

Least Squares





Numerical Analysis

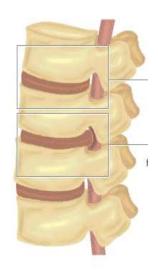
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Examples and motivations

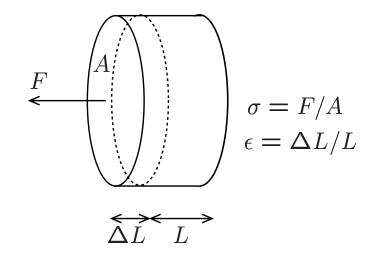
Example 1. We consider a mechanical test to establish the link between stresses $(MPa = 100N/cm^2)$ and relative deformations (cm/cm) of a sample of biological tissue (an intervertebral disc, taken from P. Komarek, Chapt. 2 of *Biomechanics of Clinical Aspects of Biomedicine*, 1993, J. Valenta ed., Elsevier).



disques intervert ebraux



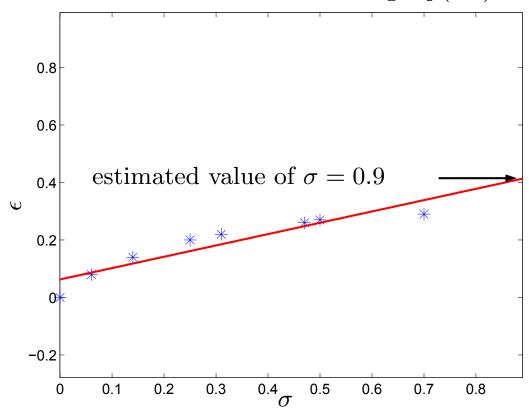
test i	pressure σ	deformation ϵ
1	0.00	0.00
2	0.06	0.08
3	0.14	0.14
4	0.25	0.20
5	0.31	0.23
6	0.47	0.25
7	0.60	0.28
8	0.70	0.29



From these data, we want to estimate the deformation corresponding to a stress $\sigma = 0.9$ MPa.

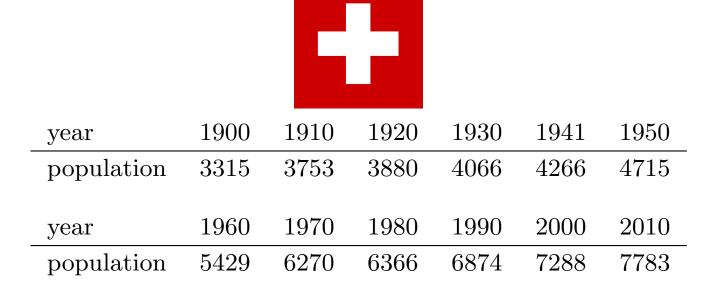


By the method of least squares, we get that best approximation for the data is p(x) = 0.3938x - 0.0629. The approximation can be used (called a linear regression) to estimate ϵ when $\sigma = 0.9$ MPa: We get $p(0.9) \simeq 0.4$.





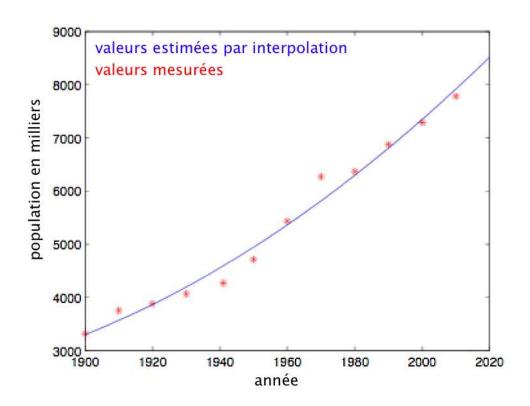
Example 2. The result of census of the population of Switzerland between 1900 and 2010 (in thousands):



- Is it possible to estimate the number of inhabitants of Switzerland during the year when there has not been census, for example in 1945 and 1975?
- Is it possible to predict the number of inhabitants of Switzerland in 2020?



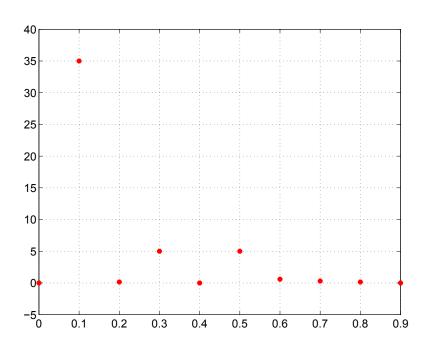
The polynomial of degree two (parabola) which approximates the data by the method of least squares is $p(x) = 0.15x^2 - 549.9x + 501600$.





Example 3. Points on the following figure represent the measurements of blood flow in a part of the common carotid artery during a heartbeat. The frequency of data collection is constant and equal to 10 / T where T = 1 sec. is the period of the beat.

We want to deduce from this discrete signal a continuous signal represented by a linear combination of known functions (eg. trigonometric functions then we can adequately approximate a periodic signal).



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Let f(t) be a signal that we know. N = 10 is a size of a sample $[f(t_0), \ldots, f(t_{N-1})]$, where $t_j = jT/N$. We are looking for $\{c_k\} \in \mathbb{C}$, $k \in [0, N-1] \subset \mathbb{N}$ such that:

$$f(t_j) = \frac{1}{N} \sum_{k=0}^{N-1} c_k \omega_N^{-kj}, \quad j = 0, \dots, N-1,$$
 (1)

where

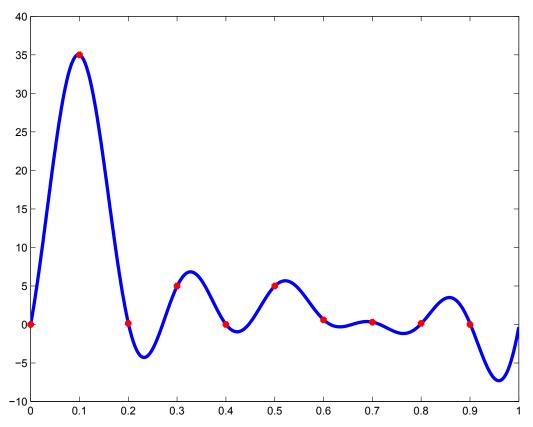
$$\omega_N = e^{(-2\pi i)/N} = \cos(2\pi/N) - i\sin(2\pi/N),$$

i is the imaginary unit. We can calculate a vector of the coefficients $\mathbf{c} = [c_1, \dots, c_{10}]^T$ by the FFT algorithm (Fast Fourier Transform, Cooley & Tuckey, 1965), implemented in Matlab/Octave by the fft command.



Using the formula (1), there are several techniques for obtaining the value of f in each point $t \in [0, T]$.

Using one of techniques we obtain a result that is plotted on a following figure:





Approximation by the least square methor

(Chapt. 3.4 of the book)

Suppose we have n+1 points x_0, x_1, \ldots, x_n and n+1 values y_0, y_1, \ldots, y_n . We have seen that if n is large, the interpolating polynomial may show large oscillations

Instead of interpolating the values, it is possible to define a polynomial of degree m < n that approximates the data "at best"



Definition 1. We call least squares polynomial approximation of degree m the polynomial $\tilde{f}_m(x)$ of degree m such that

$$\sum_{i=0}^{n} |y_i - \tilde{f}_m(x_i)|^2 \le \sum_{i=0}^{n} |y_i - p_m(x_i)|^2 \qquad \forall p_m(x) \in \mathbb{P}_m$$

Remark 4. Where $y_i = f(x_i)$ (f is a continuous function) then \tilde{f}_m is called the approximation of f in the least squares sense.



In other words, the least squares polynomial approximation is the polynomial of degree m that minimizes the distance to the data.

Let note $\tilde{f}_m(x) = a_0 + a_1x + a_2x^2 + \ldots + a_mx^m$ and define the function

$$\Phi(a_0, a_1, \dots, a_m) = \sum_{i=0}^{n} |y_i - (a_0 + a_1 x_i + a_2 x_i^2 + \dots + a_m x_i^m)|^2$$

Then the coefficients of \tilde{f}^{m} can be determined by the relation

$$\frac{\partial \Phi}{\partial a_k} = 0, \qquad k = 0, ..., m, \tag{5}$$

i.e., m+1 linear equations in with m+1 unknowns a_k , k=0,...,m.

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Example 8. Let n = 2 and m = 1, nodes $x_0 = 1$, $x_1 = 3$, $x_2 = 4$ with values $y_0 = 0$, $y_1 = 2$, $y_2 = 7$. We want to compute the (*regression line*), i.e., the the least squares polynomial approximation of degree 1, $\tilde{f}_1(x) = a_0 + a_1 x$.

We set $\Phi(a_0, a_1) = \sum_{i=0}^{2} [y_i - (a_0 + a_1 x_i)]^2$ and impose $\frac{\partial \Phi}{\partial a_0} = 0$ and $\frac{\partial \Phi}{\partial a_1} = 0$:

$$\frac{\partial \Phi}{\partial a_0} = -2\sum_{i=0}^{2} [y_i - (a_0 + a_1 x_i)] = -2\left(\sum_{i=0}^{2} y_i - 3a_0 - a_1\sum_{i=0}^{2} x_i\right)
= -2(9 - 3a_0 - 8a_1)
\frac{\partial \Phi}{\partial a_1} = -2\sum_{i=0}^{2} x_i [y_i - (a_0 + a_1 x_i)] = -2\left(\sum_{i=0}^{2} x_i y_i - a_0\sum_{i=0}^{2} x_i - a_1\sum_{i=0}^{2} x_i^2\right)
= -2(34 - 8a_0 - 26a_1)$$

Hence the coefficients a_0 and a_1 are the solution of the system

$$\begin{cases} 3a_0 + 8a_1 = 9 \\ 8a_0 + 26a_1 = 34 \end{cases}$$

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Ideally, for $\tilde{f}_m(x) = a_0 + a_1 x + a_2 x^2 + \ldots$ we would like to impose $\tilde{f}_m(x_i) = y_i$ pour $i = 0, \ldots, n$.

This can be written as a linear system with unknowns a_k , k=0,...,m: $B\mathbf{a}=\tilde{\mathbf{y}}$, where B is a matrix of dimension $(n+1)\times(m+1)$

$$B = \begin{pmatrix} 1 & x_0 & \dots & x_0^m \\ 1 & x_1 & \dots & x_1^m \\ \vdots & & & \vdots \\ 1 & x_n & \dots & x_n^m \end{pmatrix}$$

Since m < n, the system is oversized. The solution to (5) is equivalent to the square system (system of normal equations)

$$B^T B \mathbf{a} = B^T \tilde{\mathbf{y}}.$$



```
Example 9. We have 8 measures (\sigma - \epsilon):
```

```
>> sigma = [0.00 0.06 0.14 0.25 0.31 0.47 0.50 0.70];
>> epsilon = [0.00 0.08 0.14 0.20 0.22 0.26 0.27 0.29];
```

We want to extrapolate the value of ϵ for $\sigma = 0.4$. We consider two ways:

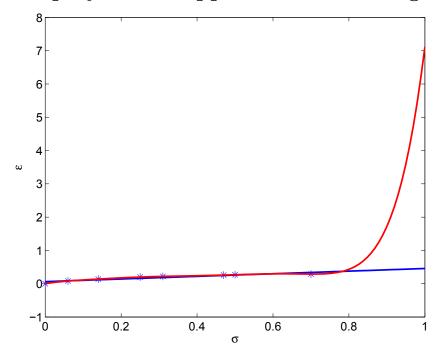
- compute the interpolating polynomial Π_7 of degree 7
- compute the least squares polynomial approximation of degree 1

On peut utiliser les commandes suivantes:

```
>> plot(sigma, epsilon, '*'); hold on; % plotting the known values
>> sigma_sample = linspace(0,1.0,100);
>> p7 = polyfit(sigma, epsilon, 7);
>> pol = polyval(p7, sigma_sample); % interpolating polynomial
>> plot(sigma_sample,pol, 'r');
>> p1 = polyfit(sigma,epsilon,1);
>> pol_mc = polyval(p1, sigma_sample); % least square
>> plot(sigma_sample, pol_mc, 'g'); hold off;
```



- the interpolating polynomial Π_7 of degree 7 is in red
- the least squares polynomial approximation of degree 1 is in blue



For $\sigma > 0.7$, the behavior of the two polynomials are very different.

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In particular, for $\sigma = 0.9$ the values of $\epsilon(\sigma)$ extrapolated with the two methods are

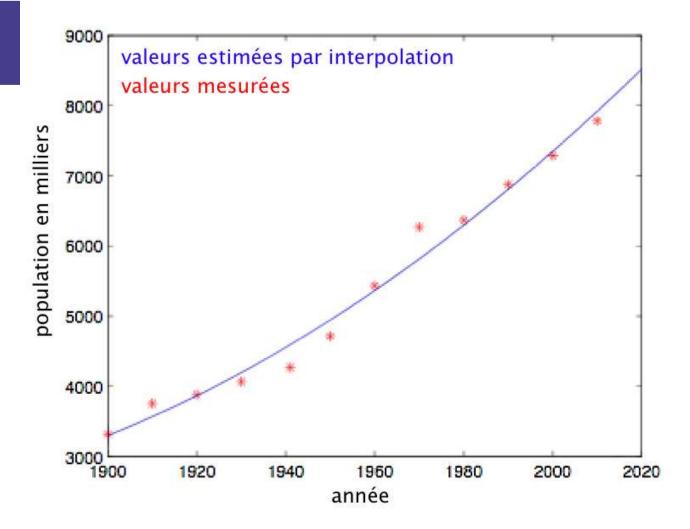
```
>> polyval(p7, 0.9)
ans =
    1.7221
>> polyval(p1, 0.9)
ans =
    0.4173
```

- The value obtained by Π_7 (172.21%) is unrealistic
- On the contrary, the value obtained with the regression line is more appropriate to compute the value at $\sigma = 0.9$.



Example 10. Swiss population Starting from the population at the 20th century decades, we extrapolate the Swiss popululation this year. We use a least square polynomial approximation of degree 2



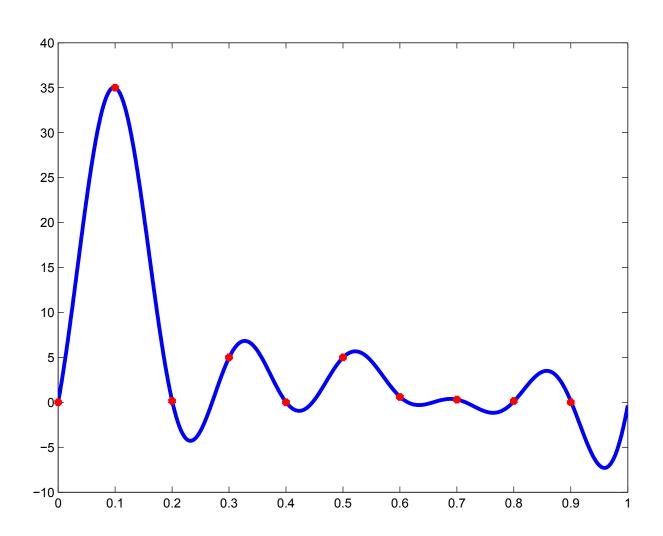




Example. Carotide flow rate We define 10 couples of data (time vs flowrate) with the vectors t and deb. With the help of the command interpft, we compute the value of the interpolating function at 1000 equidistributed points in the periodicity interval [0,1]:

```
t = [0 .1 .2 .3 .4 .5 .6 .7 .8 .9];
deb = [0 35 .15 5 0 5 .6 .3 .15 0];
f = interpft(deb, 1000);
plot(linspace(0, 1, 1000), f); hold on;
plot(t, deb, 'r*')
```







Processing of polynomials

In Matlab/Octave, there are specific commands for doing calculations with polynomials. Let x be a vector of abscissas, y be a vector of ordinates and p (respectively p_i) be the vector of coefficients of a polynomial P(x) (respectively P_i); then, we have following commands:

command	action	
y=polyval(p,x)	y = values of $P(x)$	
p=polyfit(x,y,n)	${ t p}={ t coefficients}$ of the interpolating polynomial Π_n	
z=roots(p)	z = zeros of P such that $P(z) = 0$	
$p=conv(p_1,p_2)$	$\mathtt{p}=coefficients$ of the polynomial P_1P_2	
$[q,r]=deconv(p_1,p_2)$	q = coefficients of Q, r = coefficients of R	
	such that $P_1 = QP_2 + R$	
y=polyderiv(p)	y = coefficients of P'(x)	
y=polyinteg(p)	$y = coefficients of \int P(x) dx$	