- Part II.

Math methods for data analysis:

interpolation and approximation methods

II.3 Approximation

using the Least Squares Method

***Interpolation** – a general term (concept) of constructing new data points within the range of a discrete set of known data points*

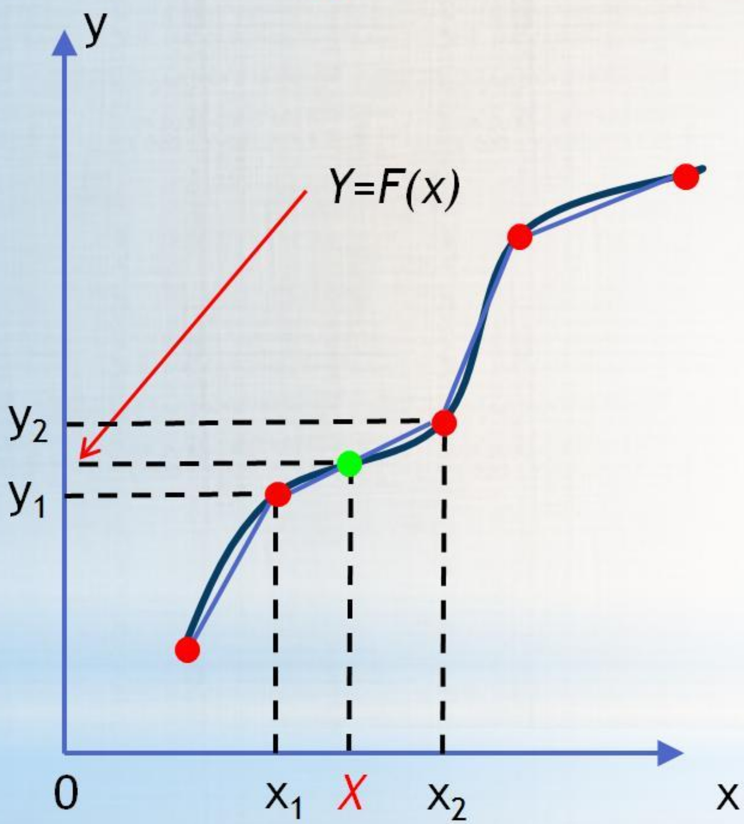
- ***the given data points** are considered to be exact nodes of the function to be constructed*

*(unlike Interpolation), **Approximation** – a concept of finding the best possible fit to the given data points, which would allow to predict values outside of the measured range of a discrete set of known data points*

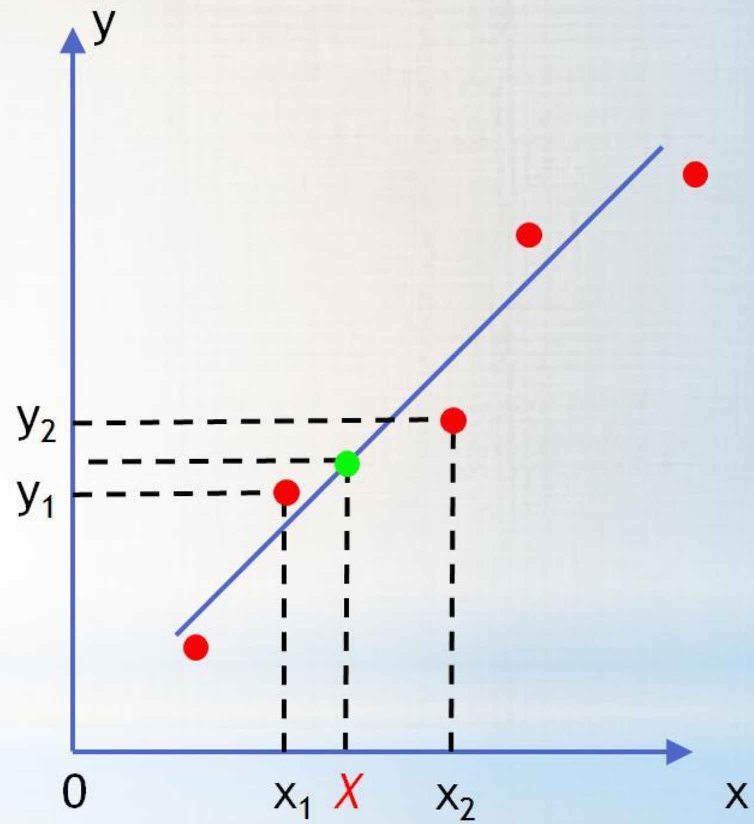
- ***the given data points** are regarded as the approximate ones*

x	x_0	x_1	x_2	…	x_n
$f(x)$	y_0	y_1	y_2	…	y_n

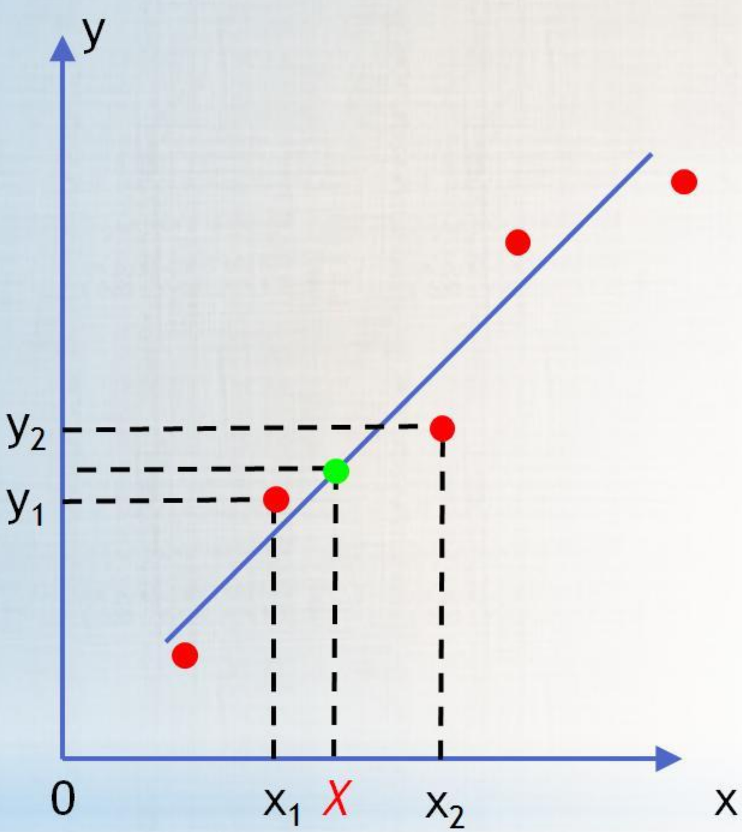
Interpolation



Approximation



Approximation



x	x_0	x_1	x_2	...	x_n
f(x)	y_0	y_1	y_2	...	y_n

Task: find a function $Y=F(X)$, which describes the observed dependence and produces values $Y_i=F(x_i)$, as close as possible to measured $y_0 \dots y_n$ at $x_0, \dots x_n$.

Condition of being as close as possible mathematically is written as follows:

$$(y_i - Y_i)^2 \rightarrow min \quad \Leftrightarrow \quad \Sigma\, (y_i - Y_i)^2 \rightarrow min$$

Standard regressions used for approximation of data points:

LS method guarantees that the found fit would be the best possible with the given type of dependence.

Standard dependences:

To choose a proper dependence type:

- perform visual analysis of the data points;
- consider physical processes the dependence should be described with;
- use analytical algorithm (Demidovitch)

A. linear:	$y=ax+b$	E. fractionally-linear:	$y=1/(ax+b)$
B. polynomial (example - square-law):	$y=ax^2+bx+c$	F. logarithmic:	$y=a\ln(x)+b$
C. power-law:	$y=ax^m$	G. inversely-proportional:	$y=a/x+b$
D. exponential:	$y=a\exp(kx)$	H. rational:	$y=x/(ax+b)$

Linear approximation:

$\{x_i, y_i\}$, $i = 1,2,..n$
$Y_i(x_i) = a + b\cdot x_i$

$\sigma^2 = \frac{1}{n}\Sigma[(a + b\cdot x_i) - y_i]^2$, σ^2 is the variance, $\sigma^2 \rightarrow \min$.

Differentiating $\Sigma[(a + b\cdot x_i) - y_i]^2$ by each parameter, and setting differential equal to 0, we obtain a system of *m+1* equations:

$$\begin{cases} \frac{\partial}{\partial a}\left[\Sigma((a + bx_i) - y_i)^2\right] = 0 \\ \frac{\partial}{\partial b}\left[\Sigma((a + bx_i) - y_i)^2\right] = 0 \end{cases} \quad => \quad \begin{cases} na + b\Sigma x_i = \Sigma y_i \\ a\Sigma x_i + b\Sigma x_i^2 = \Sigma x_i y_i \end{cases}$$

Hence, to find the best possible linear fit for $\{x_i;y_i\}$, one needs to compute :
Σx_i, Σx_i^2, Σy_i, $\Sigma x_i y_i$.

Example: *finding of coefficients a_0, a_1 for fitting curve* $y = a_0 x + a_1$:

Data table:	x_i	1	2	3	4	5	6
	y_i	2.0	4.9	7.9	11.1	14.1	17.0

$$\begin{cases} na + b\Sigma x_i = \Sigma y_i \\ a\Sigma x_i + b\Sigma x_i^2 = \Sigma x_i y_i \end{cases}$$

Calculation table:

i	x_i	x_i^2	y_i	$x_i y_i$
1	1	1	2.0	2.0
2	2	4	4.9	9.8
3	3	9	7.9	23.7
4	4	16	11.1	44.4
5	5	25	14.1	70.5
6	6	36	17.0	102
Σ	21	91	57.0	252.4

Hence, system of equations:

$$\begin{cases} a_0 \cdot 91 + a_1 \cdot 21 = 252.4 \\ a_0 \cdot 21 + a_1 \cdot 6 = 57 \end{cases}$$

Solution:

$$\begin{cases} a_0 = 3.023 \\ a_1 = -1.081 \end{cases}$$

Polynomial approximation

$$y = a_0 x^m + a_1 x^{m-1} + a_2 x^{m-2} + \cdots + a_{m-1} x^1 + a_m$$

Differentiating by free coefficients, we have a system with unknown $a_0 \dots a_m$.

$$\begin{cases} a_0 \Sigma x_i^m + a_1 \Sigma x_i^{m-1} + a_2 \Sigma x_i^{m-2} + \cdots + n a_m = \Sigma y_i \\ a_0 \Sigma x_i^{m+1} + a_1 \Sigma x_i^{m} + a_2 \Sigma x_i^{m-1} + \cdots + a_m \Sigma x_i^1 = \Sigma x_i y_i \\ a_0 \Sigma x_i^{m+2} + a_1 \Sigma x_i^{m+1} + a_2 \Sigma x_i^{m} + \cdots + a_m \Sigma x_i^2 = \Sigma x_i^2 y_i \\ \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \\ a_0 \Sigma x_i^{2m} + a_1 \Sigma x_i^{2m-1} + a_2 \Sigma x_i^{2m-2} + \cdots + a_m \Sigma x_i^m = \Sigma x_i^m y_i \end{cases}$$

Make a table for calculation:

i	x_i	x_i^2	.	x_i^{2m}	y_i	$x_i y_i$	$x_i^2 y_i$	.	$x_i^m y_i$
1	x_1	x_1^2	.	x_1^{2m}	y_1	$x_1 y_1$	$x_1^2 y_1$	.	$x_1^m y_1$
2	x_2	x_2^2	.	x_2^{2m}	y_2	$x_2 y_2$	$x_2^2 y_2$	.	$x_2^m y_2$
…	…	…	….	…	…	…	…	….	…
n	x_n	$x_n^2 y_n$	.	$x_n^2 y_n$	y_n	$x_n y_n$	$x_n^2 y_n$	.	$x_n^m y_n$
Σ	Σx_i	Σx_i^2	.	$\Sigma x_i^2 y_i$	Σy_i	$\Sigma x_i y_i$	$\Sigma x_i^2 y_i$	.	$\Sigma x_i^m y_i$

Other standard regressions. Linearization by variable(s) change

Dependence type	Regression	Rearranging	Variable(s) change	Linear regression
C. power-law:	$y=ax^m$	$\lg(y) = m\cdot\lg(x) + \lg(a)$	$Y = \lg(y)$, $X = \lg(x)$	$Y = m\cdot X + \lg(a)$
D. exponential:	$y=a\exp(kx)$	$\ln(y) = \ln(a) + kx$	$Y = \ln(y)$	$Y = kx + \ln(a)$
E. fractionally-linear:	$y=1/(ax+b)$	$1/y = ax + b$	$Y = 1/y$	$Y = ax + b$
F. logarithmic:	$y=a\ln(x)+b$		$X = \ln(x)$	$y = a\cdot X + b$
G. inversely-proportional:	$y=a/x+b$		$X = 1/x$	$y = a\cdot X + b$
H. rational:	$y=x/(ax+b)$	$1/y = a + b/x$	$Y = 1/y$, $X = 1/x$	$Y = a + b\cdot X$

Exercise 1. In the "Fundamentals of Chemistry" by D.I. Mendeleyev, data are presented on the solubility of sodium nitrate ($NaNO_3$) as a function of water temperature. In a hundred parts of water the following number of parts of the substance dissolves at the appropriate temperatures:

Plot data points and find linear approximation: $n = a + bt$.

t, °C	0	4	10	15	21	29	36	51	68
n	66.7	71.0	76.3	80.6	85.7	92.9	99.4	113.6	125.1

Exercises 2. When studying the street traffic, observations were made on the distance traveled by the vehicle by inertia (after braking), depending on the speed. The results of observations are:

u, km/h	S_1, m	S_2, m	S_3, m	S_4, m	S_5, m	<S>, m
6.44	0.61	3.05				
11.26	1.22	6.71				
12.87	4.88					
14.48	3.05					
16.09	7.93	5.49	10.37			
17.70	8.54	5.18				
19.31	6.10	4.27	7.32	8.54		
20.92	10.37	7.93	10.37	14.03		
22.53	10.98	7.93	18.30	24.40		
24.14	16.47	7.93	6.10			
25.74	9.76	12.20				
27.35	15.25	12.20	9.76			
28.96	17.08	25.62	23.18	12.81		
30.57	20.74	14.03	10.98			
32.18	14.64	17.08	19.52	15.86	9.76	
35.40	20.13					
37.01	16.47					
38.62	28.36	21.35	36.60	28.06		
40.23	25.92					

Plot data points and find linear/polynomial approximation.

Exercises 3. Data of laboratory experiments on the determination of gravity with the help of a device with a falling load, in which the load positions at the ends of consecutive intervals in ***1/30*** second were noted by the spark method, are given in the table.

The dependence s(t) has the form: $s = s_0 + u_0 t + 1/2\, g t^2$. Find ***g***.

Peg's data for determination of the free-fall acceleration:

time, in 1/30 sec	1	2	3	4	5	6	7	8	9	10	11	12	13	14
S, cm	11.86	15.67	20.60	26.69	33.71	41.93	51.13	61.49	72.90	85.44	99.08	113.77	129.54	146.48

Exercise 4. In a laboratory work on refractometry, it is required to calculate the unknown concentration of glycerin solution by its refractive index using the coefficients of solutions with known concentration. The refractive index in the work is determined with use of a refractometer:

Sample		1	2	3	4	5
Concentration, %	X	25	50	75	100	x
Refractive index, *n*	y	1.3734	1.3943	1.4244	1.4538	1.3746

Find linear dependence $y=a_0x + a_1$ and determine the unknown concentration.

http://rplab.ru/~ylobanov / Information & Communication Technologies and Media-Information Literacy / The Least Square Method Introduction / LSM.pdf