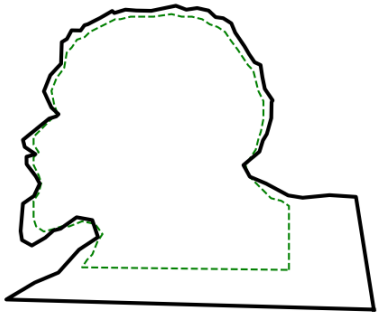
        A[n+i, i] =    1*.3 # light data fitting term
        b[n+i, 0] = x[i]*.3
    return (np.linalg.inv(A.T*A)*A.T*b).tolist()

x = [100,100,97,93,91,87,84,83,85,87,88,89,90,90,90,88,87,86,84,82,80,77,75,72,69,66,62,58,54,47,42,38,
     34,32,28,24,22,20,17,15,13,12,9,7,8,9,8,6,0,0,2,0,0,2,3,2,0,0,1,4,8,11,14,19,24,27,25,23,21,19]
y = [0,25,27,28,30,34,37,41,44,47,51,54,59,64,66,70,74,78,80,83,86,90,93,95,96,98,99,99,100,99,99,99,98,98,
    96,94,93,91,90,87,85,79,75,70,65,62,60,58,52,49,46,44,41,37,34,30,27,20,17,15,16,17,17,19,18,14,11,6,4,1]
x = amplify(x)
y = amplify(y)
```

Caricature

A quick fix:

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



Caricature

A quick fix:

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

```
from mesh import Mesh
from scipy.sparse.linalg import lsmr
from scipy.sparse import lil_matrix
m = Mesh("input-face.obj") # load mesh

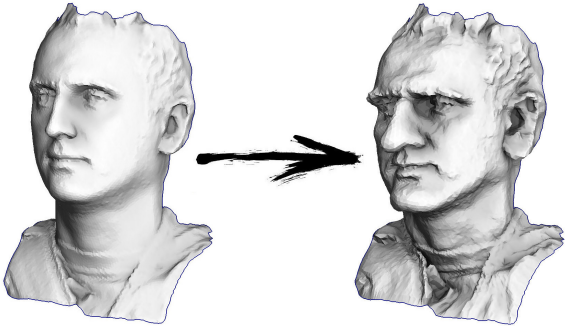
A = lil_matrix((m.nverts+m.ncorners, m.nverts))
for v in range(m.nverts): # per-vertex attachment to the original geometry
    A[v,v] = 10 if m.on_border(v) else .29  # hard on the boundary, light for the interior
for c in range(m.ncorners): # per-half-edge discretization of the derivative
    A[m.nverts+c, m.org(c)] = -1
    A[m.nverts+c, m.dst(c)] =  1
A = A.tocsr() # sparse row matrix for fast matrix-vector multiplication

for dim in range(3): # the problem is separable in x,y,z; the matrix A is the same, the right hand side changes
    b = [m.V[v][dim]*10 if m.on_border(v) else m.V[v][dim]*.29 for v in range(m.nverts)] + \
        [2.5*(m.V[m.dst(c)][dim]-m.V[m.org(c)][dim]) for c in range(m.ncorners)]
    x = lsmr(A, b)[0] # call the least squares solver
    for v in range(m.nverts): # apply the computed distortion
        m.V[v][dim] = x[v]
print(m) # output the deformed mesh
```

Caricature

A quick fix:

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



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

Caricature

A quick fix:

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

The takeaway message

Reformulating as a least squares problem allows for much easier tweaking.

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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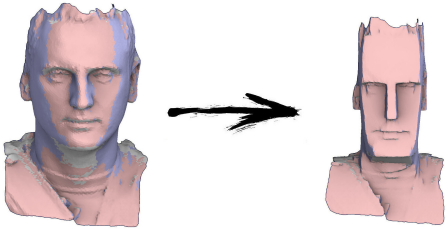


Let $\vec{e}_{ij} := \vec{x}_j - \vec{x}_i$ be the input geometry, and $\vec{e}'_{ij} := \vec{x}'_j - \vec{x}'_i$ the unknowns.

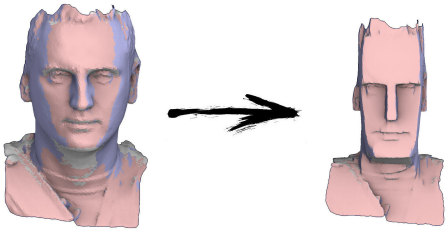
Quick test

What would be the result?

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

Cubify it!

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



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

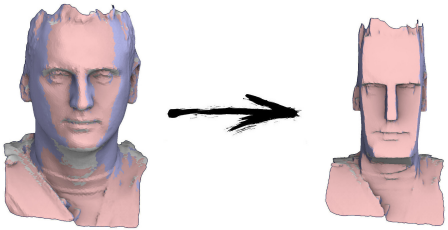
Let $\vec{e}_{ij} := \vec{x}_j - \vec{x}_i$ be the input geometry, and $\vec{e}'_{ij} := \vec{x}'_j - \vec{x}'_i$ the unknowns.

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

N.B: still a separable problem

Cubify it!

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



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.

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

N.B: still a separable problem

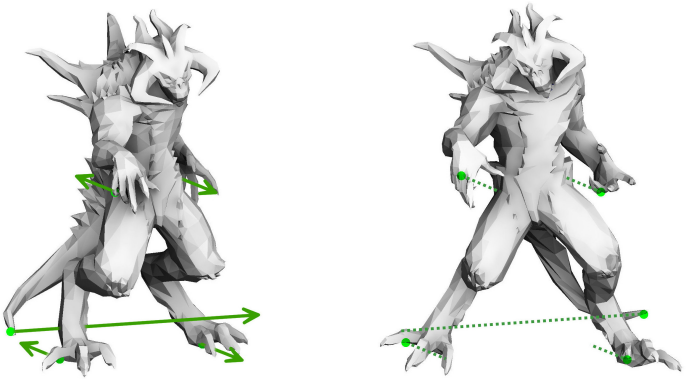
The takeaway message

And again, the same variables, but different tweaking
$\Rightarrow$ completely different results.

```python
import numpy as np
from mesh import Mesh
from scipy.sparse        import lil_matrix
from scipy.sparse.linalg import lsmr

m = Mesh("input-face.obj") # load mesh

def nearest_axis(n):
    return np.argmax([np.abs(np.dot(n, a)) for a in [[1,0,0],[0,1,0],[0,0,1]]])
for dim in range(3): # the problem is separable in x,y,z
    A = lil_matrix((m.ncorners*2, m.nverts))
    b = [m.V[m.dst(c)][dim]-m.V[m.org(c)][dim] for c in range(m.ncorners)]+[0]*m.ncorners
    for c in range(m.ncorners):
        A[c, m.org(c)] = -1 # per-half-edge discretization of the derivative
        A[c, m.dst(c)] =  1

        t = c//3 # triangle id from halfedge id
        if nearest_axis(m.normal(t))==dim:  # flatten the right dimension
            A[c+m.ncorners, m.org(c)] = -2
            A[c+m.ncorners, m.dst(c)] =  2
    A = A.tocsr() # sparse row matrix for fast matrix-vector multiplication
    x = lsmr(A, b)[0] # call the least squares solver
    for v in range(m.nverts): # apply the computed distortion
        m.V[v][dim] = x[v]
print(m) # output the deformed mesh
```

As-rigid-as-possible deformation

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



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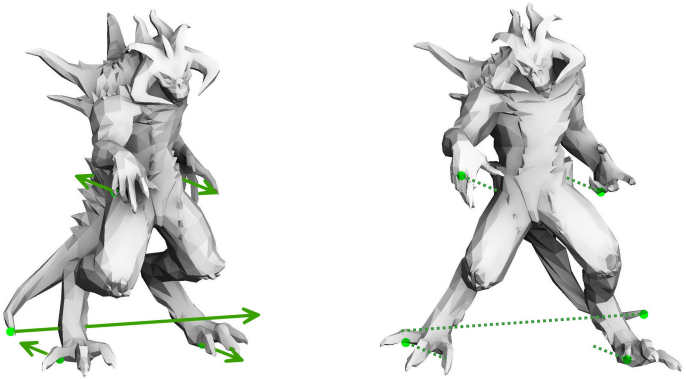

Let $\vec{e}_{ij} := \vec{x}_j - \vec{x}_i$ be the input geometry, and $\vec{e}'_{ij} := \vec{x}'_j - \vec{x}'_i$ the unknowns.
Choose a subset of vertices $\mathcal{I} \subset [0 \dots n-1]$, to have final position $\{\vec{p}_k\}_{k \in \mathcal{I}}$

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Naive solution

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

As-rigid-as-possible deformation

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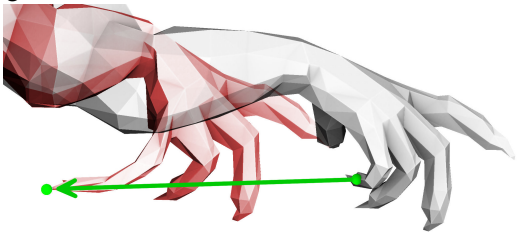
Problem: huge stretching near the constraints



As-rigid-as-possible deformation

Penalize stretching: make the deformation be a rotation locally

Introduce new variables: a rotation matrix R_i per vertex

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

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

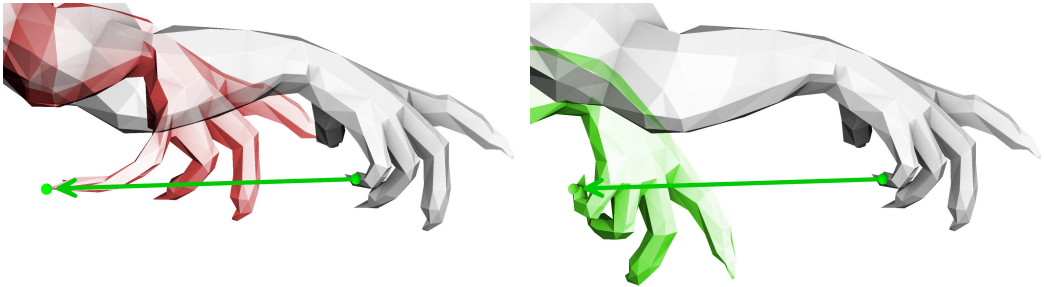
- Solving for $\{\vec{x}'_i\}_{i=0}^{n-1}$ having $\{R_i\}_{i=0}^{n-1}$ fixed is a **separable** linear problem: 3 conjugate gradients calls
- Solving for $\{R_i\}_{i=0}^{n-1}$ is the *orthogonal Procrustes problem* (closed form solution): let $U_i \Sigma_i V_i^\top$ be the s.v.d. of the 3×3 matrix $\sum_{j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

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



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Penalize stretching: make the deformation be a rotation locally

Introduce new variables: a rotation matrix R_i per vertex

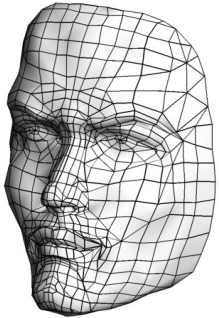
$$\underset{\{\vec{x}'_i, R_i\}_{i=0}^{n-1}}{\arg\min} \sum_{\forall \text{ edge } ij} \left\| \vec{e}'_{ij} - R_i \times \vec{e}_{ij} \right\|^2$$

The takeaway message

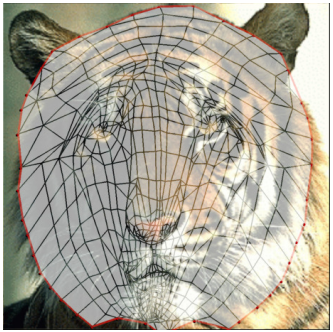
Many nonlinear problems can be solved as a series of linear ones.

```python
from mesh import Mesh
import numpy as np
from scipy.sparse import lil_matrix
from scipy.sparse.linalg import lsmr
from scipy.linalg import svd
m = Mesh("diablo.obj")
eij = [np.matrix(m.V[m.dst(c)] - m.V[m.org(c)]).T for c in range(m.ncorners)] # reference geometry for each half-edge
lock = [1175, 1765, 381, 2383, 1778] # id of the vertices to constrain
disp = [[0,0,-0.5], [0,0,0.5], [0,0,-0.5], [0,0,0.5], [1.5,0,0]] # displacement for the constrained vertices
for v,d in zip(lock, disp): # apply the displacement
    m.V[v] = m.V[v] + d
A = lil_matrix((m.ncorners+len(lock), m.nverts))
for c in range(m.ncorners): # Least-squares verion of Poisson's problem
    A[c, m.dst(c)], A[c, m.org(c)] =  1, -1
for i,v in enumerate(lock):  # the vertices are locked
    A[m.ncorners+i, v] = 100 # via quadratic penalty
A = A.tocsr() # convert to compressed sparse row format for faster matrix-vector muliplications
for _ in range(100):
    R = [] # rotation per vertex
    for v in range(m.nverts): # solve for rotations
        M = np.zeros(3)
        c = m.v2c[v] # half-edge departing from v
        while True: # iterate through all half-edges departing from v
            M = M + np.matrix(m.V[m.dst(c)] - m.V[m.org(c)]).T*eij[c].T
            c = m.c2c[c] # next around vertex
            if c==m.v2c[v]: break
        U, s, VT = svd(M)
        R.append(np.dot(U,VT)) # rotation matrix for the neighborhood of vertex v
    for dim in range(3): # the problem is separable in x,y,z
        b = [(R[m.org(c)]*eij[c])[dim,0] for c in range(m.ncorners)] + [100*m.V[v][dim] for v,d in zip(lock, disp)]
        x = lsmr(A, b)[0] # call the least squares solver
        for v in range(m.nverts): # apply the computed deformation
            m.V[v][dim] = x[v]
print(m) # output the deformed mesh
```

Mix the coordinates: least squares conformal maps

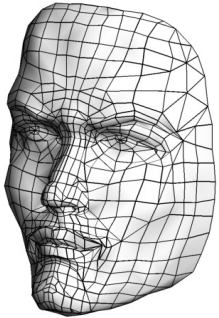


$$U(x, y, z) = (u, v)$$



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

Mix the coordinates: least squares conformal maps



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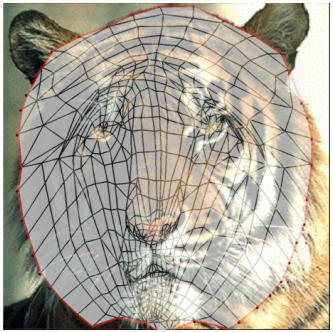
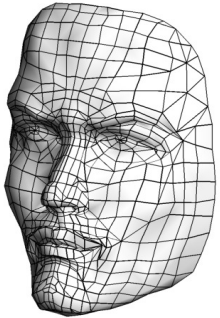


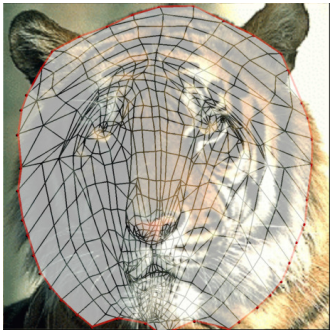
$$U^{-1}(u, v) = (x, y, z)$$

How to create such a map?

Mix the coordinates: least squares conformal maps



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



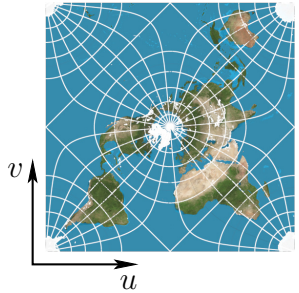
$$U^{-1}(u, v) = (x, y, z)$$

How to create such a map?

Let us compute a conformal map!

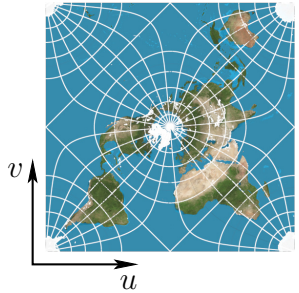
Mix the coordinates: least squares conformal maps

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



Mix the coordinates: least squares conformal maps

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

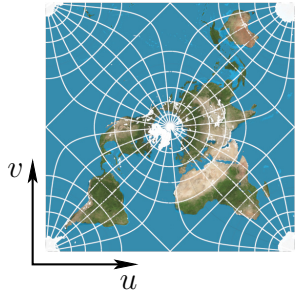


Cauchy–Riemann condition:

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

Mix the coordinates: least squares conformal maps

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



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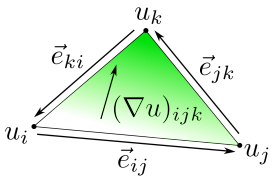
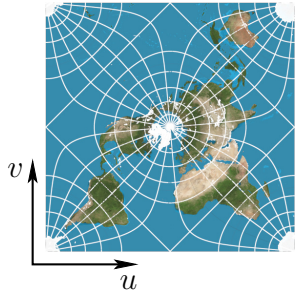


Sample tex coords at vertices: (u_i, v_i), interpolate linearly inside triangles.

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

Mix the coordinates: least squares conformal maps

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



Cauchy–Riemann condition:

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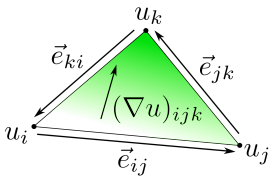

Sample tex coords at vertices: (u_i, v_i), interpolate linearly inside triangles.

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

Very simple formula for a gradient over a triangle:

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

Mix the coordinates: least squares conformal maps

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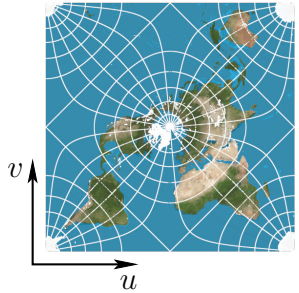

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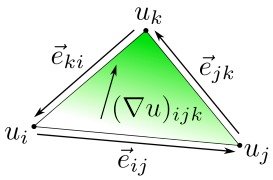

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Sum failure of Cauchy–Riemann condition to hold:

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

N.B: Beware of the zero solution!

Mix the coordinates: least squares conformal maps

Quick hack: pin two arbitrary vertices.

```
import mesh
import numpy as np
import scipy.sparse
from scipy.sparse.linalg import lsmr

m = mesh.Mesh("input-face.obj") # load mesh
lock1, lock2 = 10324%m.nverts, 35492%m.nverts  # select two arbitrary vertices to pin

A = scipy.sparse.lil_matrix((2*m.ntriangles+4, 2*m.nverts)) # the variables are packed as u0,v0,u1,v1, ...
for (t,[i,j,k]) in enumerate(m.T): # for each triangle ijk
    [eij, ejk, eki] = mesh.project_triangle(m.V[i], m.V[j], m.V[k]) # project the triangle to a local 2d basis
    A[t*2+0, i*2  ] =  ejk[0] # (grad u)[0] = (grad v)[1]
    A[t*2+0, j*2  ] =  eki[0]
    A[t*2+0, k*2  ] =  eij[0]
    A[t*2+0, i*2+1] =  ejk[1]
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    A[t*2+0, k*2+1] =  eij[1]
    A[t*2+1, i*2  ] =  ejk[1] # (grad u)[1] = -(grad v)[0]
    A[t*2+1, j*2  ] =  eki[1]
    A[t*2+1, k*2  ] =  eij[1]
    A[t*2+1, i*2+1] = -ejk[0]
    A[t*2+1, j*2+1] = -eki[0]
    A[t*2+1, k*2+1] = -eij[0]
A[-1,lock2*2+1] = A[-2,lock2*2+0] = A[-3,lock1*2+1] = A[-4,lock1*2+0] = 10 # quadratic penalty
A = A.tocsr() # convert to compressed sparse row format for faster matrix-vector muliplications

b = [0]*(2*m.ntriangles) + [0,0,10,10] # one pinned to (0,0), another to (1,1)
x = lsmr(A, b)[0] # call the least squares solver

for v in range(m.nverts): # apply the computed flattening
    m.V[v] = np.array([x[v*2], x[v*2+1], 0])
print(m) # output the deformed mesh
```

Table of Contents

Binary classification: a naive approach

Learning database: n real numbers and the corresponding colors (red and green).
Problem: build a classifying function $\mathbb{R} \to \{\text{red}, \text{green}\}$.

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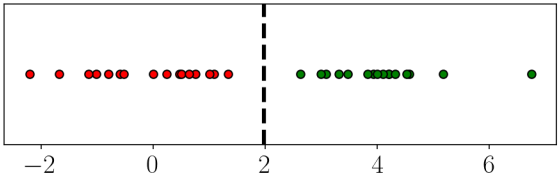

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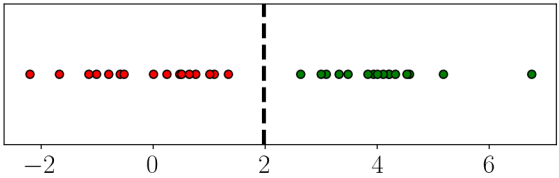
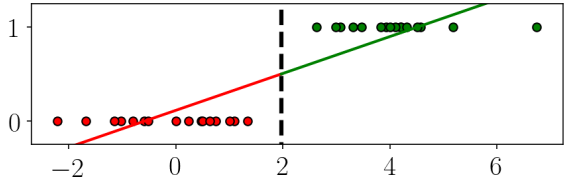



Encode red as 0 and green as 1, compute the regression line over $\{(x_i, y_i)\}_{i=1}^{n}$, $x_i \in \mathbb{R}$ and $y_i \in \{0, 1\}$. The decision rule: if $y(x) > 1/2$ then x is green, otherwise it is red.



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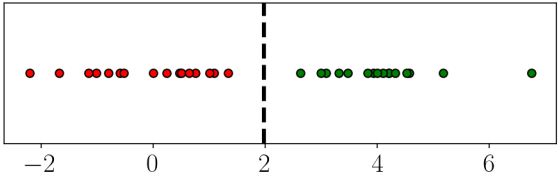


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n = len(samples)
labels = [0]*(n//2) + [1]*(n-n//2)
A = np.matrix(samples)
b = np.matrix(labels).transpose()
print(np.linalg.inv(A.transpose()*A)*A.transpose()*b)
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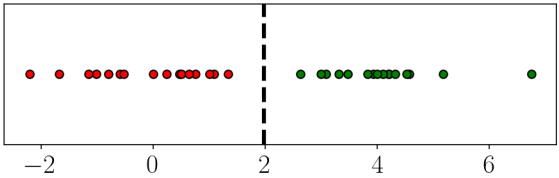


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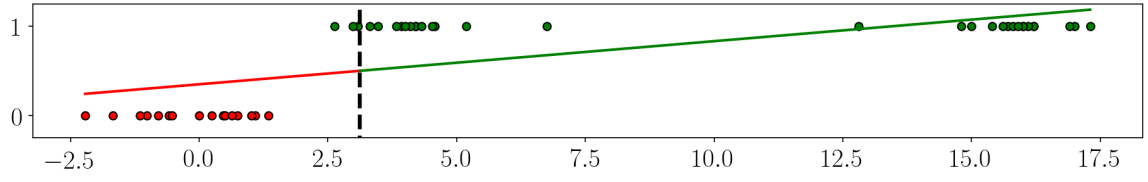

Logistic growth

Limited ressources model: a colony of the bacteria *B. dendroides* is growing in a Petri dish. The colony's area a can be modeled as a function of time t:

$$a(t) = \frac{c}{1 + e^{-wt - w_0}},$$

where c is the carrying capacity, w_0 is the initial population size and w is the growth rate.

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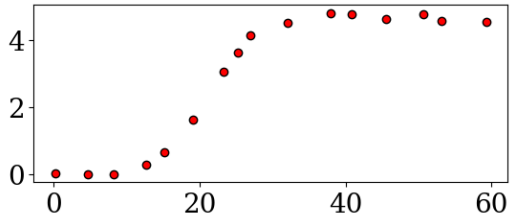

A series of n measurements $\{(a_i, t_i)\}_{i=1}^{n}$.

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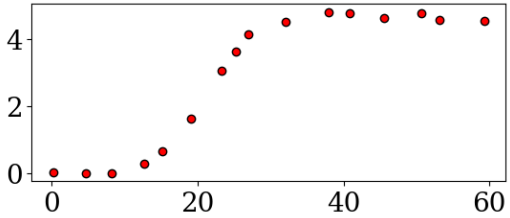

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$$\arg\min_{c,w_0,w} \sum_{i=1}^{n} (a(t_i) - a_i)^2$$

N.B: nonlinear problem!

Solve a nonlinear problem

Transform the model!

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```
import numpy as np
X = [0.2,37.9,32.0,12.7,23.3,8.2,25.2,27.0,
     40.9,4.7,19.1,50.7,53.2,59.3,15.2,45.5]
Y = [0.04,4.79,4.51,0.30,3.05,0.01,3.61,4.14,
     4.77,0.01,1.64,4.77,4.56,4.53,0.67,4.61]
c = np.max(Y)+0.01 # +eps to avoid division by zero
A = np.matrix(np.column_stack(([1.]*len(X), X)))
b = np.matrix([np.log(y/(c-y)) for y in Y]).T
print(np.linalg.inv(A.T*A)*A.T*b)
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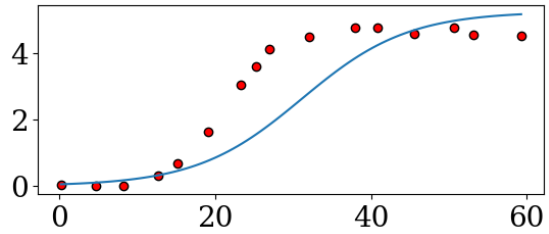

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Solve a nonlinear problem: linearization

Denote by $\vec{r}(c, w_0, w)$ the residual between the input labels and the predictions:

$$\vec{r}(c, w_0, w) := (a(t_1) - a_1, \dots \; a(t_n) - a_n)$$

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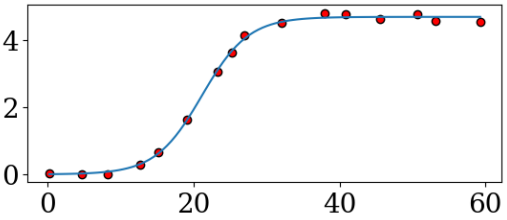

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           [6.75,1],[3.47,1],[4.32,1],[3.08,1],[4.10,1],[4.00,1],[2.99,1],[3.83,1]]
n = len(samples)
labels = [0]*(n//2) + [1]*(n-n//2)
U = np.matrix([[1],[0]])
for _ in range(5):
    JR = np.matrix(np.zeros((n+2, 2)))
    R  = np.matrix(np.zeros((n+2, 1)))
    for i in range(n):
        ei = np.exp(-U[1,0] - samples[i][0]*U[0,0])
        R[i,0] = -1/(1+ei) + labels[i]
        for j in range(3):
            JR[i, 0] = samples[i][0]*ei/(1+ei)**2
            JR[i, 1] = ei/(1+ei)**2
    l = .001 # regularization
    JR[n,0] = JR[n+1, 1] = 1.*l
    R[n,0] = -U[0]*l
    R[n+1,0] = -U[1]*l
    U = U + np.linalg.inv(JR.T*JR)*JR.T*R
print(U.T)
```
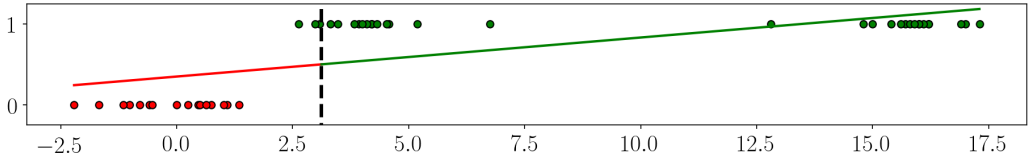

Back to the classification: quadratic loss function



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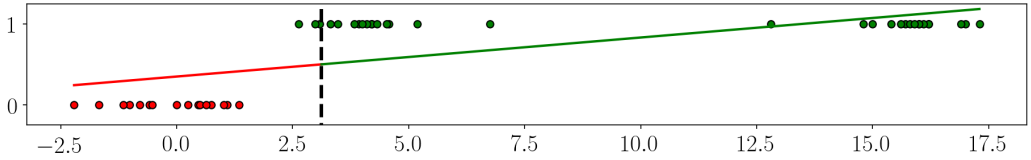
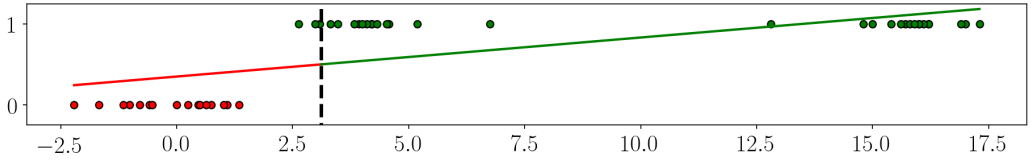


Fit a sigmoid! $1/(1 + e^{-wx-w_0})$

Leave the same decision rule: $y(x) > 1/2$ then x is green, red otherwise.

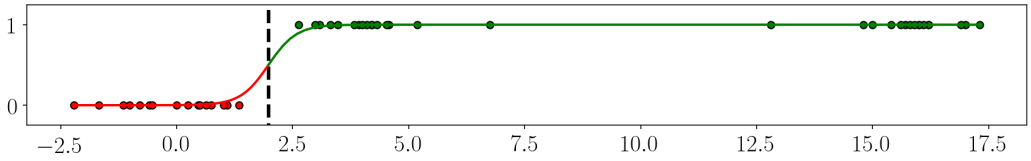
Back to the classification: quadratic loss function



Fit a sigmoid! $1/(1 + e^{-wx-w_0})$

Leave the same decision rule: $y(x) > 1/2$ then x is green, red otherwise.

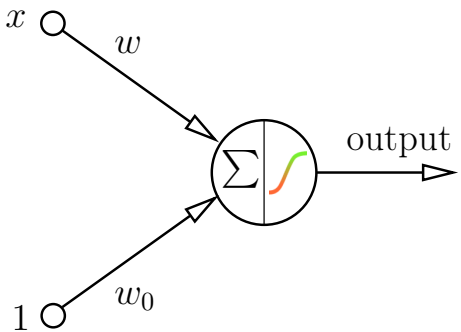
Two parameters only, call Gauß–Newton:



N.B: attention to overfitting! May need to regularize the objective function.

Good news, bad news

Good news:
we have just trained a neural network



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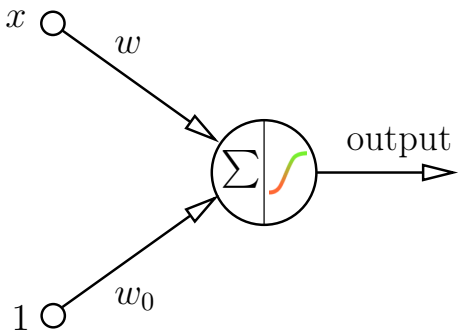
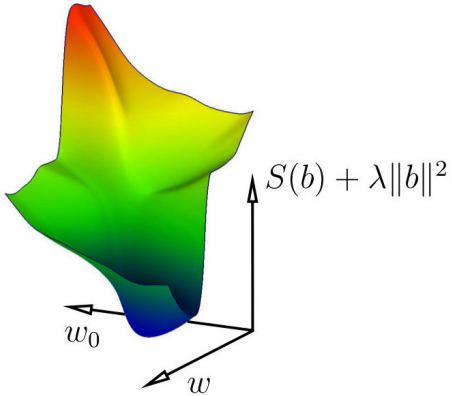


Bad news:
the energy is not convex :(



Cross-entropy loss function

As before, let two possible classes encoded as $y \in \{0, 1\}$ and assume

$$p(y = 1|x, w) := \frac{1}{1 + e^{-w^\top x}},$$

where w is a $(m + 1)$-parameter vector and the last element of x is the constant 1.

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The game changer: Bernoulli's scheme

$\log \mathcal{L}(w) = \log \prod_{i=1}^{n} p_i(w)^{y_i}(1 - p_i(w))^{1-y_i}$, where $p_i(w) := p(y_i = 1|x_i, w)$.

Problem: $\arg\max_w \log \mathcal{L}(w)$

Refer to the course notes for all details of the derivation.

Cross-entropy loss function

Problem: $\arg\max_{w} \log \mathcal{L}(w)$

Cross-entropy loss function

Problem: $\arg\max_w \log \mathcal{L}(w) \quad \Leftrightarrow \quad \frac{\partial \log \mathcal{L}}{\partial w}(w) = X^\top (y - p) = 0$, where

$X := \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}^\top$, $y := \begin{bmatrix} y_1 & \dots & y_n \end{bmatrix}^\top$ and $p := \begin{bmatrix} p_1(w) & \dots & p_n(w) \end{bmatrix}^\top$.

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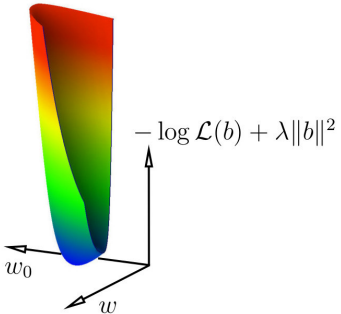
N.B: Non-linear problem, but the Hessian matrix $\frac{\partial^2 \log \mathcal{L}}{\partial w \partial w^\top}$ is definite positive, so the problem is **convex**!



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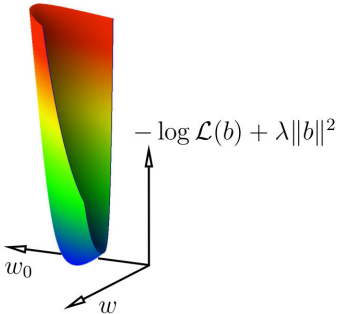
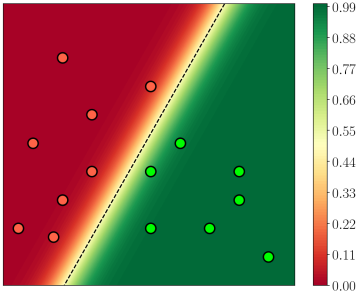
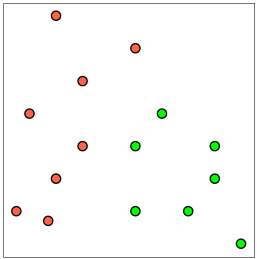




```
import numpy as np
import math

def p(x, w):
    return 1./(1.+math.exp(-np.dot(x,w)))

samples = [[.5,.7,1.],[.1,.5,1.],[.3,.6,1.],[.2,.8,1.],
           [.17,.17,1.],[.2,.3,1.],[.3,.4,1.],[.05,.2,1.],
           [.2,.3,1.],[.8,.3,1.],[.5,.2,1.],[.7,.2,1.],
           [.9,.1,1.],[.8,.4,1.],[.6,.5,1.],[.5,.4,1.]]
labels = [0.,0.,0.,0.,0.,0.,0.,0.,1.,1.,1.,1.,1.,1.,1.]

n = len(samples)
X = np.matrix(samples)
y = np.matrix(labels).T
wk = np.matrix([[.3], [.7], [-.02]]) # small random numbers

l = -0.001 # regularization coefficient
for _ in range(5):
    pk = np.matrix([p(xi,wk) for xi in samples]).T
    Vk = np.matrix(np.diag([pk[i,0]*(1.-pk[i,0]) for i in range(n)]))
    wk += np.linalg.inv(X.T*(Vk-l*np.matrix(np.identity(n)))*X)*(X.T*(y-pk) + l*wk)

print(wk)
```

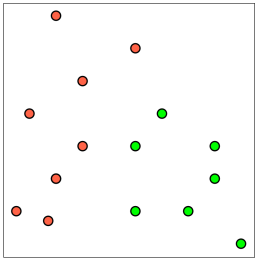
Nonlinear decision boundary: logistic regression



Linear decision boundary:

$$\frac{1}{1 + e^{-w^\top x}} = \frac{1}{2}$$

Nonlinear decision boundary: logistic regression



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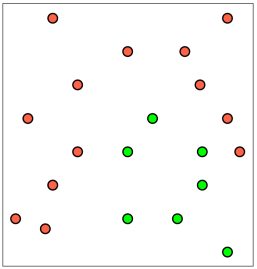


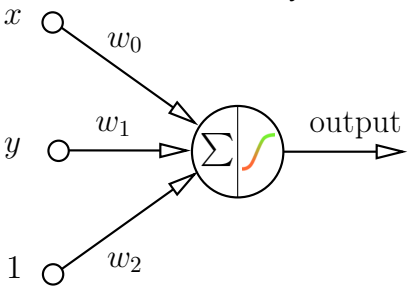
Quadratic decision boundary:

$$\frac{1}{1 + e^{-x^\top A x}} = \frac{1}{2}$$

But where is the fun in that...

Nonlinear decision boundary: 3 neurons

Linear decision boundary:

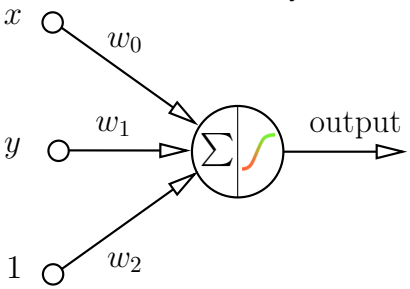


$$\arg\min_{w} \sum_{i=1}^{n} \left(\sigma\left(w^\top x_i\right) - y_i\right)^2,$$

where $\sigma(x, w) := \frac{1}{1+e^{-w^\top x}}$

Nonlinear decision boundary: 3 neurons

Linear decision boundary:



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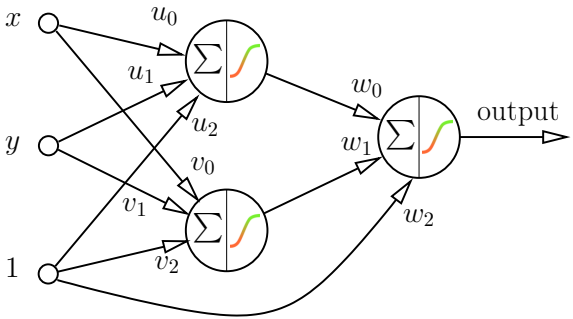


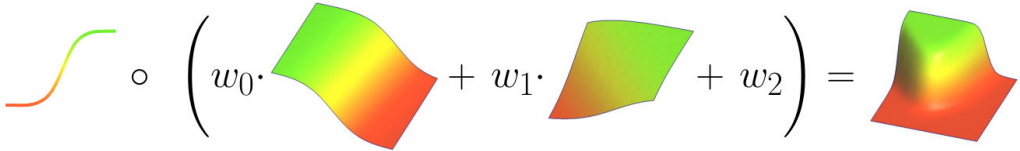
$$\arg\min_{u,v,w} \sum_{i=1}^{n} \left(\sigma\left(w^\top x_i'\right) - y_i\right)^2,$$

where $x_i' := \begin{pmatrix}\sigma(u^\top x_i) & \sigma(v^\top x_i) & 1\end{pmatrix}^\top$

```
import numpy as np
samples = [[.5,.7,1.],[.1,.5,1.],[.3,.6,1.],[.2,.8,1.],[.17,.17,1.],[.2,.3,1.],
           [.3,.4,1.],[.05,.2,1.], [.2,.3,1.],[.8,.3,1.],[.5,.2,1.],[.7,.2,1.],
           [.9,.1,1.],[.8,.4,1.],[.6,.5,1.], [.5,.4,1.], [.9, .5, 1.],[.79, .6, 1.],
           [.73, .7, 1.],[.9, .8, 1.],[.95, .4, 1.]]
labels = [0,0,0,0,0,0,0,0,0,1,1,1,1,1,1,1,0,0,0,0,0]

def neuron(x, w):
    return 1./(1.+np.exp(-np.dot(x,w)))
u = np.array([0.814, 0.779, 0.103]) # small random values
v = np.array([0.562, 0.310, 0.591])
w = np.array([0.884, 0.934, 0.649])
alpha = 1. # learning rate
for _ in range(0,3000):
    E = 0
    for x, label in zip(samples,labels):
        E += (label - neuron([neuron(x, u), neuron(x, v), 1.],w))**2
    for x, label in zip(samples,labels):
        out_u = neuron(x, u)
        out_v = neuron(x, v)
        out_w = neuron([out_u, out_v, 1.], w)
        u += alpha*(label-out_w)*out_w*(1.-out_w)*out_u*(1.-out_u)*np.array(x)
        v += alpha*(label-out_w)*out_w*(1.-out_w)*out_v*(1.-out_v)*np.array(x)
        w += alpha*(label-out_w)*out_w*(1.-out_w)*np.array([out_u, out_v, 1.])
print(u,v,w)
```

Nonlinear decision boundary: 3 neurons



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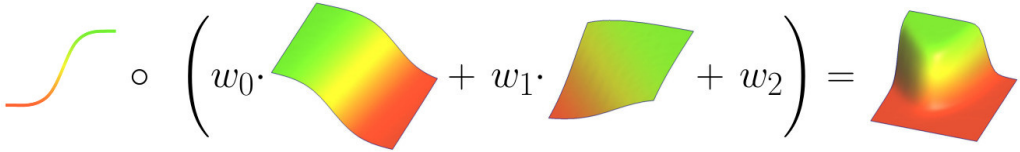

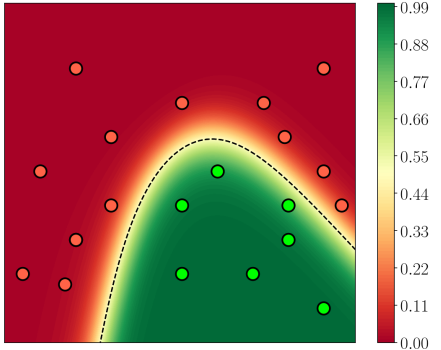

The takeaway message

Surprisingly, there are two irreconcilable camps: those for whom neural networks are the *answer to everything*, and those who *despise* neural networks.

I do not advocate for either party, two main points of this chapters are:

- neural networks are not the only machine learning tool;
- there is no clear boundary between least squares methods and neural networks.

Concluding remarks

Linear regression is often underestimated being considered only as a sub-domain of statistics, but it is much more than that.

It offers a different view on programming:

- Traditionally, we break down complex tasks into a sequence of elementary operations that manipulate combinatorial structures (trees, graphs, meshes...).
- Instead, we can describe what a good result looks like, and let numerical optimization algorithms find it for us.

For any questions/remarks/corrections you are very welcome to contact me:
dmitry.sokolov@univ-lorraine.fr

Dmitry Sokolov, Nicolas Ray, Étienne Corman

Least squares for programmers

— with color plates —