Approximation of function

outline

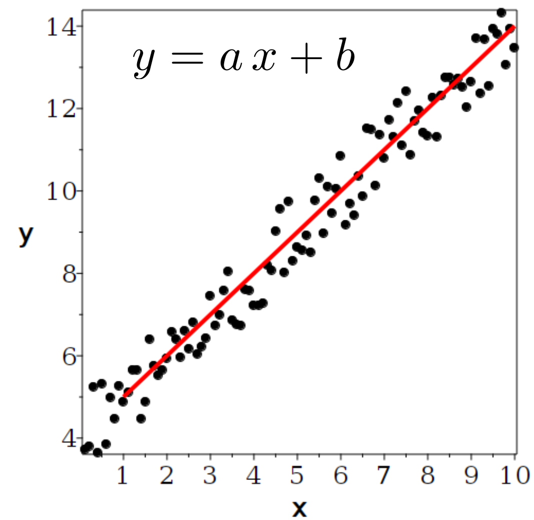
- approximation – general considerations
- linear mean-square approximation
    - for general basis
    - for basis of monomials
    - for basis of trigonometric function
- Pade approximation
- examples

Approximation of function

- approximation means fitting an unknown or a known function *f(x)* with another one *F(x)* requiring the „distance” between both (the norm) to be minimal

$$f(x) \approx F(x)$$

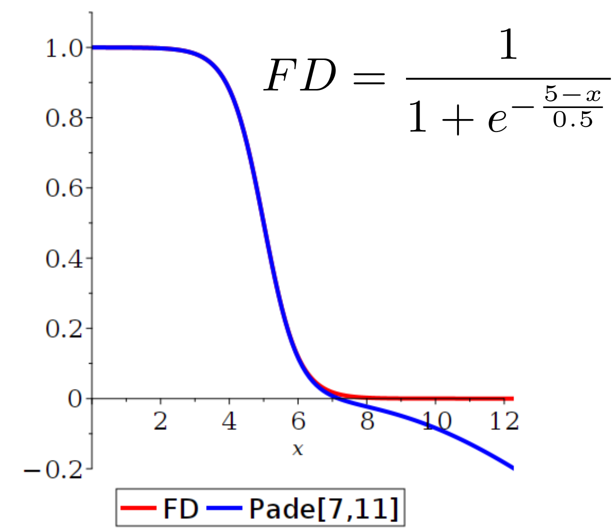
$$\|f(x) - F(x)\| = \min$$



- information about uknown function is usually given in the tabulated form (nodes+function values) and one looks for the best smooth fitting function of some predefined shape what is assessed by particular norm
  – this kind of approximation is usually done for the experimental data

  example: linear regression known from physics laboratory

$$\{(x_0, y_0),\, (x_1, y_1),\, \ldots,\, (x_m, y_m)\} \quad \rightarrow \quad F(x)$$



- in some, mainly theoretical, applications we approximate the known function with another one so as to get and operate on simpler formula or to directly exploit properties of the approximating function

$$f(x) \quad \rightarrow \quad F(x)$$

Before conducting an approximation we need to precisely define what kind of functions we will use in calculations, usually we need a single or a group of functions, called basis functions

$$\Phi = \{\varphi_0(x;\vec{c}_1),\ \varphi_1(x;\vec{c}_2),\ \ldots,\varphi_m(x;\vec{c}_m)\}$$

Approximation can be generally expressed as follows

$$F(x) = \sum_{i=0}^{m} a_i \varphi(x;\vec{c}_m)$$

and our task is to find the linear coefficients $\mathbf{a_i}$ and nonlinear coefficients $\mathbf{c_m}$ in such a way to minimize the norm

$$\|f(x) - F(x)\| = \min$$

Generally approximation we may divide into two categories

- **linear approximation** – coefficients $\mathbf{c_m}$ are fixed (basis functions shapes are fixed) and we only need to find the linear coeffcients, this is usually done with some of the linear algebra methods

- **nonlinear approximation** – nonlinear coefficients $\mathbf{c_m}$ are free parameters which need to be found, they can shape approximating function F(x) more than the linear ones, but the problem transforms into nonlinear equation that can be solved iteratively making it harder

Choice of basis functions

The choice of functions we will use in approximation depends on the problem we try to solve and the solution we expect or want to get. Solution is in fact an element of finite-dimensional subspace of function, example subspace could be following

- subspace of harmonic function for problems which are periodic in space

$$\{1,\, \sin(x),\, \cos(x),\, \sin(2x),\, \cos(2x), \ldots,\, \sin(kx),\, \cos(kx)\}$$

- subspace of polynomials of m-degree with basis composed of monomials

$$\{1,\, x,\, x^2,\, \ldots, x^m\}$$

- subspace of functions of given properties, like e.g. exponential/logarithmic shape

$$\{\exp(c_0 + c_1 x + c_2 x^2),\, \exp\left(ln(s_0 + s_1 x + s_2 x^2)\right)\}$$

Norms

In order to consider „the distance" between original function and its approximation we need to define a measure that allow us to assess the quality of solution. For this purpose there are commonly used the following norms, as usual norm must be non-negative real number

- Chebyshev norm

$$\|f(x) - F(x)\| = \sup_{[a,b]} |f(x) - F(x)|$$

- 2-nd norm

$$\|f(x) - F(x)\| = \left(\int_a^b |f(x) - F(x)|^2 dx \right)^{\frac{1}{2}}$$

- 2-nd norm with weight w(x)>0

$$\|f(x) - F(x)\| = \left(\int_a^b w(x) |f(x) - F(x)|^2 dx \right)^{\frac{1}{2}}$$

- 2-nd norm with weight w(x)>0 for discrete problems

$$\|f(x) - F(x)\| = \left(\sum_{i=0}^{n} w(x_i) \left[f(x_i) - F(x_i) \right]^2 \right)^{\frac{1}{2}}$$

Mean-square approximation

For a set of approximation nodes, tabulated unknown function's values and weights

$$\{(x_0, y_0, w_0),\ (x_1, y_1, w_1),\ \ldots,\ (x_n, y_n, w_n)\}$$

we define basis of functions

$$\Phi = \{\varphi_0(x),\ \varphi_1(x),\ \ldots,\ \varphi_m(x)\}$$

and express the approximation function as linear combination of basis elements (linear approximation)

$$F(x) = \sum_{i=0}^{m} a_i \varphi_i(x)$$

We need to determine the values of the coefficients a_i, for this purpose we will use 2-nd norm with weight

$$\begin{aligned} &H(a_0, a_1, \ldots, a_m) = \\ &= \sum_{j=0}^{n} w(x_j) \left[f(x_j) - \sum_{i=0}^{m} a_i \varphi_i(x_j) \right]^2 \\ &= \sum_{j=0}^{n} w(x_j) R_j^2 \end{aligned}$$

R_j – is the difference between f(x) and F(x)

Approximation of function

The norm is in fact a new function for variables a_0, a_1,... which are the free parameters.
We are looking for minimal „distance” between f(x) and F(x) or in other words the minimum of the norm.
This minimum can be found in standard way, at minimum the gradient of norm vanishes

$$\nabla_{\vec{a}} H(\vec{a}) = 0 \quad \rightarrow \quad \frac{\partial H}{\partial a_k} = 0, \quad k = 0, 1, \ldots, m$$

$$\frac{\partial H}{\partial a_k} = \sum_{j=0}^{n} w(x_j) \frac{\partial}{\partial a_k} \left[f(x_j) - \sum_{i=0}^{m} a_i \varphi_i(x_j) \right]^2 = 0$$

$$\frac{\partial H}{\partial a_k} = -2 \sum_{j=0}^{n} w(x_j) \left[f(x_j) - \sum_{i=0}^{m} a_i \varphi_i(x_j) \right] \varphi_k(x_j) = 0$$

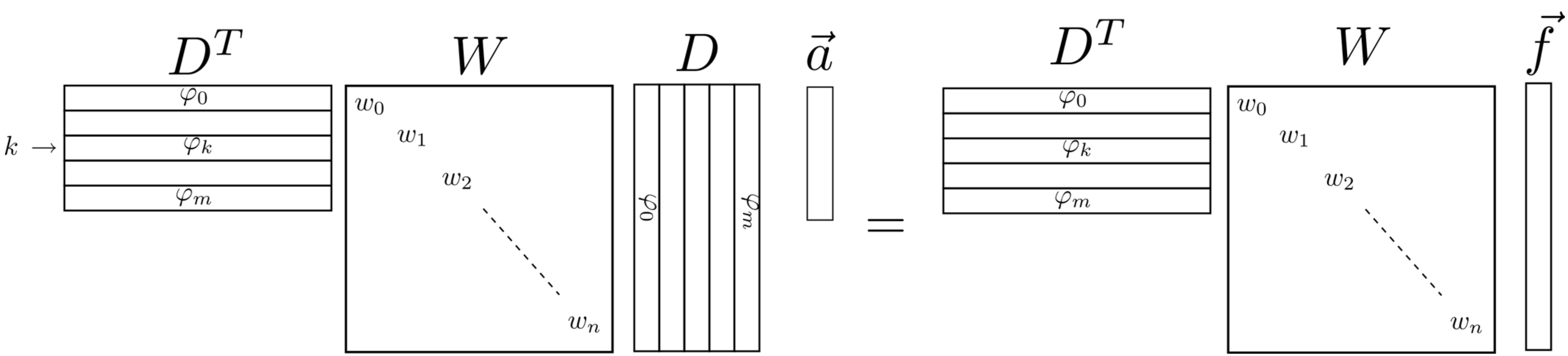
$$\vec{a} = [a_0, a_1, \ldots, a_m]$$

$$\vec{f} = [f_0, f_1, \ldots, f_n]$$

$$\vec{\varphi}_k = [\varphi_{k,0}, \varphi_{k,1}, \ldots, \varphi_{k,n}]$$

$$D = [\vec{\varphi}_0, \vec{\varphi}_1, \ldots, \vec{\varphi}_m]$$

$$W = diag\{w_0, w_1, \ldots, w_n\}$$



Because the weights are non-negative and nonzero, the diagonal matrix W can written as a product of $W^{1/2}$

$$W^{\frac{1}{2}} = diag\left\{w_0^{\frac{1}{2}},\ w_1^{\frac{1}{2}}, \ldots, w_n^{\frac{1}{2}}\right\}$$

$$W = W^{\frac{1}{2}} W^{\frac{1}{2}}$$

by making an assumption

$$W^{\frac{1}{2}} D = D_w$$

allows the matrix equation

$$D^T W D \vec{a} = D^T W \vec{f}$$

to be written in more commonly recognized form

$$D_w^T D_w \vec{a} = D_w^T \vec{f}$$

we have transformed an approximation problem into the least-squared one,
this can be effectively solved with QR decomposition of D_W matrix

Mean-square approximation in basis of monomials

Let's assume the explicit form of basis elements as monomials

$$\Phi = \{1,\ x,\ x^2,\ \ldots,\ x^m\}$$

Minimization of the 2-nd norm for this functions provides the following expression

$$\sum_{j=0}^{n}\left[f(x_j) - \sum_{i=0}^{m} a_i x_j^i\right] x_j^k = 0 \qquad k = 0, 1, 2, \ldots, m$$

after changing the sequence of summation and shifting terms with f(x) to rhs we get

$$\sum_{i=0}^{m} a_i \left(\sum_{j=0}^{n} x_j^{i+k}\right) = \sum_{j=0}^{n} f(x_j) x_j^k$$

This equation can be rewritten in more compact form if we introduce abbreviations for summation over nodes

$$\boxed{g_{ik} = \sum_{j=0}^{n} x_j^{i+k}} \qquad \boxed{b_k = \sum_{j=0}^{n} f(x_j) x_j^k} \longrightarrow \boxed{\sum_{i=0}^{m} a_i g_{ik} = \rho_k}$$

$$\downarrow$$

$$\boxed{G\vec{a} = \vec{b}}$$

We get system of linear equations with symmetric square matrix

$$G \in \mathbb{R}^{m+1 \times\, m+1}, \quad G = G^T, \quad \vec{a}, \vec{b} \in \mathbb{R}^{m+1},$$

Mean-squared approximation in basis of trigonometric function

When we expect the unknown tabulated function is periodic, then we can use the basis of trigonometric functions

$$\Phi = \{1,\ \sin(k_1 x),\ \cos(k_1 x),\ \sin(k_2 x),\ \cos(k_2 x), \ldots\}$$

and write the approximation function as linear combination of basis elements

$$F(x) = \frac{a_0}{2} + \sum_{j=1}^{m} [a_j \cos(k_j\, x) + b_j \sin(k_j\, x)]$$

Let's make two additional assumptions, approximation interval starts at x=0 (simple shift of the interval) and the nodes are equidistant

$$x \in [0, x_{max}], \quad x_i = \Delta \cdot i, \quad \Delta = \frac{x_{max}}{2n}, \quad i = 0, 1, 2, \ldots, 2n-1$$

$$\boxed{\sin(k_j x_{max}) = 0 \quad \rightarrow \quad k_j \cdot x_{max} = 2\pi \cdot j \quad \rightarrow \quad k_j = \frac{2\pi \cdot j}{x_{max}} = \frac{2\pi \cdot j}{\Delta 2n} = \frac{j \cdot \pi}{n\Delta}}$$

then we may exploit one of the main features of basis functions – **they are orthogonal**

$$\boxed{\sum_{i=0}^{2n-1} \sin(k_p x_i) \sin(k_s x_i) = \begin{cases} 0, & p \neq s \\ n, & p = s \neq 0 \\ 0, & p = s = 0 \end{cases}}$$

$$\boxed{\sum_{i=0}^{2n-1} \cos(k_p x_i) \cos(k_s x_i) = \begin{cases} 0, & p \neq s \\ n, & p = s \neq 0 \\ 2n, & p = s = 0 \end{cases}}$$

$$\boxed{\sum_{i=0}^{2n-1} \cos(k_p x_i) \sin(k_s x_i) = 0 \quad \text{p,s - any combination}}$$

For approximation funtion

$$F(x) = \frac{a_0}{2} + \sum_{j=1}^{m} [a_j \cos(k_j\, x) + b_j \sin(k_j\, x)]$$

the coefficents a_j and b_j can be found by minimizing the 2-nd norm

$$\sum_{i=0}^{2n-1} [f(x_i) - F(x_i)]^2 = \min$$

Again we would get the normal equation with matrix D, however the columns of D are orthogonal discretized basis functions → **orthogonal vectors**. Therefore, we immediately recognize

$$D^T D = diag\{2n, n, \ldots, n\}$$

what provides the solution without the need of using any numerical routine

$$\vec{v} = [\underbrace{a_0, a_1, \ldots, a_m}_{\cos(k_j x)}, \underbrace{b_1, b_2, \ldots, b_m}_{\sin(k_j x)}]$$

$$D^T D \vec{v} = D^T \vec{f}$$

$$diag(2n, n, \ldots, n)\vec{v} = D^T \vec{f}$$

$$\vec{v} = diag\left(\frac{1}{2n}, \frac{1}{n}, \ldots, \frac{1}{n}\right) D^T \vec{f}$$

$$a_0 = \frac{1}{2n} \sum_{i=0}^{2n-1} f(x_i)$$

$$a_j = \frac{1}{n} \sum_{i=0}^{2n-1} f(x_i) cos(k_j x_i)$$

$$b_j = \frac{1}{n} \sum_{i=0}^{2n-1} f(x_i) sin(k_j x_i)$$

Pade approxiamtion

Second purpose of approximation, namely, replacing the known function f(x) with another one F(x) often is conducted with rational functions

$$R_{n,k}(x) = \frac{L_n(x)}{M_k(x)}$$

where L_n and M_k are algebraic polynomias

$$L_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

$$M_k(x) = b_0 + b_1 x + b_2 x^2 + \ldots + b_k x^k, \qquad (b_0 = 1)$$

Usually b_0 is assumed as unit so we need to find n+k+1 polynomials coefficients.
These are calculated by comparing coefficents standing at monomials of the same degree in MacLaurin expansion (Taylor for x=0) with polynomials' coefficients in Pade formula.

First, we calculate the MacLaurin series for function f(x)

$$f(x) = \sum_{i=0}^{\infty} c_i x^i$$

it is infinite expansion so comparison with Pade approximation gives an error

$$f(x) - \frac{L_n(x)}{M_k(x)} = \frac{\left(\sum_{i=0}^{\infty} c_i x^i\right)\left(\sum_{i=0}^{k} b_i x^i\right) - \sum_{i=0}^{n} a_i x^i}{\sum_{i=0}^{k} b_i x_i}$$

Now we impose the continuity condition on the low order derivatives of the error, these must vanish

$$f^{(m)}(x)\Big|_{x=0} - R_{n,k}^{(m)}(x)\Big|_{x=0} = 0, \qquad m = 0, 1, 2, \ldots, k+n$$

For 0-th order derivative, we expect vanishing of numerator of error up to n+k degree monomials

$$\left(\sum_{i=0}^{\infty} c_i x^i\right)\left(\sum_{i=0}^{k} b_i x^i\right) - \sum_{i=0}^{n} a_i x^i = \sum_{j=1}^{\infty} d_{n+k+j} x^{n+k+j}$$

Condition for function vaule can be written as follows

$$f(0) - R_{n,k} = 0$$

$$(b_0 + b_1 x + \ldots + b_k x^k)(c_0 + c_1 x + \ldots) = (a_0 + a_1 x + \ldots + a_n x^n)$$

Direct comparison of coefficients standing at the monomials of the same degree on both sides delivers set of dependences

$$\begin{array}{lcl} a_0 & = & b_0 c_0 \\ a_1 & = & b_0 c_1 + b_1 c_0 \\ a_2 & = & b_0 c_2 + b_1 c_1 + b_2 c_0 \\ \ldots & \ldots & \ldots\ldots\ldots\ldots \end{array}$$

(1)

$$a_r = \sum_{j=0}^{r} c_{r-j} b_j, \quad r = 0, 1, 2, \ldots, n$$

Fulfilling the condition of vanishing the derivatives gives additional k equations

(2)

$$\sum_{j=0}^{k} c_{n+k-s-j} b_j = 0, \quad s = 0, 1, 2, \ldots, k-1$$

Set **(2)** forms the system of k linear equations, if it be solved then calculation of the coefficients a_r in **(1)** is straighforward.

In order to form the SLE for (2) we need to keep in mind that coefficent b_0 is fixed, this allows to find the right hand side of SLE

$$s = 0, 1, 2, \ldots, k-1$$
$$\sum_{j=0}^{k} c_{n+k-s-j} b_j = 0$$

$$j = 0 \rightarrow b_0 = 1$$

$$\begin{bmatrix} c_{n-m+1} & c_{n-m+2} & \cdots & c_n \\ c_{n-m+2} & c_{n-m+3} & \cdots & c_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_n & c_{n+1} & \cdots & c_{n+m-1} \end{bmatrix} \begin{bmatrix} b_m \\ b_{m-1} \\ \vdots \\ b_1 \end{bmatrix} = \begin{bmatrix} -c_{n+1} \\ -c_{n+2} \\ \vdots \\ -c_{n+m} \end{bmatrix}$$

elements c_k we get from Maclaurin expansion

$$C\vec{b} = \vec{c}, \qquad C \in \mathbb{R}^{m\times m}, \quad \vec{b}, \vec{c} \in \mathbb{R}^m$$

Solution of above SLE gives coefficients bj, coefficients aj we get from simple summation

$$a_i = \sum_{j=0}^{i} c_{i-j} \cdot b_j, \quad i = 0, 1, \ldots, n$$

Example: approximation of Gauss function around the point x=0

$$f(x) = \exp(-x^2), \quad x \in [-5, 5]$$

First 12 terms in Maclaurin expansion
(odd parity terms vanish)

$$T_{12}\{f(x)\} \approx 1 - x^2 + \frac{x^4}{2} - \frac{x^6}{6} + \frac{x^8}{24} - \frac{x^{10}}{120} + \frac{x^{12}}{720}$$