Introduction to Numerical Analysis

Marek Kręglewski

Course content

Week 1	Solutions of nonlinear equations in one variable: the bisection algorithm.
Week 2	Differential calculus.
Week 3	The Newton-Raphson method, the secant method.
Week 4	Integral calculus.
Week 5	Numerical integration: trapezoidal rule and Simpson's rule.
Week 6	Taylor expansion – error of a numerical method
Week 7	Numerical differentiation: forward and backward-difference formula. Three-point formula of numerical differentiation.
Week 8	The Richardson's extrapolation.
Week 9	Initial value-problem for differential equations: Euler's method, the Runge-Kutta methods.
Week 10	Polynomial interpolation: Newton and Lagrange polynomials.
Week 11	Methods for solving linear systems: linear systems of equations, Cramer's rule, Gaussian elimination.
Week 12	Approximation theory: least-squares approximation.
Week 13	Linear algebra, matrix inversion and the determinant of a matrix.
Week 14	Round-off errors: absolute error, relative error, significant digits.

Course content 2

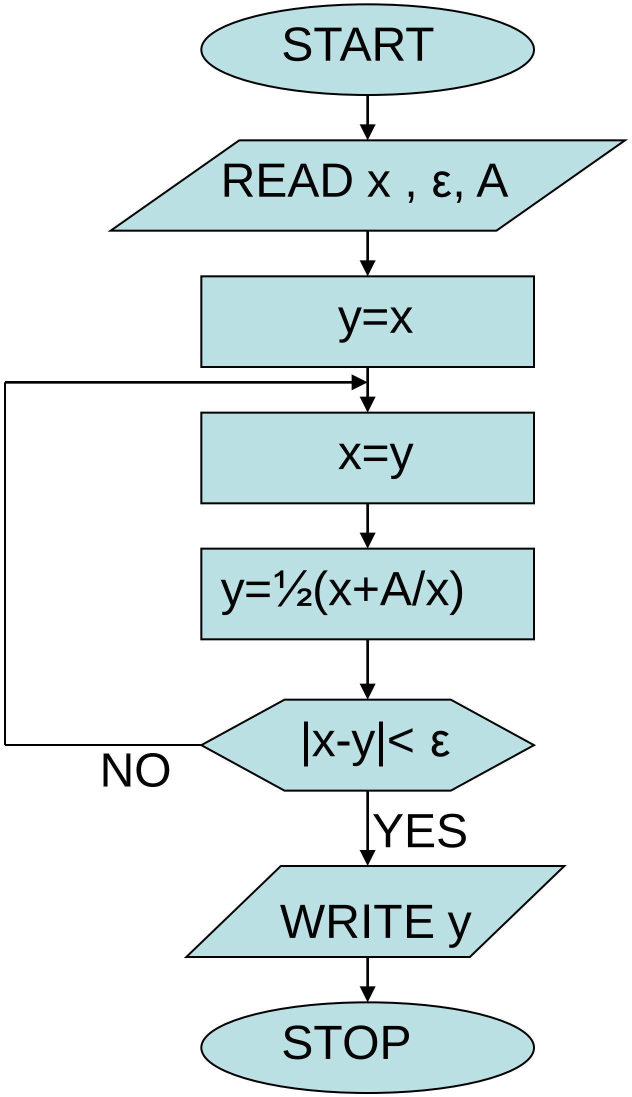
LABORATORY CLASSES

1. MS Excel – general introduction
2. Application of the MS Excel in solving numerical problems

MANUALS:

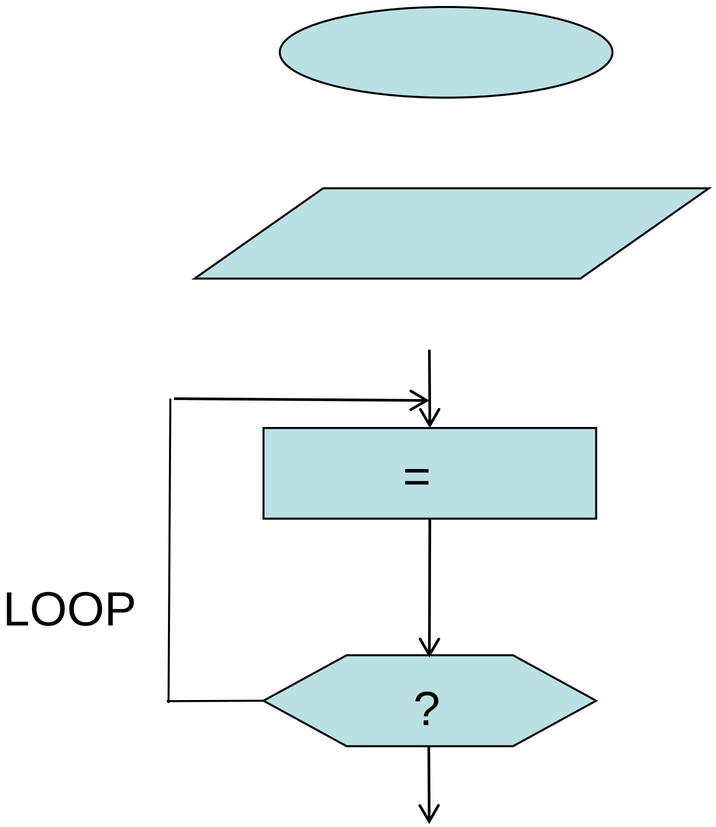
1. E. Steiner, Mathematics for chemists, Oxford.
2. A. Ralston, Introduction to numerical analysis.

Solution of equation in one variable x=f(x)



Trace of operations

Algorithm notation



START and STOP of a sequential algorithm

INPUT and OUTPUT operations

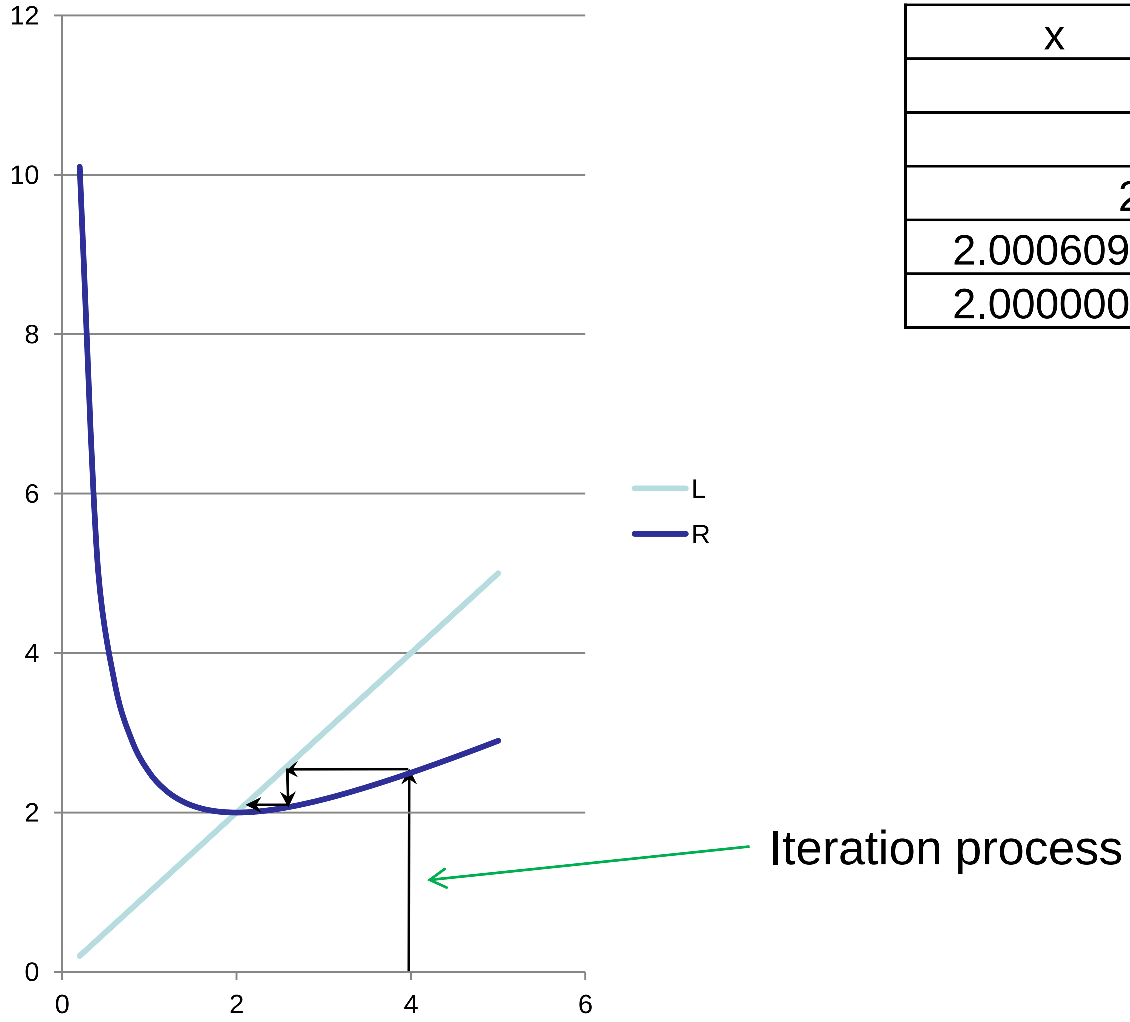
SUBSTITUTION operations

CONDITIONAL operation

SUBSTITUTION   variable = expression

Calculate the value of the expression and save it under the name of the variable

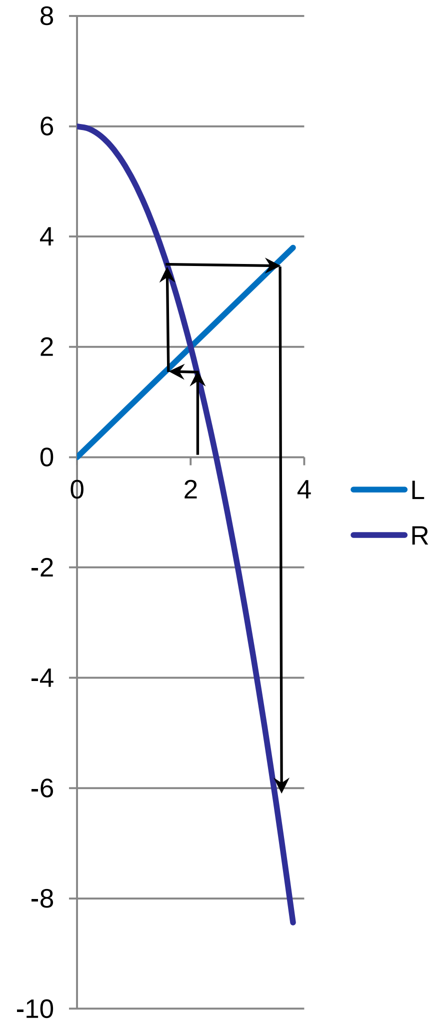
Convergent process: $x=\frac{1}{2}(x+4/x)$



x	y
4	2.5
2.5	2.05
2.05	2.000609756
2.000609756	2.000000093
2.000000093	2

Divergent process: x=6-x*x

x	y
2.1	1.59
1.59	3.4719
3.4719	-6.05408961
-6.05408961	-30.65200101
-30.65200101	-933.5451657
-933.5451657	-871500.5763
-871500.5763	-7.59513E+11
-7.59513E+11	-5.7686E+23
-5.7686E+23	-3.32768E+47
-3.32768E+47	-1.10734E+95

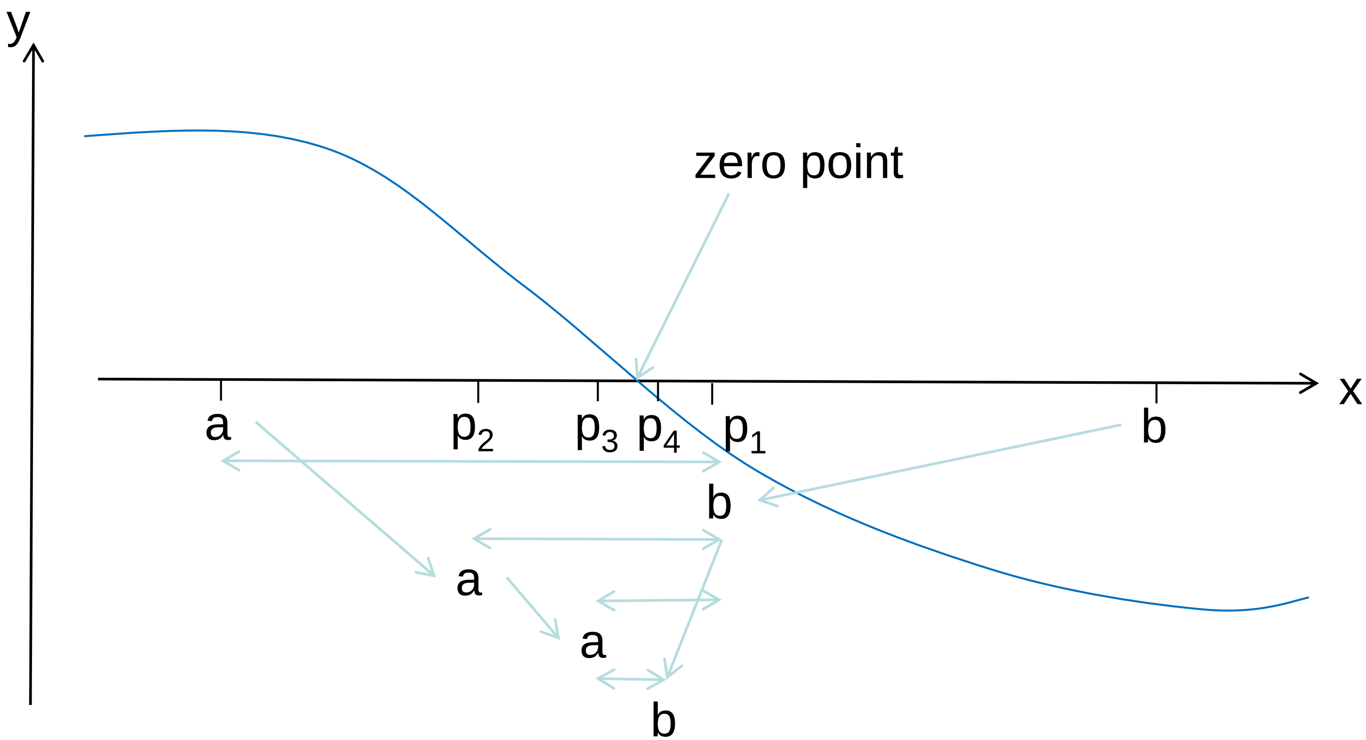


Solution of equation in one variable

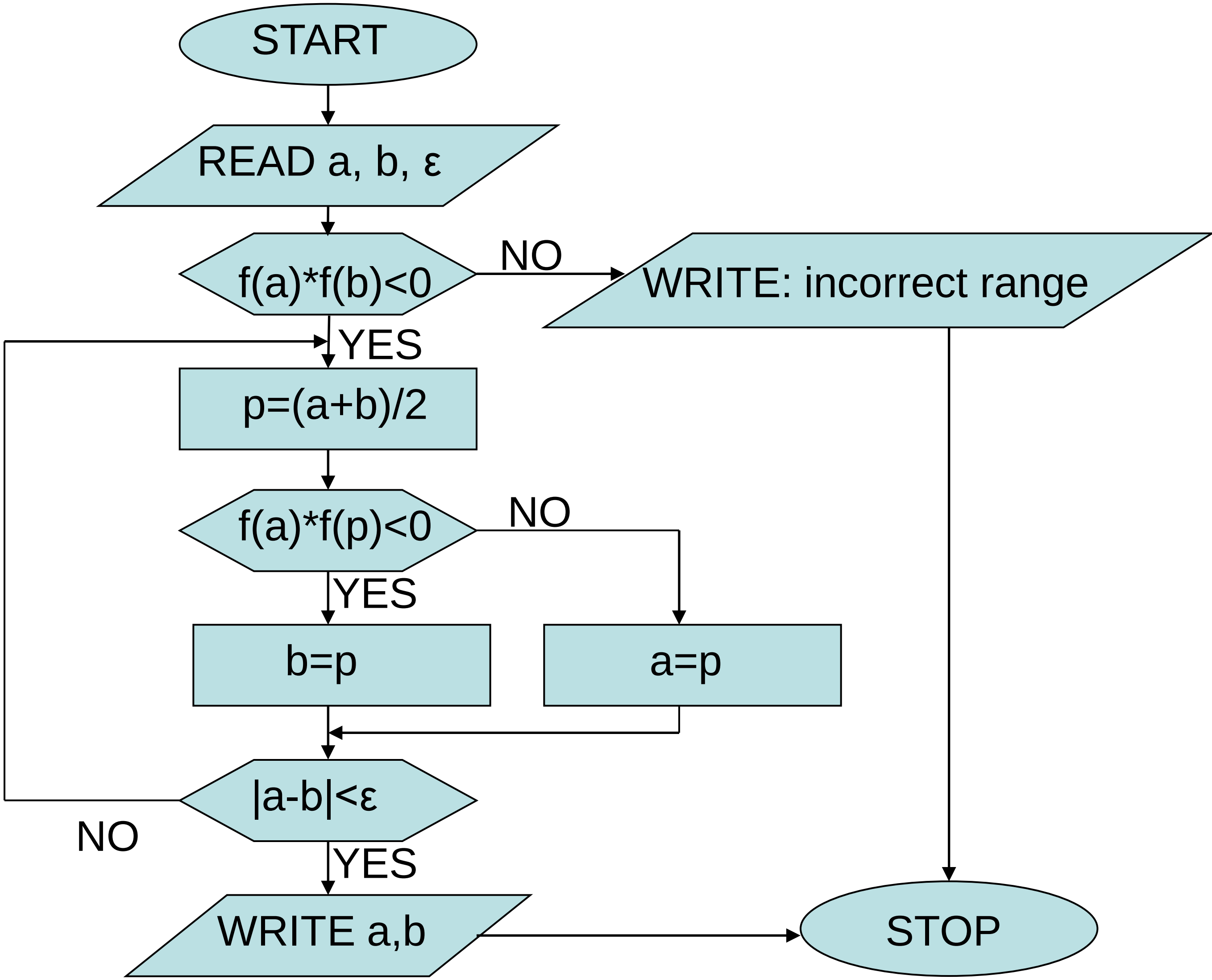
Bisection method

Solution of an equation f(x)=0, i.e. search for zero points of the function f(x).
Search for the a zero point in the range <a,b>, in which:

1) the function f(x) is continuous
2) f(x) changes the sign in the range <a,b>, i.e. f(a)*****f(b)<0



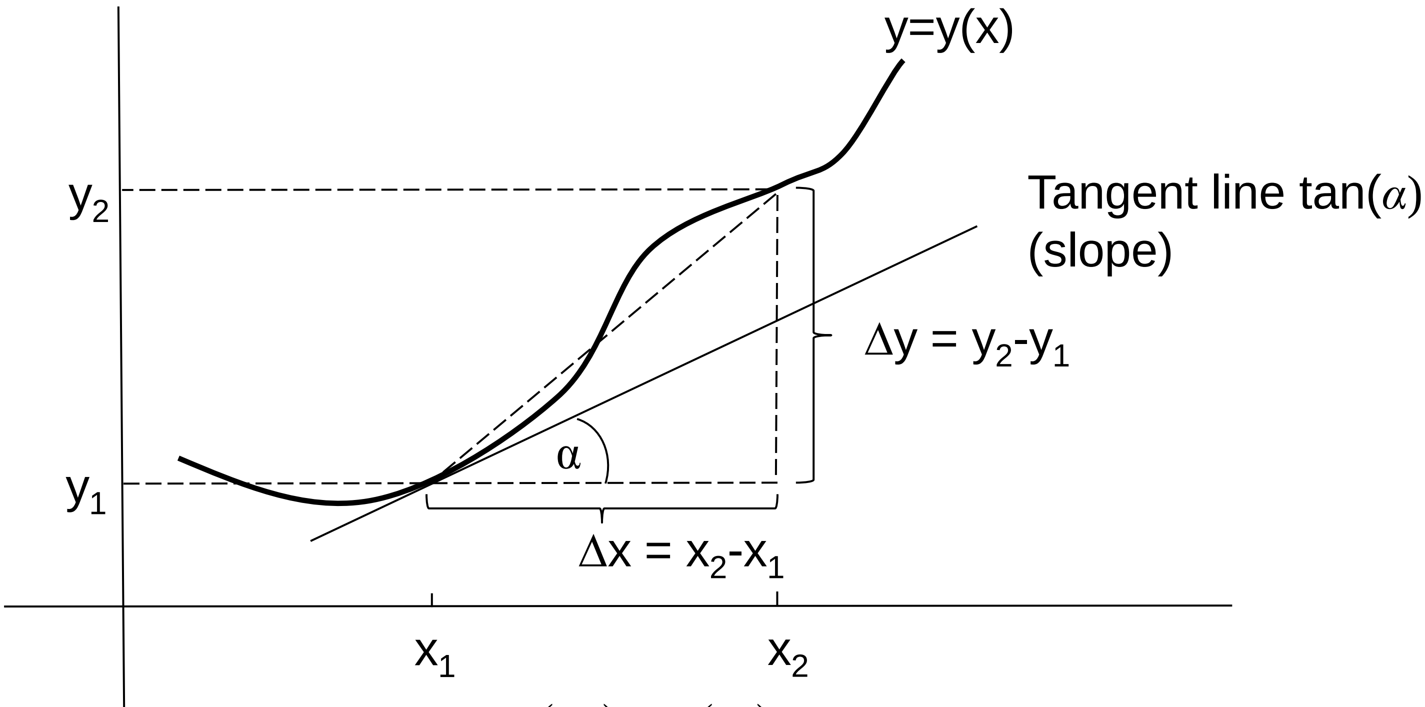
Bisection Algorithm



Trace of operations

Differential Calculus

Derivative of a function – a measure how rapidly the dependent variable changes with changes of the independent variable



$$\tan(\alpha) = \lim_{x_2 \to x_1} \frac{y(x_2) - y(x_1)}{x_2 - x_1} = \lim_{x_2 \to x_1} \frac{\Delta y}{\Delta x} = \frac{dy}{dx}$$

derivative

Differential Calculus

Find the derivative of the function
$y = a\,x^2$
Let $\Delta x = x_2 - x_1$ and $\Delta y = y(x_2) - y(x_1)$

$$\Delta y = a(x_2)^2 - a(x_1)^2 = a(x_1+\Delta x)^2 - a(x_1)^2 = a[(x_1)^2 + 2x_1\Delta x + (\Delta x)^2] - a(x_1)^2 =$$
$$= a[2x_1\Delta x + (\Delta x)^2]$$

After dividing by Δx

$$\frac{\Delta y}{\Delta x} = 2a\,x_1 + a\,\Delta x$$

In the limit as $x_2 \rightarrow x_1$ (i.e. $\Delta x \rightarrow 0$)

$$\frac{d\left(ax^2\right)}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = 2a\,x$$

The derivative of the function $y=ax^2$ is $dy/dx=2ax$

Differential Calculus

Derivatives of some elementary functions (*a* is a constant):

Function *y=y(x)*	**Derivative *dy/dx=y'(x)***
x^n	$n\, x^{n-1}$
a^x	$a^x \ln(a)$
$ln(x)$	$1/x$
$sin(x)$	$cos(x)$
$cos(x)$	$-sin(x)$
a	0

Let y(x) and z(x) are differentiable functions of x:

$$\frac{d(y+z)}{dx} = \frac{dy}{dx} + \frac{dz}{dx} \qquad \frac{d(y-z)}{dx} = \frac{dy}{dx} - \frac{dz}{dx} \qquad \frac{d(yz)}{dx} = y\frac{dz}{dx} + z\frac{dy}{dx} \qquad \frac{d(y/z)}{dx} = \frac{z\left(\frac{dy}{dx}\right) - y\left(\frac{dz}{dx}\right)}{z^2}$$

Composite function f(u(x)) $\qquad \frac{df}{dx} = \frac{df}{du} * \frac{du}{dx}$

Derivatives - examples

d/dx($4*x^5$ – $0.3*x^3$+10) =4 d/dx x^5 – 0.3 d/dx x^3 + d/dx(10)= 4*(5*x^4)-0.3*(3*x^2) +0 = 20*x^4-0.9*x^2

d/dx(sin(x)*cos(x)) = d/dx(sin(x))*cos(x)+sin(x)*d/dx(cos(x))=
=cos(x)*cos(x) +sin(x)*(-sin(x))=$\cos^2$(x)-$\sin^2$(x)=cos(2x)

d/dx(½ sin(2x))= ½ d/dx(sin(2x)) = ½ cos(2x)*2 =cos(2x)

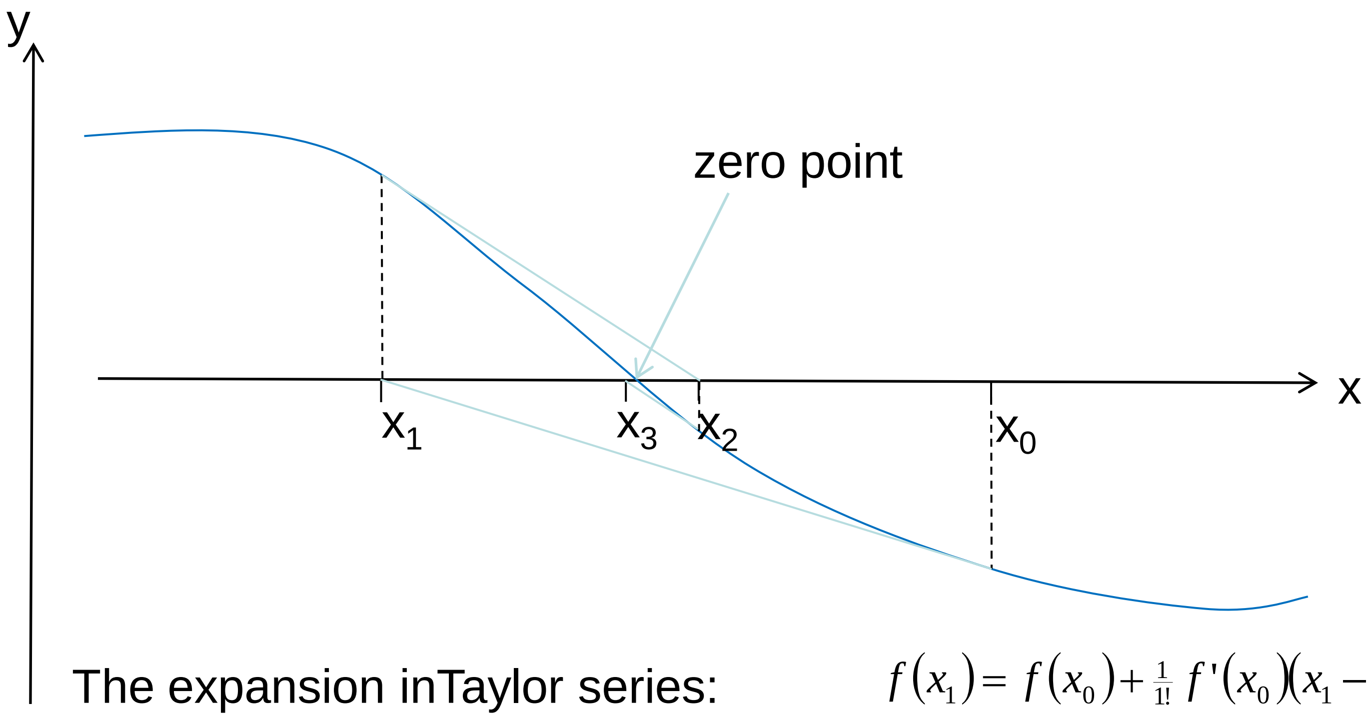
d/dx(4*x^5/(1 – x^3)) =[d/dx(4*x^5)*(1-x^3)-4*x^5*d/dx(1-x^3)]/$(1-x^3)^2$ =
=[20*x^4*(1-x^3)+12*x^7]/ $(1-x^3)^2$=[20*x^4-8x^7]/ $(1-x^3)^2$

Solution of equation in one variable

Newton-Raphson method

The search of a zero point begins at any point x_0, if:

1) the function f(x) and its first derivative are continuous
2) the first derivative is different from zero

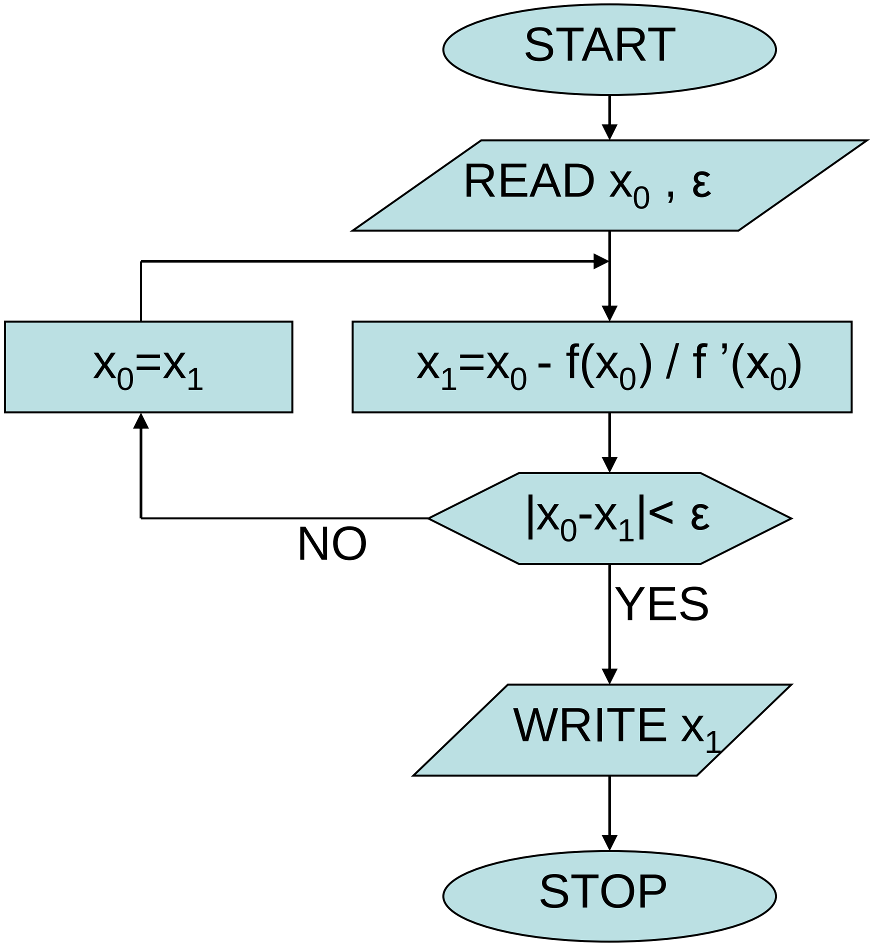


The expansion inTaylor series:

$$f(x_1) = f(x_0) + \tfrac{1}{1!} f'(x_0)(x_1 - x_0) + \ldots$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Newton-Raphson algorithm



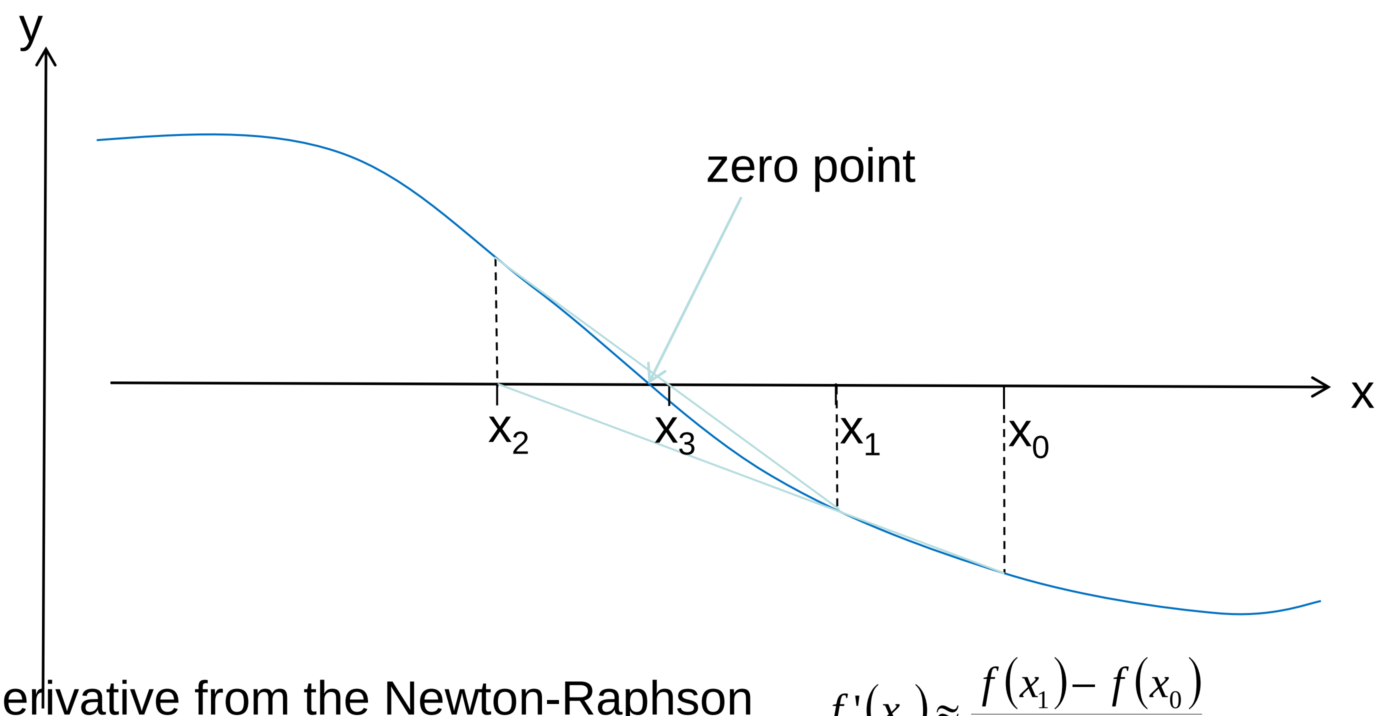
Trace of operations

Solution of equation in one variable

Secant Method

The search for the zero point begins from a pair of points(x_0, x_1), if:

1) the function f(x) is continuous
2) $f(x_0) \neq f(x_1)$, when $x_0 \neq x_1$

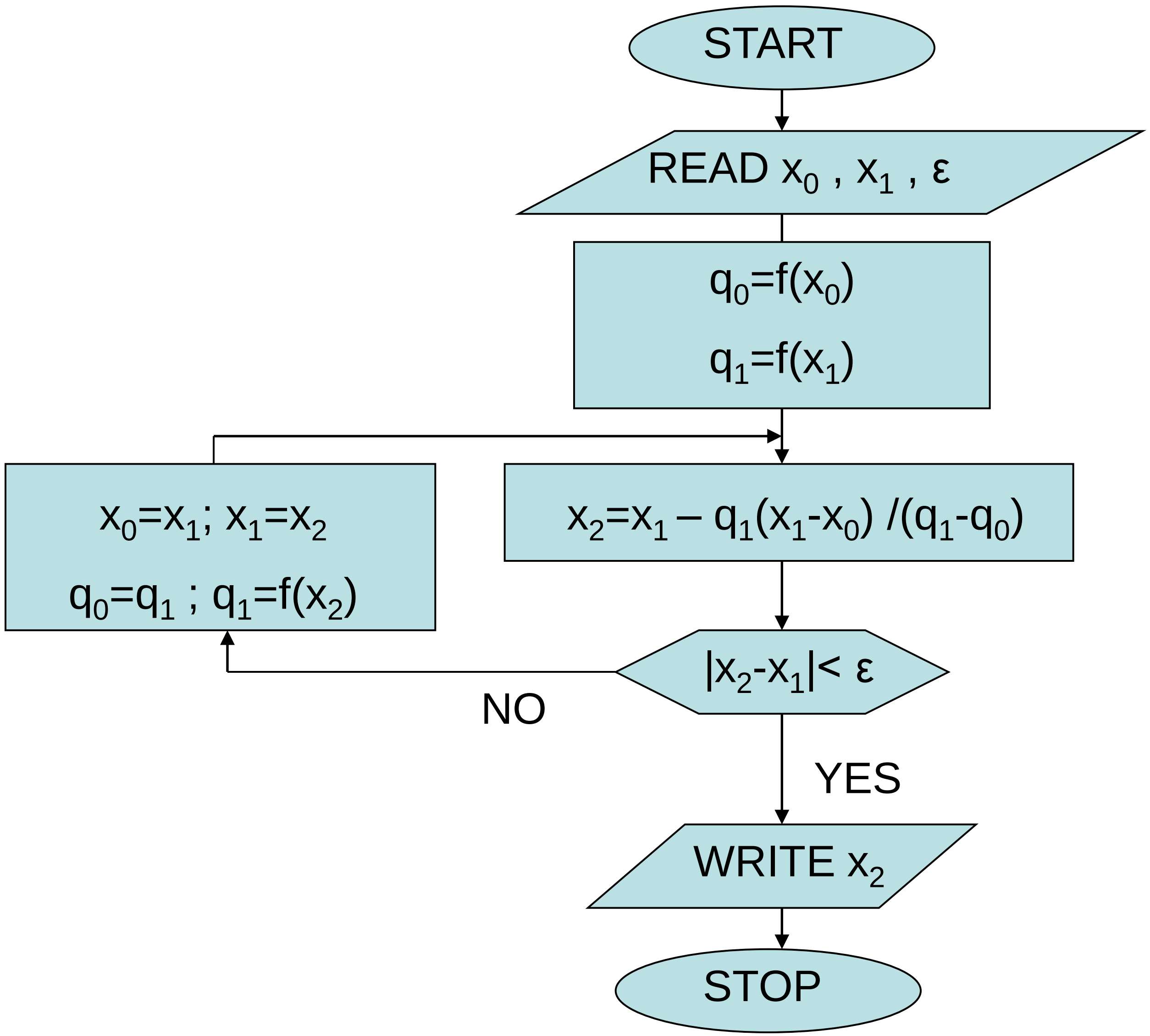


The first derivative from the Newton-Raphson method approximated with an expression:

$$f'(x_1) \approx \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$x_2 = x_1 - \frac{f(x_0)(x_1 - x_0)}{f(x_1) - f(x_0)}$$

Secant method algorithm



Trace of operations

Integral Calculus – principal facts

- The antiderivative *F(x)* of *f(x)* is the function such that *dF(x)/dx=f(x)*
- The indefinite integral is the same thing as the antiderivative function
- A definite integral is the limit of a sum of terms *f(x)Δx*

$$\int_a^b f(x)dx = F(b) - F(a)$$

Integral Calculus - examples

A car moves with constant velocity v(t)=50 km/h. Calculate the distance it covers in 2 hours.

$$s = v(t)\Delta t = 50km/h*2h = 100km$$

$$s = \int_0^2 v(t)dt = \int_0^2 50dt = 50t\Big|_0^2 = 50*2 - 50*0 = 100km$$

A stone is falling with the acceleration g(t) = 10 m/s^2. At the begining its velocity is 0 m/s. Calculate the distance the stone covers between 2nd and 4th second of the fall.

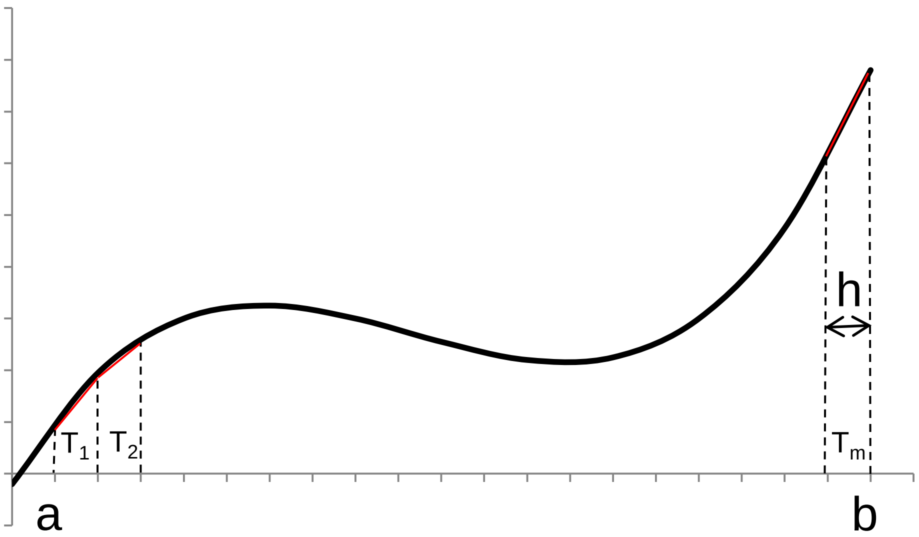
$$v(t) = \int g(t)dt = \int 10dt = 10t + const$$

$$v(0) = 0 \quad \Rightarrow \quad const = 0$$

$$s = \int_2^4 v(t)dt = \int_2^4 10tdt = 5t^2\Big|_2^4 = 5*4^2 - 5*2^2 = 80 - 20 = 60m$$

Numerical integration

Trapezoidal rule



$$\int_a^b f(x)dx$$

$$h = \frac{b-a}{m}$$

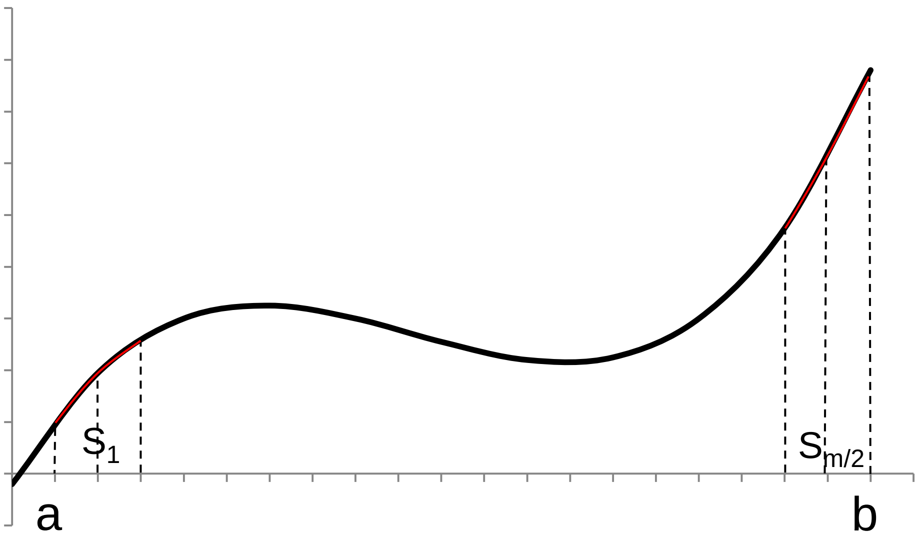
$$T_1 = \frac{h}{2}[f(a) + f(a+h)] \qquad T_2 = \frac{h}{2}[f(a+h) + f(a+2h)] \qquad \ldots \qquad T_m = \frac{h}{2}[f(a+(m-1)*h) + f(a+m*h)]$$

$$T_1 = \frac{h}{2}[f_0 + f_1] \qquad T_2 = \frac{h}{2}[f_1 + f_2] \qquad \ldots \qquad T_m = \frac{h}{2}[f_{m-1} + f_m], \qquad f_i = f(a+i*h)$$

$$T = T_1 + T_2 + \ldots + T_m = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \ldots + f_m]$$

Numerical integration

Simpson's rule



$$\int_a^b f(x)dx$$

$$h = \frac{b-a}{m}$$

m must be even

$S_1 = \frac{h}{3}[f_0 + 4f_1 + f_2]$ $S_2 = \frac{h}{3}[f_2 + 4f_3 + f_4]$ ... $S_{m/2} = \frac{h}{3}[f_{m-2} + 4f_{m-1} + f_m]$, $f_i = f(a + i * h)$

$$S = S_1 + S_2 + ... + S_{m/2} = \frac{h}{3}[f_0 + 4f_1 + 2f_2 + ... + 2f_{m-2} + 4f_{m-1} + f_m]$$

Analytical integration – an example

$$I = \int_{10}^{12} f(x)dx$$

f(x)=x^3

$$\int_{10}^{12} x^3 dx = \left.\frac{x^4}{4}\right|_{10}^{12} = \frac{12^4}{4} - \frac{10^4}{4} = 2684$$

f(x)=x^4

$$\int_{10}^{12} x^4 dx = \left.\frac{x^5}{5}\right|_{10}^{12} = \frac{12^5}{5} - \frac{10^5}{5} = 29766{,}4$$

Numerical integration – an example

$$I = \int_{10}^{12} f(x)dx$$

	f(x)	
x	x^3	x^4
10	1000	10000
11	1331	14641
12	1728	20736

Calculation results

	x^3	x^4
T(h=2)	2728	30736
T(h=1)	2695	30009
S(h=1)	2684	29766,67
I (accurate)	2684	29766,4

f(x)=x³

$$T(h=2) = \frac{2}{2}(1000 + 1728) = 2728$$

$$T(h=1) = \frac{1}{2}(1000 + 2*1331 + 1728) = 2695$$

$$S(h=1) = \frac{1}{3}(1000 + 4*1331 + 1728) = 2684$$

f(x)=x⁴

$$T(h=2) = \frac{2}{2}(10000 + 20736) = 30736$$

$$T(h=1) = \frac{1}{2}(10000 + 2*14641 + 20736) = 30009$$

$$S(h=1) = \frac{1}{3}(10000 + 4*14641 + 20736) = 29766\tfrac{2}{3}$$

h	T(h)	T(h)-I
2	2728	44
1	2695	11

Errors of the trapezoidal rule

error ~ h^2

h	T(h)	T(h)-I
2	30736	969,6
1	30009	242,6

Geometric series

$$S_n = \sum_{r=0}^{n-1} ax^r = ax^0 + ax^1 + ax^2 + ... + ax^{n-1} \qquad /* \, x$$

$$xS_n = ax^1 + ax^2 + ax^3 + ... + ax^n$$

$$S_n - xS_n = a - ax^n = a(1 - x^n)$$

$$S_n(1 - x) = a(1 - x^n)$$

$$S_n = a\frac{1 - x^n}{1 - x} \qquad x \neq 1$$

When a=1 $$\frac{1 - x^n}{1 - x} = 1 + x + x^2 + ... + x^{n-1}$$

i) The sum $(1 + x + x^2 + ... + x^{n-1})$ is equal to $\left(\frac{1 - x^n}{1 - x}\right)$

ii) $(1 + x + x^2 + ... + x^{n-1})$ is a series expansion of the function $\left(\frac{1 - x^n}{1 - x}\right)$

Maclaurin Series

$$f(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + \dots$$

$c_0, c_1, c_2, c_3 \dots$ constants

$$f'(x) = \frac{df}{dx} = c_1 + 2c_2 x^1 + 3c_3 x^2 + 4c_4 x^3 + \dots$$

$$f''(x) = \frac{d^2 f}{dx^2} = 2c_2 + 6c_3 x^1 + 12c_4 x^2 + \dots$$

Thus

$$f(0) = c_0 \qquad f'(0) = c_1 \qquad f''(0) = 2!c_2 \qquad f'''(0) = 3!c_3$$

$$f^{(n)}(0) = n!c_n \qquad\qquad c_n = \frac{1}{n!} f^{(n)}(0)$$

$$f(x) = f(0) + \frac{1}{1!} f'(0)x + \frac{1}{2!} f''(0)x^2 + \frac{1}{3!} f'''(0)x^3 + \dots$$

Taylor Series

$$f(x) = c_0 + c_1(x-a) + c_2(x-a)^2 + c_3(x-a)^3 + c_4(x-a)^4 + \ldots$$

$c_0, c_1, c_2, c_3 \ldots$ constants

$$f'(x) = \frac{df}{dx} = c_1 + 2c_2(x-a)^1 + 3c_3(x-a)^2 + 4c_4(x-a)^3 + \ldots$$

$$f''(x) = \frac{d^2 f}{dx^2} = 2c_2 + 6c_3(x-a)^1 + 12c_4(x-a)^2 + \ldots$$

Thus

$$f(a) = c_0 \qquad f'(a) = c_1 \qquad f''(a) = 2!c_2 \qquad f'''(a) = 3!c_3$$

$$f^{(n)}(a) = n!c_n \qquad\qquad c_n = \frac{1}{n!} f^{(n)}(a)$$

$$f(x) = f(a) + \frac{1}{1!} f'(a)(x-a) + \frac{1}{2!} f''(a)(x-a)^2 + \frac{1}{3!} f'''(a)(x-a)^3 + \ldots$$

Maclaurin Series - an example

$$f(x) = y_0 e^{-kx}$$

$$y_0 = 1000 \qquad\qquad k = 0{,}2$$

Calculate the value f(6) using the Maclaurin series

$$f'(x) = -k y_0 e^{-kx}$$

$$f''(x) = k^2 y_0 e^{-kx}$$

$$f^{(n)}(x) = (-1)^n k^n y_0 e^{-kx}$$

$$f^{(n)}(x) = -k * f^{(n-1)}(x)$$

Call the Taylor series

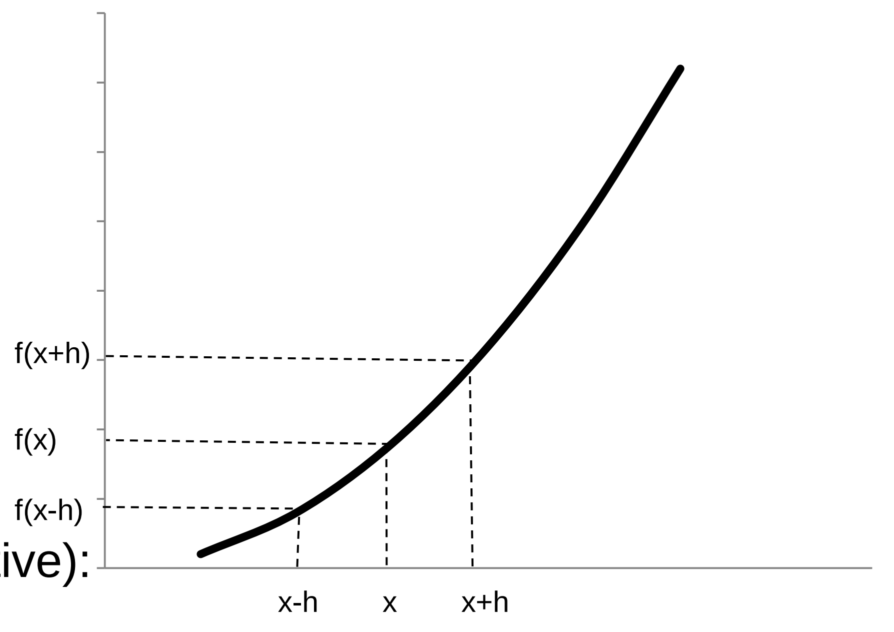
Numerical differentiation

Definition of derivative $$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h}$$

One-side approximation:

$$\tilde{f}_R'(x) = \frac{f(x+h) - f(x)}{h}$$

$$\tilde{f}_L'(x) = \frac{f(x) - f(x-h)}{h}$$



The average of R i L (central derivative):

$$\tilde{f}(x) = \frac{\tilde{f}_R'(x) + \tilde{f}_L'(x)}{2} = \frac{f(x+h) - f(x-h)}{2h}$$

Differentiation – the error

$$f(x+h) = f(x) + \frac{1}{1!} f'(x)h + \frac{1}{2!} f''(x)h^2 + \frac{1}{3!} f'''(x)h^3 + \ldots$$

$$f(x-h) = f(x) - \frac{1}{1!} f'(x)h + \frac{1}{2!} f''(x)h^2 - \frac{1}{3!} f'''(x)h^3 + \ldots$$

$-$

One-side derivative

$$f(x+h) \approx f(x) + \frac{1}{1!} f'(x)h + \frac{1}{2!} f''(x)h^2$$

$$f'(x)h \approx f(x+h) - f(x) - \frac{1}{2!} f''(x)h^2 \quad / : h$$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} - \frac{1}{2!} f''(x)h$$

derivative error ~ h^1

Central derivative

$$f(x+h) - f(x-h) \approx 2f'(x)h + \frac{2}{3!} f'''(x)h^3$$

$$2f'(x)h \approx f(x+h) - f(x-h) - \frac{2}{3!} f'''(x)h^3 \quad / : (2h)$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{3!} f'''(x)h^2$$

derivative error ~ h^2

Calculation of a derivative

Calculate the derivative of ln(x) at the point x=3 using the central derivative method and one-side method for different step length h:

f(x)=ln(x)   ln'(3)=1/3   ln(3)=1.098612

f'(x)=[f(x+h)-f(x-h)]/(2*h)

h	x±h	f(x±h)	f'(3)	error	h^2	error/h^2
1	4	1.386294	0.346574	0.01324	1	0.01324
	2	0.693147				
0.5	3.5	1.252763	0.336472	0.003139	0.25	0.012556
	2.5	0.916291				
0.1	3.1	1.131402	0.333457	0.000124	0.01	0.012354
	2.9	1.064711				

f'(x)=[f(x+h)-f(x)]/h

h	x+h	f(x+h)	f'(3)	error	h	error/h
1	4	1.386294	0.287682	-0.04565	1	-0.04565
0.5	3.5	1.252763	0.308301	-0.02503	0.5	-0.05006
0.1	3.1	1.131402	0.327898	-0.00544	0.1	-0.05435

The decreasing step minimizes the error. The results are different for different methods.

Differential equation 1st order

Differential equation for radioactive decay

$$\frac{dN(t)}{dt} = -kN(t)$$

Suggested solution:

$$N(t) = ae^{bt}$$

Checking the correctness:

$$\frac{dN(t)}{dt} = abe^{bt}$$

Substitution:

$$abe^{bt} = -kae^{bt}$$

Left side equal to right side, when:

$$b = -k$$

$$N(t) = ae^{-kt}$$

Constant „a” determined from the initial condition:

$$N(0) = N_0$$

$$ae^{-k0} = N_0$$

$$a = N_0$$

Final analytic solution:

$$N(t) = N_0 e^{-kt}$$

k – radioactive decay constant

Radioactive decay

Differential equation for the radioactive decay

$$\frac{dN(t)}{dt} = -kN(t)$$

Analytic solution:

$$N(t) = N_0 e^{-kt}$$

Half-life period τ:

$$N(\tau) = \tfrac{1}{2} N_0$$

$$N_0 e^{-k\tau} = \tfrac{1}{2} N_0$$

$$e^{-k\tau} = \tfrac{1}{2}$$

$$-k\tau = \ln\left(\tfrac{1}{2}\right)$$

$$-k\tau = -\ln(2)$$

$$\boxed{\tau = \frac{\ln(2)}{k}}$$

Differetial equation – the Euler method

The equation (f is a known function):

$$\frac{dy(x)}{dx} = f\left(x, y(x)\right)$$

Approximate expression for the derivative:

$$\frac{dy(x)}{dx} = \frac{y(x+h) - y(x)}{h}$$

After transformation:

$$y(x+h) = y(x) + h\,\frac{dy(x)}{dx}$$

Simplified notation:

$$y_i = y(x+ih) \qquad f_i = f\left(x+ih, y_i\right)$$

$$y_{i+1} = y_i + h\left(\frac{dy(x)}{dx}\right)_i$$

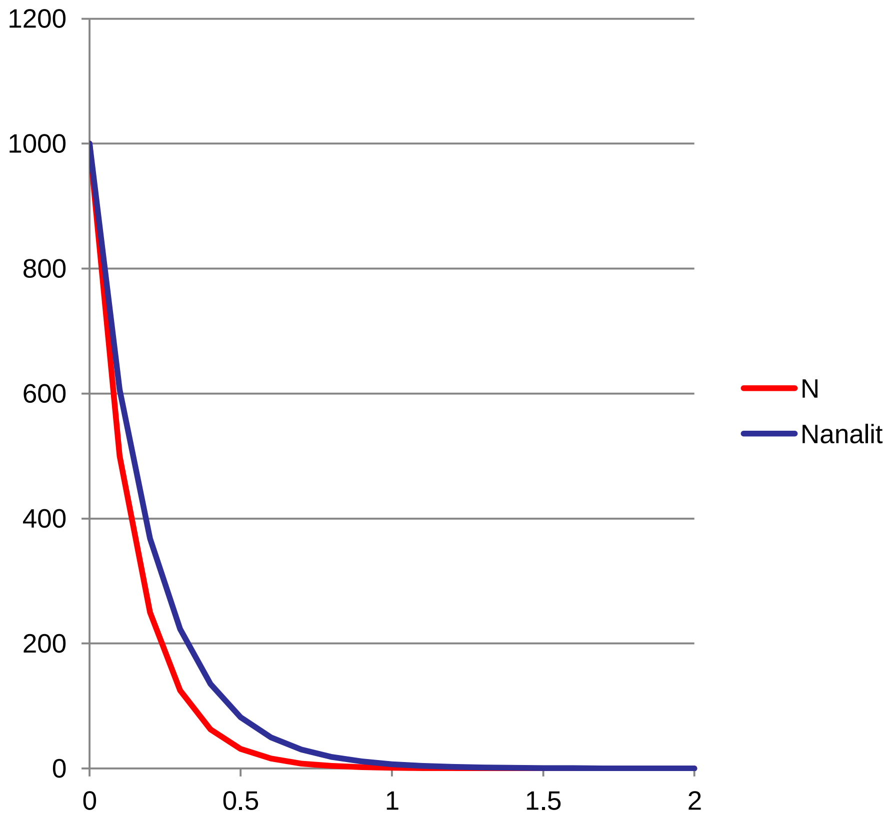
$$y_{i+1} = y_i + hf_i$$

The last expression allows for step by step calculation of the function y(x).
The value of the function in the zeroth step y_0 determined from initial condition.

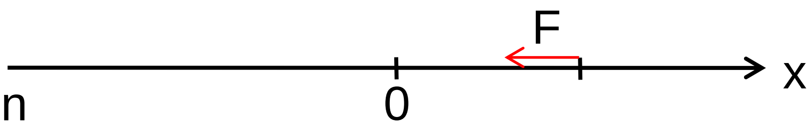
Differential equation 1st order

$$\frac{dN}{dt} = -kN \qquad k = 5 \qquad \tau = 0.1386 \qquad h = 0.1$$

i	t	N	dN/dt	Nanalit
0	0	1000	-5000	1000
1	0.1	500	-2500	606.5307
2	0.2	250	-1250	367.8794
3	0.3	125	-625	223.1302
4	0.4	62.5	-312.5	135.3353
5	0.5	31.25	-156.25	82.085
6	0.6	15.625	-78.125	49.78707
7	0.7	7.8125	-39.0625	30.19738
8	0.8	3.90625	-19.5313	18.31564
9	0.9	1.953125	-9.76563	11.109
10	1	0.976563	-4.88281	6.737947
11	1.1	0.488281	-2.44141	4.086771
12	1.2	0.244141	-1.2207	2.478752
13	1.3	0.12207	-0.61035	1.503439
14	1.4	0.061035	-0.30518	0.911882
15	1.5	0.030518	-0.15259	0.553084
16	1.6	0.015259	-0.07629	0.335463
17	1.7	0.007629	-0.03815	0.203468
18	1.8	0.003815	-0.01907	0.12341
19	1.9	0.001907	-0.00954	0.074852
20	2	0.000954	-0.00477	0.0454



Differential equation 2nd order



Harmonic oscillation

$F_p = ma$ a - acceleration

$F_w = -kx$ x - position

Assumption: m=1 k=1

The balance of forces: $F_p = F_w$

Thus a=-x

$$\frac{d^2x(t)}{dt^2} = -x(t)$$

$$x(t) = ce^{bt}$$

$$x'(t) = cbe^{bt}$$

$$x''(t) = cb^2e^{bt}$$

$$cb^2e^{bt} = -ce^{bt}$$

$$b^2 = -1$$

$$b = \pm i$$

Specific solutions:

$$x_1(t) = ce^{it}$$

$$x_2(t) = ce^{-it}$$

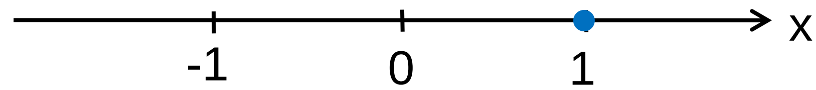
General solution:

$$x(t) = c_1e^{it} + c_2e^{-it}$$

Constants c_1 i c_2 determined from intial conditions

Differential equation 2nd order

$$x(t) = c_1 e^{it} + c_2 e^{-it}$$



Initial conditions:

$$x(0) = 1$$

$$x'(0) = 0$$

$$x(0) = c_1 e^{i0} + c_2 e^{-i0} = c_1 + c_2 = 1$$

$$x'(0) = c_1 i e^{i0} - c_2 i e^{-i0} = ic_1 - ic_2 = 0$$

$$c_1 = c_2$$

$$2c_1 = 1$$

$$c_1 = \tfrac{1}{2} \qquad c_2 = \tfrac{1}{2}$$

General solution including the initial conditions:

$$x(t) = \tfrac{1}{2} e^{it} + \tfrac{1}{2} e^{-it} = \boxed{\cos(t)}$$

Numerical solution I

$$a(t) = -x(t) \qquad where: \quad a(t) = \frac{dv}{dt} = \frac{d^2x}{dt^2} \qquad v(t) = \frac{dx}{dt}$$

Succesive application of approximate expressions for the first derivative:

$$v(t) = \frac{x(t+\Delta t) - x(t)}{\Delta t}$$

$$a(t) = \frac{v(t+\Delta t) - v(t)}{\Delta t}$$

$$\Rightarrow \quad x(t+\Delta t) = x(t) + v(t)\Delta t$$

$$v(t+\Delta t) = v(t) + a(t)\Delta t$$

Notation:

$$x_k = x(t_0 + k\Delta t)$$

$$v_k = v(t_0 + k\Delta t)$$

$$\Rightarrow \quad x_{k+1} = x_k + v_k \Delta t$$

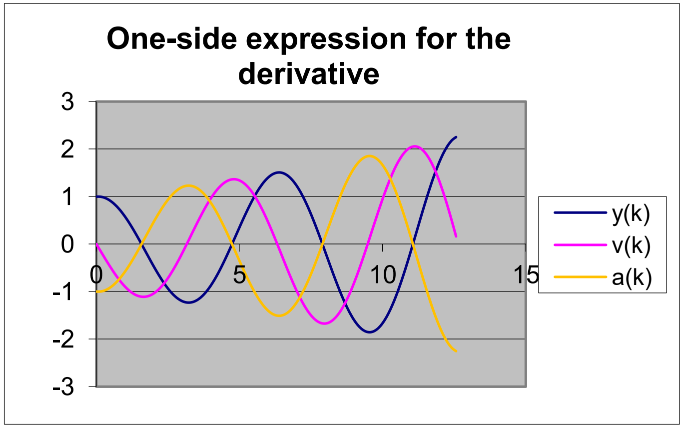
$$v_{k+1} = v_k + a_k \Delta t$$

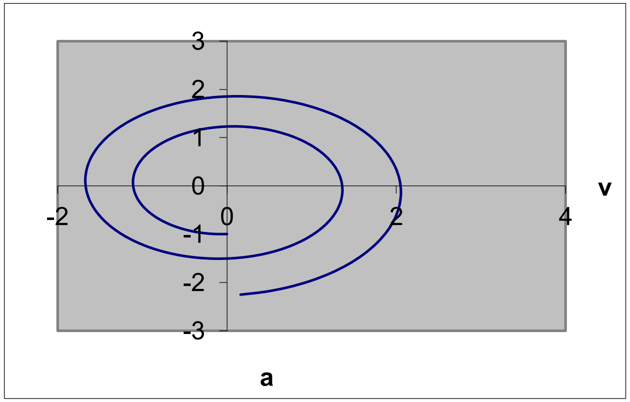
From the equation it results: $a_k = -x_k$

Numerical solution I cont.

For t=0 : $x_0 = 1[m]$ $v_0 = 0\left[\frac{m}{s}\right]$ $\Delta t = \frac{\pi}{24}$

k	t(k)	x(k)	v(k)	a(k)
0	0	1	0	-1
1	0.1308997	1	-0.1309	-1
2	0.2617994	0.9828653	-0.261799	-0.982865
3	0.3926991	0.9485958	-0.390456	-0.948596
4	0.5235988	0.8974852	-0.514627	-0.897485
5	0.6544985	0.8301207	-0.632108	-0.830121
6	0.7853982	0.747378	-0.74077	-0.747378
7	0.9162979	0.6504114	-0.838602	-0.650411
8	1.0471976	0.5406387	-0.92374	-0.540639
9	1.1780972	0.4197214	-0.99451	-0.419721
10	1.3089969	0.2895404	-1.049451	-0.28954
11	1.4398966	0.1521675	-1.087352	-0.152168
12	1.5707963	0.0098335	-1.107271	-0.009833
13	1.701696	-0.135108	-1.108558	0.1351079
14	1.8325957	-0.280218	-1.090872	0.2802178
15	1.9634954	-0.423013	-1.054192	0.4230126
16	2.0943951	-0.561006	-0.99882	0.561006
17	2.2252948	-0.691751	-0.925384	0.6917512
18	2.3561945	-0.812884	-0.834834	0.8128837
19	2.4870942	-0.922163	-0.728428	0.9221632
20	2.6179939	-1.017514	-0.607717	1.0175142
21	2.7488936	-1.097064	-0.474525	1.0970641
22	2.8797933	-1.159179	-0.330919	1.1591793
23	3.010693	-1.202497	-0.179183	1.2024965
24	3.1415927	-1.225952	-0.021777	1.2259515





Numerical solution II

$$a(t) = -x(t) \qquad where: \quad a(t) = \frac{dv}{dt} = \frac{d^2x}{dt^2} \qquad v(t) = \frac{dx}{dt}$$

Approximate expressions for the central-derivatives:

$$v\left(t + \tfrac{1}{2}\Delta t\right) = \frac{x(t+\Delta t) - x(t)}{\Delta t}$$

$$a(t+\Delta t) = \frac{v\left(t+\tfrac{3}{2}\Delta t\right) - v\left(t + \tfrac{1}{2}\Delta t\right)}{\Delta t}$$

$$\Rightarrow$$

$$x(t+\Delta t) = x(t) + v\left(t+\tfrac{1}{2}\Delta t\right)\Delta t$$

$$v\left(t+\tfrac{3}{2}\Delta t\right) = v\left(t+\tfrac{1}{2}\Delta t\right) + a(t+\Delta t)\Delta t$$

Notation:

$$x_k = x(t_0 + k\Delta t)$$

$$v_k = v(t_0 + k\Delta t)$$

$$\Rightarrow$$

$$x_{k+1} = x_k + v_{k+\frac{1}{2}}\Delta t$$

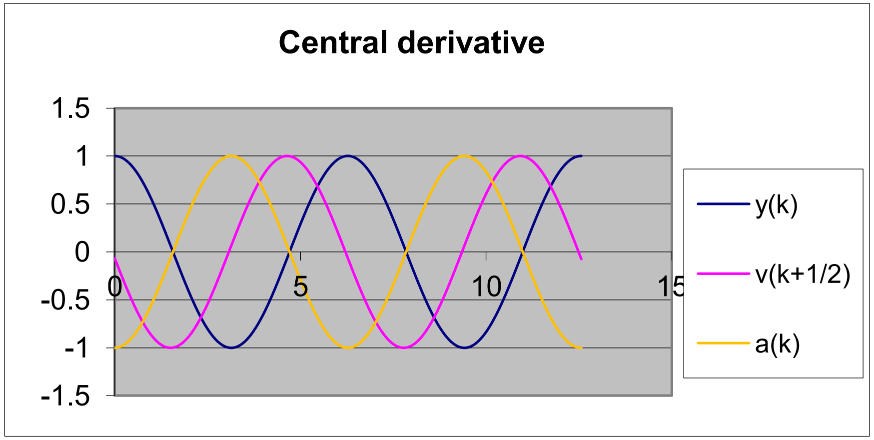
$$v_{k+\frac{3}{2}} = v_{k+\frac{1}{2}} + a_{k+1}\Delta t$$

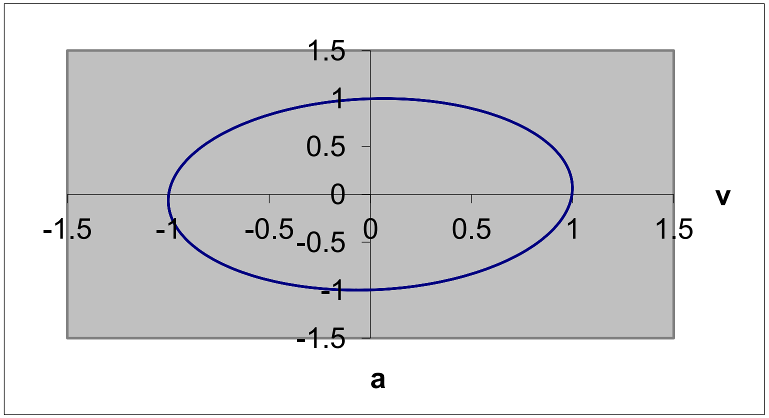
From the equation it results: $a_{k+1} = -x_{k+1}$

Numerical solution II cont.

For t=0 : $x_0 = 1[m]$ $v_0 = 0\left[{m}/{s}\right]$ $v_{\frac{1}{2}} = v_0 + a_0 {\Delta t}/{2}$ $\Delta t = \frac{\pi}{24}$

k	t(k)	x(k)	v(k+1/2)	a(k)
0	0	1	-0.06545	-1
1	0.1308997	0.9914326	-0.195228	-0.991433
2	0.2617994	0.9658773	-0.321661	-0.965877
3	0.3926991	0.923772	-0.442583	-0.923772
4	0.5235988	0.8658381	-0.555921	-0.865838
5	0.6544985	0.7930682	-0.659733	-0.793068
6	0.7853982	0.7067094	-0.752241	-0.706709
7	0.9162979	0.6082413	-0.83186	-0.608241
8	1.0471976	0.4993511	-0.897224	-0.499351
9	1.1780972	0.3819047	-0.947216	-0.381905
10	1.3089969	0.2579145	-0.980977	-0.257914
11	1.4398966	0.1295049	-0.997929	-0.129505
12	1.5707963	-0.001124	-0.997782	0.0011236
13	1.701696	-0.131733	-0.980538	0.131733
14	1.8325957	-0.260085	-0.946493	0.2600851
15	1.9634954	-0.383981	-0.89623	0.3839807
16	2.0943951	-0.501297	-0.83061	0.5012969
17	2.2252948	-0.610024	-0.750758	0.6100235
18	2.3561945	-0.708298	-0.658042	0.7082976
19	2.4870942	-0.794435	-0.554051	0.7944351
20	2.6179939	-0.86696	-0.440566	0.8669602
21	2.7488936	-0.92463	-0.319532	0.9246302
22	2.8797933	-0.966457	-0.193024	0.9664569
23	3.010693	-0.991724	-0.063207	0.9917237
24	3.1415927	-0.999997	0.0676921	0.9999975





Richardson’s extrapolation

When calculating the numerical result with a finite step h, is it possible to estimate the result at the limit h $\rightarrow$ 0 ?

$$F(h) = a_0 + a_1 h^p + O(h^r) \qquad\qquad r > p$$

F(h) – the result for the step *h*
$a_0 = F(0)$ hypotetical result for h=0
p – the order of the numerical error

Let’s calculate the numerical result *F* for two different step lengths *h* i (*qh*)

$$\begin{cases} F(h) = a_0 + a_1 h^p + O(h^r) \\ F(qh) = a_0 + a_1 (qh)^p + O(h^r) \end{cases} \qquad\qquad q > 1$$

$$\begin{cases} F(h) = a_0 + a_1 h^p & /{*}\, q^p \\ F(qh) = a_0 + a_1 q^p h^p \end{cases}$$

Richardson's extrapolation cont.

$$\begin{cases} q^p F(h) = q^p a_0 + a_1 q^p h^p \\ F(qh) = a_0 + a_1 q^p h^p \end{cases}$$

Substruction of both equations

$$q^p F(h) - F(qh) = a_0 (q^p - 1)$$

$$a_0 = F(h) + \frac{F(h) - F(qh)}{q^p - 1} + O(h^t) \qquad t > r$$

a_0 has an error of higher order and the process can be continued.

The most frequent step change q=2, and then:

$$a_0 = F(h) + \frac{F(h) - F(2h)}{2^p - 1} + O(h^t) \qquad t > r$$

Richardson's extrapolation example 1

$$I = \int_{10}^{12} x^3 dx = 2684$$

Numerical results with the trapezoid method:

h	T(h)
2	2728
1	2695

$$a_0 = T(1) + \frac{T(1) - T(2)}{2^2 - 1} = 2695 + \frac{2695 - 2728}{3} = 2695 - 11 = 2684$$

Richardson’s extrapolation example 2

f(x)=ln(x) f'(x)=[f(x+h)-f(x-h)]/(2*h)

ln'(3)=1/3

h			F(h)	$\Delta/3$	a_0
0.8	3.8	1.335001	0.341590		
	2.2	0.788457			
0.4	3.4	1.223775	0.335330	-0.002087	0.333243
	2.6	0.955511			
0.2	3.2	1.163151	0.333828	-0.000501	0.333328
	2.8	1.029619			
0.1	3.1	1.131402	0.333457	-0.000124	0.333333
	2.9	1.064711			

The central derivative method error~ h^2, thus p=2.

Δ = F(h)-F(2h)

The interpolation polynomial

The function f(x) is given as a table, i.e. its values are known in (n+1) points (nodes)

$$f(x_0),\ f(x_1),\ f(x_2),\ ...,\ f(x_n).$$

Problem: find a polynomial of the n-th order such as:

$$w(x_0)= f(x_0)$$
$$w(x_1)= f(x_1)$$
$$...$$
$$w(x_n)= f(x_n)$$

$w_n(x)$ is called the interpolation polynomial.

Goals of the interpolation:

- simple presentation of the function values (coefficients)
- execution of mathematical operations using the polynomial
- determination of the intermediate values of the function

Calculation of the polynomial value

Natural form of the polynomial

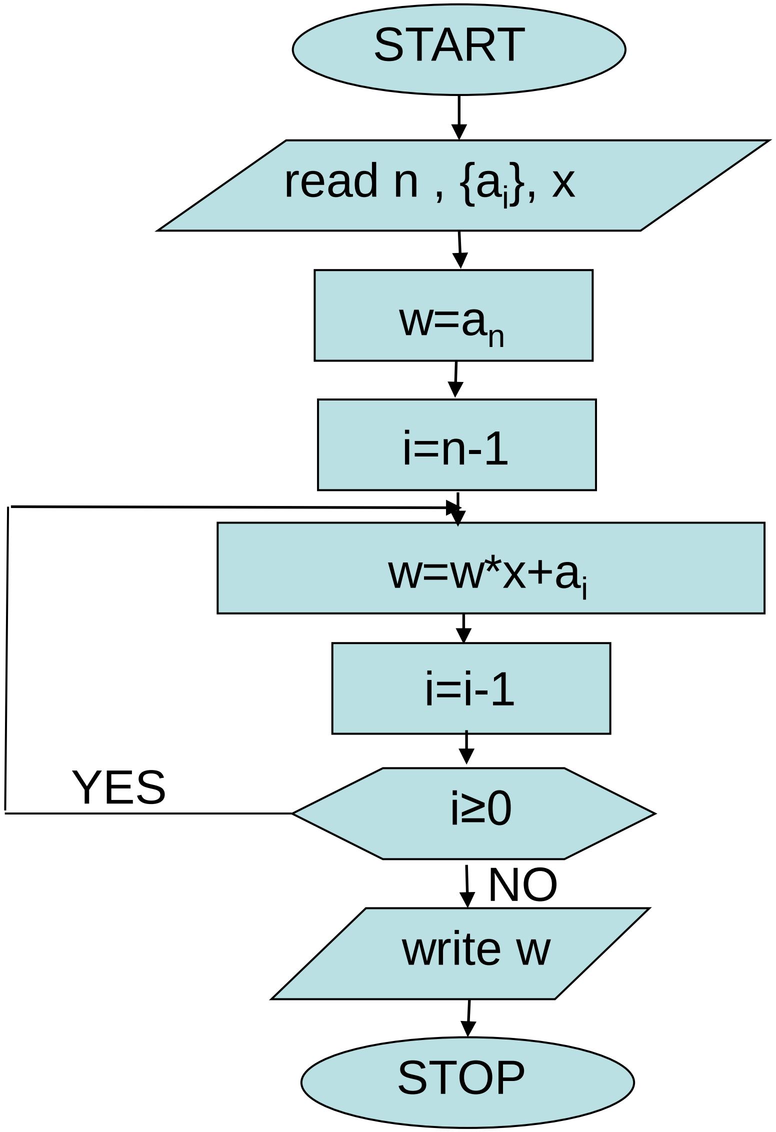
$$w_n(x) = \sum_{k=0}^{n} a_k x^k = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

The Horner's scheme of the calculation

$$w_n(x) = (\ldots(a_n x + a_{n-1})x + \ldots + a_1)x + a_0$$

Calculation of the polynomial value

Algorithm



Trace of the calculation

$w_3(x)=1+3x-2x^2+4x^3$

$n=3$ $a_0=1$ $a_1=3$ $a_2=-2$ $a_3=4$

Calculate the value of the polynomial at x=3.

n	**w**	**i**
3	4	2
	4*3-2=10	1
	10*3+3=33	0
	33*3+1=100	-1

The value at x=3 is 100.

Newton form of the polynomial

Let x_0, x_1, x_2,..., x_{n-1} are given numbers, where the values of a polynomial are given (the data).

Auxiliary polonomial p_k (k=0,1,2,...,n) are defined

$p_0(x) = 1$

$p_1(x) = x-x_0$

$p_2(x) = (x-x_0)(x-x_1)$

...

$p_k(x)= (x-x_0)(x-x_1)... (x-x_{k-1})$

The polynomial $w_n(x)$ is given as

$$w_n(x) = \sum_{k=0}^{n} b_k p_k(x)$$

How to determine the coefficients b_k?

Determination of the coefficients b_k

x	f(x)	$f[x_l,x_{l+1}]$	$f[x_l,x_{l+1},x_{l+2}]$
x_0	$f(x_0)$		
x_1	$f(x_1)$	$f[x_0,x_1]=\dfrac{f(x_1)-f(x_0)}{x_1-x_0}$	
x_2	$f(x_2)$	$f[x_1,x_2]=\dfrac{f(x_2)-f(x_1)}{x_2-x_1}$	$f[x_0,x_1,x_2]=\dfrac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$
…			
x_n	$f(x_n)$	$f[x_{n-1},x_n]=\dfrac{f(x_n)-f(x_{n-1})}{x_n-x_{n-1}}$	$f[x_{n-2},x_{n-1},x_n]=\dfrac{f[x_{n-1},x_n]-f[x_{n-2},x_{n-1}]}{x_n-x_{n-2}}$

$$b_k = f[x_0, x_1, \ldots, x_k]$$

Example

x	f(x)	f[x_0,x_1]	f[x_0,..,x_2]	f[x_0,...,x_3]
3	100			
5	466	183		
7	1296	415	58	
9	2782	743	82	4

$b_0 = 100$
$b_1 = 183$
$b_2 = 58$
$b_3 = 4$

$$p_0(x) = 1$$

$$p_1(x) = x - 3$$

$$p_2(x) = (x-3)(x-5)$$

$$p_3(x) = (x-3)(x-5)(x-7)$$

$$w_3(x) = b_0 + (x - x_0)(b_1 + (x - x_1)(b_2 + (x - x_3)b_3))$$

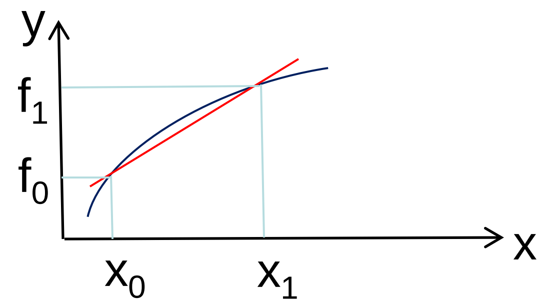
$$w_3(x) = 100 + (x-3)*(183 + (x-5)*(58 + (x-7)*4))$$

$$= 1 + x*(3 + x*(-2 + x*4)) =$$

$$= 1 + 3x - 2x^2 + 4x^3$$

Linear interpolation

linear function: $w_1(x)=a_0+a_1x$



$f(x_0) = f_0 = a_0+a_1x_0 \ \ (/\ x_1)$
$f(x_1) = f_1 = a_0+a_1x_1 \ \ (/\ x_0)$

Calculate a_0, a_1

$f_1 - f_0 = a_1x_1 - a_1x_0$ $\qquad a_1=(f_1-f_0)/(x_1-x_0)$
$f_0x_1-f_1x_0 = a_0x_1 - a_0x_0$ $\qquad a_0=(f_0x_1 - f_1x_0)/(x_1-x_0)$

$w_1(x)= [(f_0x_1 - f_1x_0)/(x_1-x_0)] + [(f_1-f_0)/(x_1-x_0)]\ x$
$w_1(x)= [(f_0x_1 - f_0x_0 + f_0x_0 - f_1x_0)/(x_1-x_0)] + [(f_1-f_0)/(x_1-x_0)]\ x$

$\boldsymbol{w_1(x)=f_0 + [(f_1-f_0)/(x_1-x_0)]\ (x-x_0)}$

It is a Newton polynomial

$w_1(x) = b_0\,p_0(x) + b_1\,p_1(x)$, where

$p_0(x) = 1$ $\qquad b_0 = f_0$
$p_1(x) = x-x_0$ $\qquad b_1 = (f_1-f_0)/(x_1-x_0)$

The Runge effect

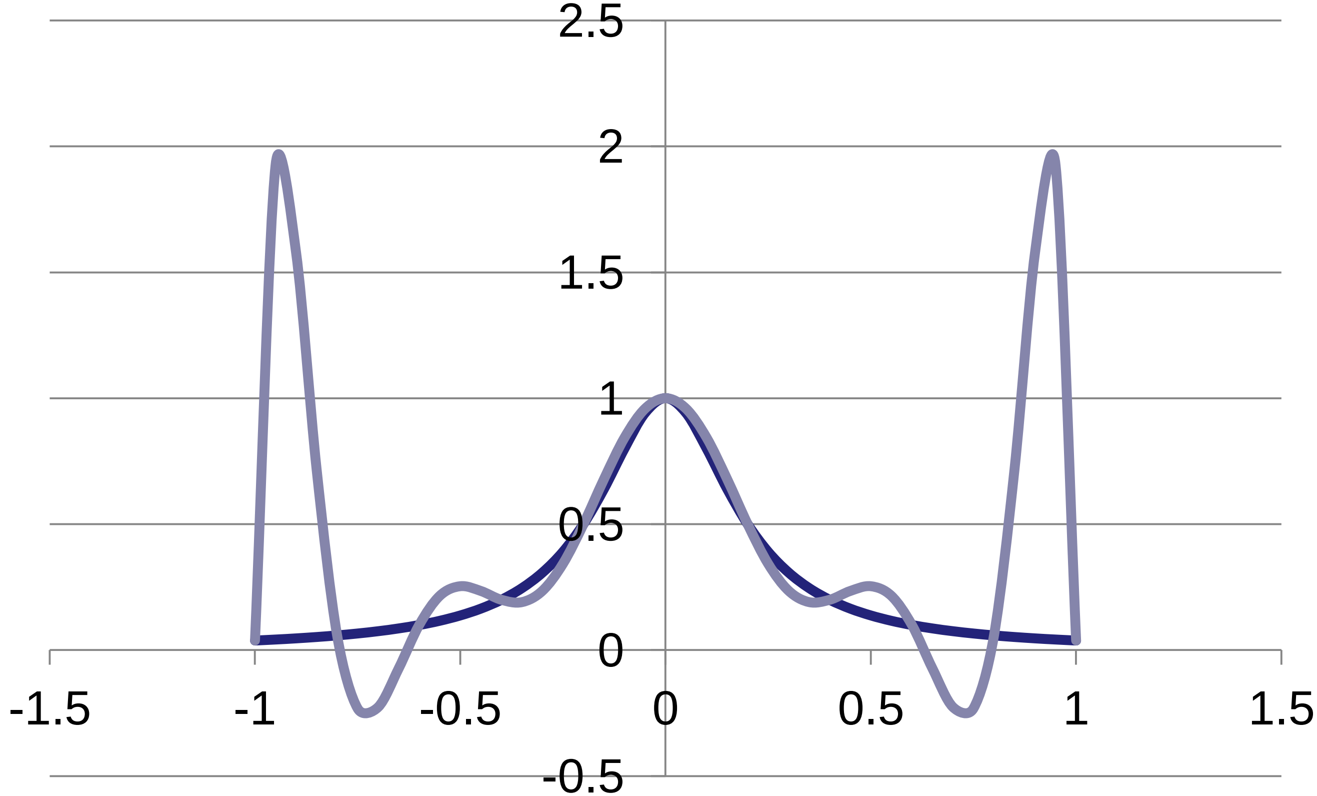
When interpolating with a polynomial of high order, eg. of the 10-th order for the function $f(x) = \frac{1}{1+25x^2}$ in the range[-1,1] for eqidistant nodes

$x_i = -1 + i * 0,2$ $\quad$ $i = 0,1,2,...,10$

x	f(x)											w(x)
-1	**0.038462**											0.038462
-0.8	0.058824	**0.10181**										0.058824
-0.6	0.1	0.205882	**0.260181**									0.1
-0.4	0.2	0.5	0.735294	**0.791855**								0.2
-0.2	0.5	1.5	2.5	2.941176	**2.686652**							0.5
0	1	2.5	2.5	1.48E-15	-3.67647	**-6.36312**						1
0.2	0.5	-2.5	-12.5	-25	-31.25	-27.5735	**-17.6753**					0.5
0.4	0.2	-1.5	2.5	25	62.5	93.75	101.1029	**84.84163**				0.2
0.6	0.1	-0.5	2.5	-1.5E-15	-31.25	-93.75	-156.25	-183.824	**-167.916**			0.1
0.8	0.058824	-0.20588	0.735294	-2.94118	-3.67647	27.57353	101.1029	183.8235	229.7794	**220.9417**		0.058824
1	0.038462	-0.10181	0.260181	-0.79186	2.686652	6.363122	-17.6753	-84.8416	-167.916	-220.942	**-220.942**	0.038462

The Runge effect

Compare the expressions for the function (dark line)and polynomial (grey line):



Calculation accuracy

Error sources:

- Errors of input data
- Rounding errors
- Cutting errors
- Simplification of a model
- Random errors

Absolute and relative erros:

$\tilde{x}$ – Approximate value

x – Exact value

Absolute error $\Delta x = \tilde{x} - x$

Relative error $r = \dfrac{\tilde{x} - x}{x} = \dfrac{\Delta x}{x}$

Rounding and cutting

		rounding		cutting
0,2397	$\rightarrow$	0,240	$\rightarrow$	0,239
-0,2397	$\rightarrow$	-0,240	$\rightarrow$	-0,239

Rounding to t decimal digits
Error of the number $\pm \frac{1}{2} \cdot 10^{-t}$

Example: $0{,}240 \pm \frac{1}{2} \cdot 10^{-3} = 0{,}240 \pm 0{,}0005$

Rounding of numbers ending with a digit 5?
0,2345 $\rightarrow$ 0,234
0,2435 $\rightarrow$ 0,244
Error reduction when calculating a sum

Errors of calculated quantities

Addition and Subtraction

$$\tilde{x}_1 = 2{,}33 \pm 0{,}02$$

What is the error of a sum?

$$\tilde{x}_2 = 1{,}42 \pm 0{,}03$$

$$\max\left(\tilde{x}_1 + \tilde{x}_2\right) = 2{,}33 + 0{,}02 + 1{,}42 + 0{,}03 = 3{,}80$$

$$\min\left(\tilde{x}_1 + \tilde{x}_2\right) = 2{,}33 - 0{,}02 + 1{,}42 - 0{,}03 = 3{,}70$$

$$\tilde{x}_1 + \tilde{x}_2 = 3{,}75 \pm 0{,}05$$

What is the error of a difference?

$$\max\left(\tilde{x}_1 - \tilde{x}_2\right) = 2{,}33 + 0{,}02 - 1{,}42 + 0{,}03 = 0{,}94$$

$$\min\left(\tilde{x}_1 - \tilde{x}_2\right) = 2{,}33 - 0{,}02 - 1{,}42 - 0{,}03 = 0{,}84$$

$$\tilde{x}_1 - \tilde{x}_2 = 0{,}89 \pm 0{,}05$$

Errors of calculated quantities

Addition and Subtraction

$$\tilde{x}_1 = x_1 \pm \Delta x_1 \qquad \tilde{x}_2 = x_2 \pm \Delta x_2$$

$$x_1 - \Delta x_1 - \left(x_2 + \Delta x_2\right) \leq \tilde{x}_1 - \tilde{x}_2 \leq x_1 + \Delta x_1 - \left(x_2 - \Delta x_2\right)$$

$$x_1 - x_2 - \left(\Delta x_1 + \Delta x_2\right) \leq \tilde{x}_1 - \tilde{x}_2 \leq x_1 - x_2 + \left(\Delta x_1 + \Delta x_2\right)$$

$$\tilde{x}_1 - \tilde{x}_2 = x_1 - x_2 \pm \left(\Delta x_1 + \Delta x_2\right)$$

$$\Delta\left(\tilde{x}_1 - \tilde{x}_2\right) = \left|\Delta x_1 + \Delta x_2\right|$$

Similarly:

$$\tilde{x}_1 + \tilde{x}_2 = x_1 + x_2 \pm \left(\Delta x_1 + \Delta x_2\right)$$

$$\Delta\left(\tilde{x}_1 + \tilde{x}_2\right) = \left|\Delta x_1 + \Delta x_2\right|$$

The absolute error of a sum or difference is equal to the sum of absolute errors of components.

Reduction of significant digits

$$\tilde{x}_1 = 0{,}5764 \pm \tfrac{1}{2}10^{-4}$$

$$\tilde{x}_2 = 0{,}5763 \pm \tfrac{1}{2}10^{-4}$$

$$\tilde{x}_1 - \tilde{x}_2 = 0{,}5764 - 0{,}5763 \pm \left(\tfrac{1}{2}10^{-4} + \tfrac{1}{2}10^{-4}\right)$$

$$\tilde{x}_1 - \tilde{x}_2 = 0{,}0001 \pm 0{,}0001$$

$$\Delta\left(\tilde{x}_1 - \tilde{x}_2\right) = 0{,}0001$$

Absolute error

$$r = \frac{0{,}0001}{0{,}0001} = 1 = 100\%$$

Relative error

Errors of calculated quantities

Multiplication and division

$$\tilde{x}_1 = x_1 \pm \Delta x_1 = x_1\left(1 \pm r_1\right) \qquad \tilde{x}_2 = x_2 \pm \Delta x_2 = x_2\left(1 \pm r_2\right)$$

$$\tilde{x}_1 * \tilde{x}_2 = x_1\left(1 \pm r_1\right) * x_2\left(1 \pm r_2\right) = x_1 x_2\left(1 \pm r_1\right)\left(1 \pm r_2\right) =$$

$$= x_1 x_2\left(1 \pm r_1 \pm r_2 \pm r_1 r_2\right) \approx x_1 x_2\left(1 \pm r_1 \pm r_2\right)$$

$$\tilde{x}_1 * \tilde{x}_2 = x_1 x_2\left[1 \pm \left(r_1 + r_2\right)\right]$$

Similarly: $$\frac{\tilde{x}_1}{\tilde{x}_2} = \tilde{x}_1 \frac{1}{\tilde{x}_2} = x_1\left(1 \pm r_1\right)\frac{1}{x_2}\left(1 \pm r_2\right)$$

$$\frac{\tilde{x}_1}{\tilde{x}_2} = \frac{x_1}{x_2}\left[1 \pm \left(r_1 + r_2\right)\right]$$

The relative error of a product or division is equal to the sum of relative errors of the factors.

Use of different rules for the error transfer

Calculate the roots of the algebraic quadratic equation with the accuracy of 5 significant digits.

$$\tfrac{1}{2}x^2 - 28x + \tfrac{1}{2} = 0$$

$$\sqrt{\Delta} = \sqrt{28^2 - 4 * \tfrac{1}{2} * \tfrac{1}{2}} = \sqrt{784 - 1} = \sqrt{783} = 27{,}982$$

$$x_1 = 28 - 27{,}982 = 0{,}018 \pm \tfrac{1}{2}10^{-3}$$

Only 2 significant digits

$$x_2 = 28 + 27{,}982 = 55{,}982 \pm \tfrac{1}{2}10^{-3}$$

5 significant digits

$$r_1 = \frac{0{,}0005}{0{,}018} = 3 * 10^{-2}$$

$$r_2 = \frac{0{,}0005}{55{,}982} = 9 * 10^{-6}$$

Use of different rules for the error transfer

The Viete's relations

$$ax^2 + bx + c = 0$$

$$x_1 * x_2 = \frac{c}{a}$$

$$\tfrac{1}{2}x^2 - 28x + \tfrac{1}{2} = 0$$

$$\sqrt{\Delta} = \sqrt{28^2 - 4 * \tfrac{1}{2} * \tfrac{1}{2}} = \sqrt{784 - 1} = \sqrt{783} = 27{,}982$$

$$x_2 = 28 + 27{,}982 = 55{,}982 \pm \tfrac{1}{2}10^{-3}$$

$$x_1 x_2 = 1 \qquad x_1 = \frac{1}{x_2} = \frac{1}{55{,}982} = 0{,}017863 \pm \tfrac{1}{2} * 10^{-6}$$

$$r_1 = \frac{0{,}0000005}{0{,}017863} = 3 * 10^{-5}$$

$$r_2 = \frac{0{,}0005}{55{,}982} = 9 * 10^{-6}$$

Maximal errors of calculated quantities

$$y = y(x_1, x_2, ..., x_n)$$

The function is given

All variables xi are given with errors. What is the error of a calculated quantity y?

$$\tilde{y} = y(\tilde{x}_1, \tilde{x}_2, ..., \tilde{x}_n)$$

$$\tilde{x}_1 = x_1 \pm \Delta x_1 \qquad \tilde{x}_2 = x_2 \pm \Delta x_2 \quad ... \quad \tilde{x}_n = x_n \pm \Delta x_n$$

$$\Delta y = \sum_{i=1}^{n} \left| \left(\frac{\partial y}{\partial x_i} \right)_{\tilde{x}} * \Delta x_i \right|$$

$$\Delta y = \left| \left(\frac{\partial y}{\partial x_1} \right)_{\tilde{x}} * \Delta x_1 \right| + \left| \left(\frac{\partial y}{\partial x_2} \right)_{\tilde{x}} * \Delta x_2 \right| + ... + \left| \left(\frac{\partial y}{\partial x_n} \right)_{\tilde{x}} * \Delta x_n \right|$$

$$r_y = \frac{\Delta y}{y}$$

Maximal error – an example

$$a = 320 \pm 2 \qquad \Delta a = 2$$

$$b = -300 \pm 1 \qquad \Delta b = 1$$

$$c = 10{,}0 \pm 0{,}1 \qquad \Delta c = 0{,}1$$

$$y = \frac{a+b}{c} = \frac{320-300}{10} = 2$$

$$\Delta y = \left|\left(\frac{\partial y}{\partial a}\right) * \Delta a\right| + \left|\left(\frac{\partial y}{\partial b}\right) * \Delta b\right| + \left|\left(\frac{\partial y}{\partial c}\right) * \Delta c\right| =$$

$$= \left|\left(\frac{1}{c}\right) * \Delta a\right| + \left|\left(\frac{1}{c}\right) * \Delta b\right| + \left|\left(\frac{a+b}{c^2}\right) * \Delta c\right| =$$

$$= \left|\frac{1}{10} * 2\right| + \left|\frac{1}{10} * 1\right| + \left|\frac{-20}{10^2} * 0{,}1\right| = 0{,}32$$

$$r_y = \frac{0{,}32}{2} = 0{,}16 = 16\%$$

Standard errors of complex expressions

$$y = y\left(x_1, x_2, \ldots, x_n\right)$$

A given function

The s_i are standard errors of parameters x_i. What is the standard error of a complex value y?

$$\tilde{y} = y\left(\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n\right)$$

$$\tilde{x}_1 = \left\{x_1, s_1\right\} \qquad \tilde{x}_2 = \left\{x_2, s_2\right\} \quad \ldots \qquad \tilde{x}_n = \left\{x_n, s_n\right\}$$

$$s_y = \sqrt{\sum_{i=1}^{n} \left| \left(\frac{\partial y}{\partial x_i}\right)_{\tilde{x}}^2 * s_i^2 \right|}$$

$$s_y = \sqrt{\left| \left(\frac{\partial y}{\partial x_1}\right)_{x}^2 * s_1^2 \right| + \left| \left(\frac{\partial y}{\partial x_2}\right)_{\tilde{x}}^2 * s_2^2 \right| + \ldots + \left| \left(\frac{\partial y}{\partial x_n}\right)_{\tilde{x}}^2 * s_n^2 \right|}$$

Example

$$a = 320 \pm 2 \qquad s_a = 2$$

$$b = -300 \pm 1 \qquad s_b = 1$$

$$c = 10{,}0 \pm 0{,}1 \qquad s_c = 0{,}1$$

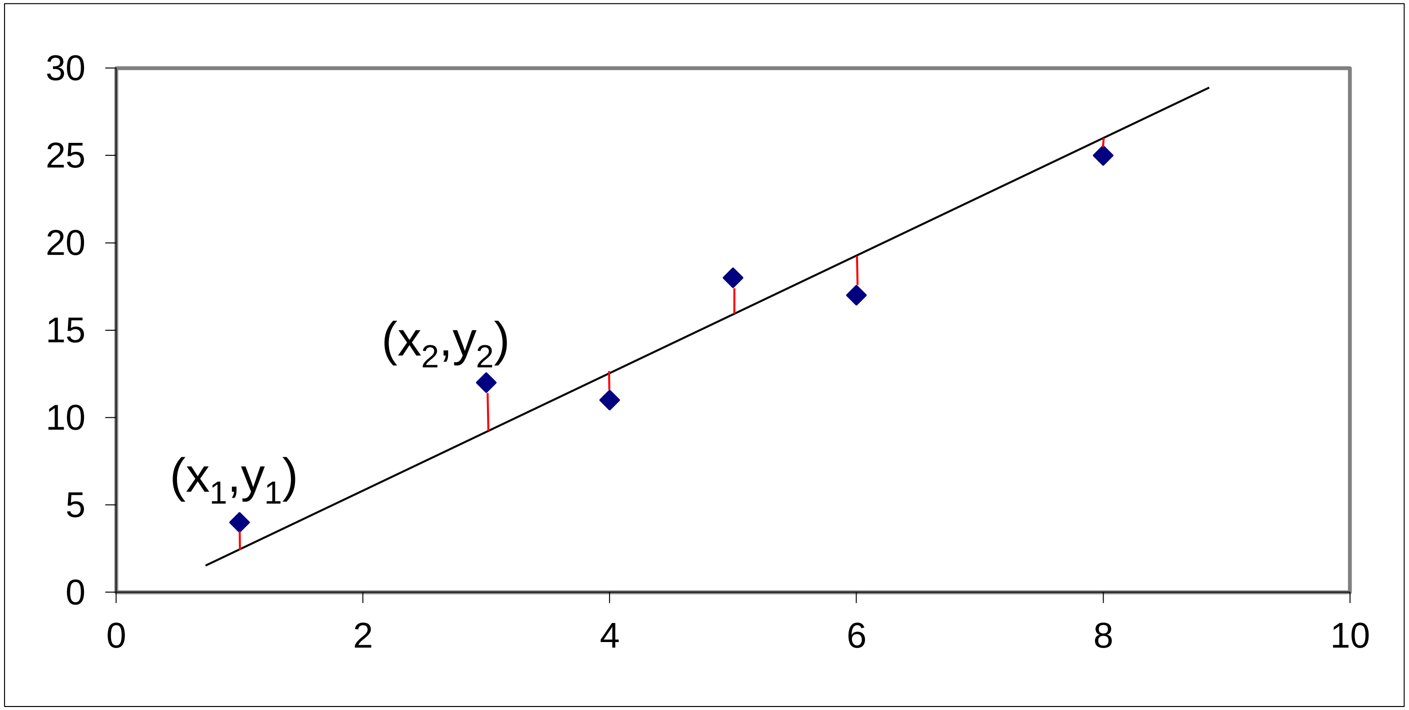
$$y = \frac{a+b}{c} = \frac{320-300}{10} = 2$$

$$s_y = \sqrt{\left|\left(\frac{\partial y}{\partial a}\right)^2 * s_a^2\right| + \left|\left(\frac{\partial y}{\partial b}\right)^2 * s_b^2\right| + \left|\left(\frac{\partial y}{\partial c}\right)^2 * s_c^2\right|} =$$

$$= \sqrt{\left|\left(\frac{1}{c}\right)^2 * s_a^2\right| + \left|\left(\frac{1}{c}\right)^2 * s_b^2\right| + \left|\left(\frac{a+b}{c^2}\right)^2 * s_c^2\right|} =$$

$$= \sqrt{\left|\left(\frac{1}{10}\right)^2 * 2^2\right| + \left|\left(\frac{1}{10}\right)^2 * 1^2\right| + \left|\left(\frac{-20}{10^2}\right)^2 * 0{,}1^2\right|} = 0{,}22$$

Linear regression



Linear regression:

$$y=a*x+b$$

Goal: Determination of optimum values of a and b.

Linear regression

Basic assumptions:

1) Random distribution of y_i around the straight line

2) The variation σ_y^2 independent of x

Least squares method:

$$\Phi(a,b) = \sum_{i=1}^{n} \left[y_i - (a\,x_i + b) \right]^2$$

Determination of min Φ(a,b) with respect to a and b:

$$\frac{\partial \Phi(a,b)}{\partial a} = -2 \sum_{i=1}^{n} \left[y_i - (a\,x_i + b) \right](x_i) = 0$$

$$\frac{\partial \Phi(a,b)}{\partial b} = -2 \sum_{i=1}^{n} \left[y_i - (a\,x_i + b) \right] = 0$$

Linear regression

$$\begin{cases} \sum_{i=1}^{n} x_i y_i - a\sum_{i=1}^{n} x_i^2 - b\sum_{i=1}^{n} x_i = 0 \\ \sum_{i=1}^{n} y_i - a\sum_{i=1}^{n} x_i - bn = 0 \end{cases}$$

$$\begin{cases} a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} x_i y_i \\ a\sum_{i=1}^{n} x_i + bn = \sum_{i=1}^{n} y_i \end{cases}$$

Solution of the equations system with respect to a, b:

$$a = \frac{n\left(\sum_{i=1}^{n} x_i y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$b = \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

Linear regression

Estimation of variance for y_i:

$$s^2 = \frac{\sum_{i=1}^{n} \left(y_i - a\,x_i - b\right)^2}{n-2}$$

Estimation of variance for parameters a and b:

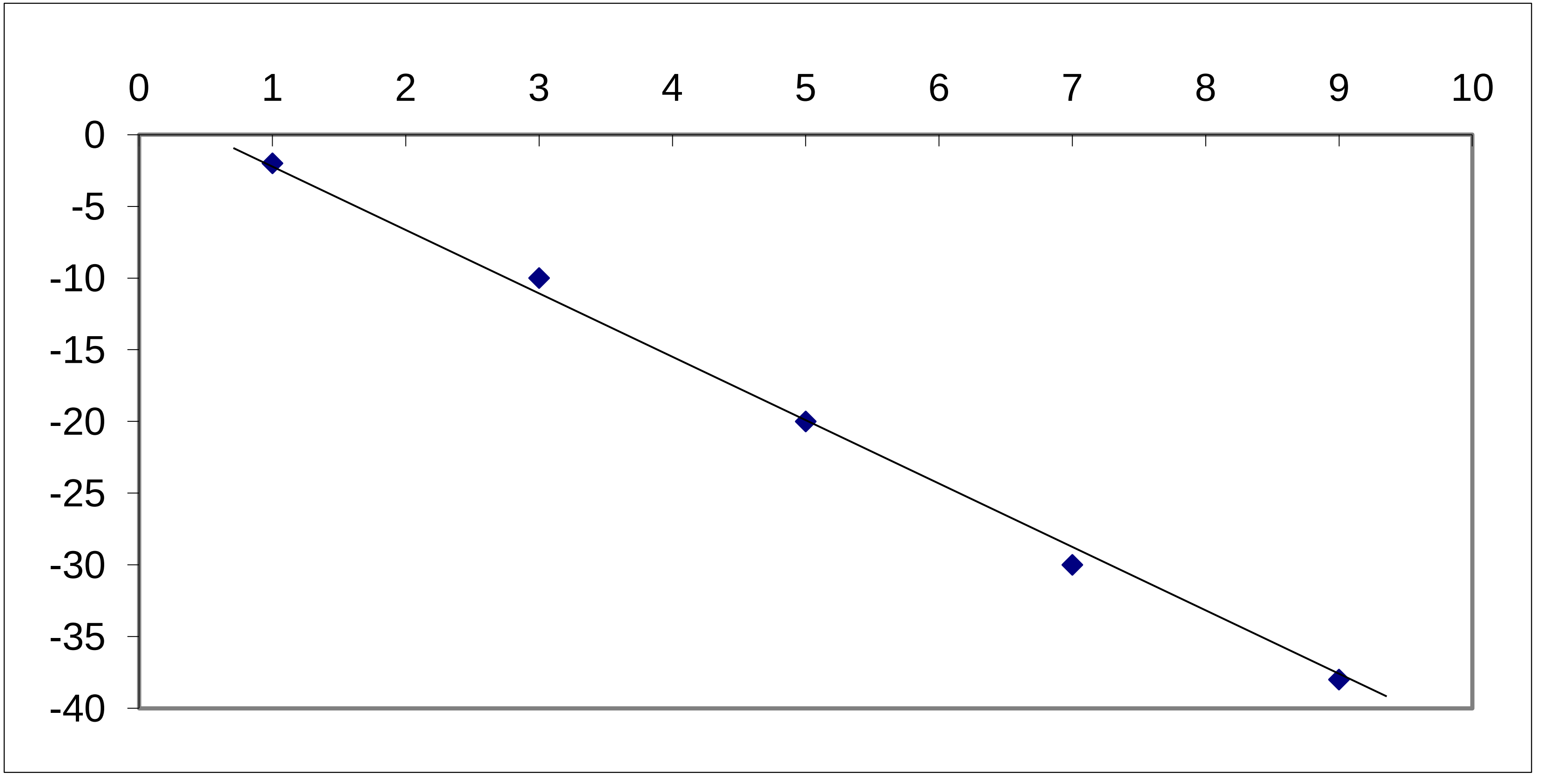
$$s_a^2 = s^2 \frac{n}{n\left(\sum x_i^2\right) - \left(\sum x_i\right)^2} \qquad s_b^2 = s^2 \frac{\left(\sum x_i^2\right)}{n\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}$$

Linear correlation coefficient r

$$r = \frac{cov\left(x_i, y_i\right)}{\sqrt{var\left(x_i\right) var\left(y_i\right)}} = \frac{S_{xy}}{\sqrt{S_{xx}\, S_{yy}}}$$

The value of r spans from -1 to +1. r>0 indicates a positive correlation, r<0 a negative correlation between x and y. r=0 indicates the lack of linear correlation between x and y.

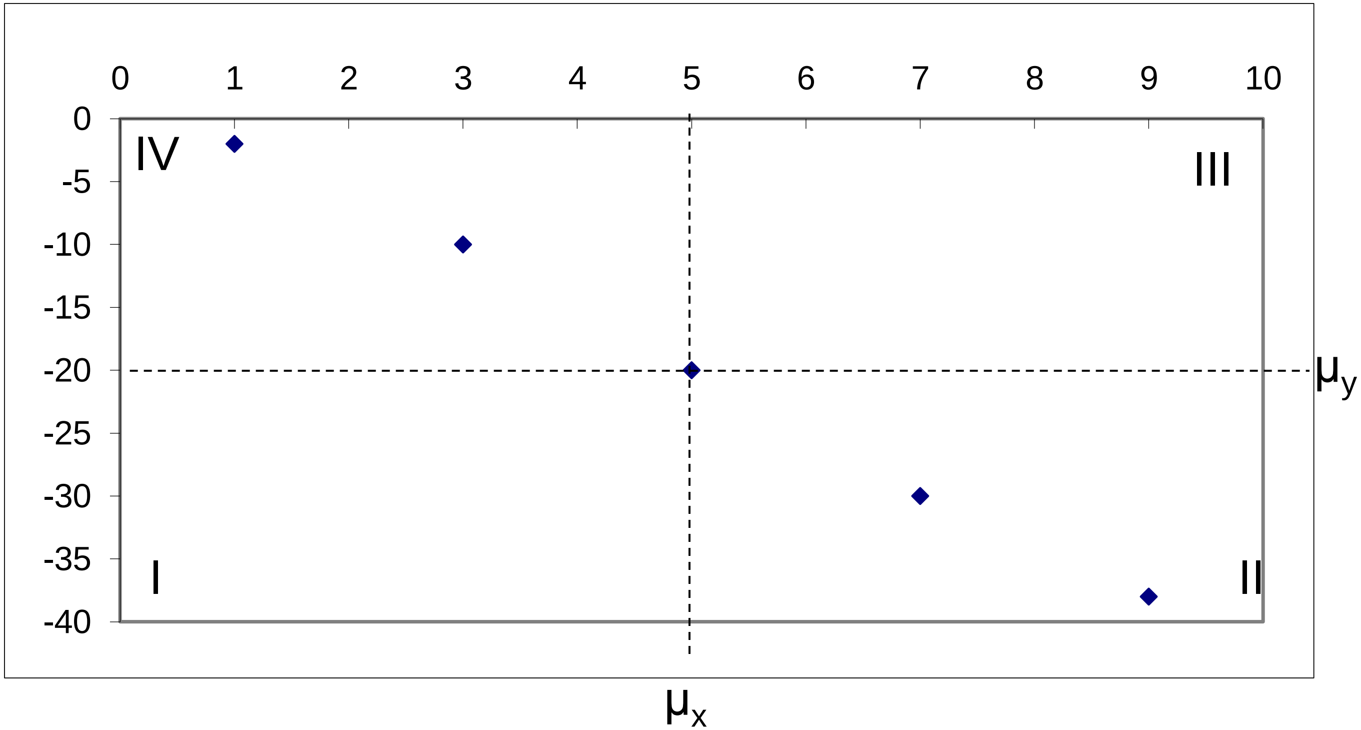
Linear regression – an example



	x [km]	y [kg]	x*x	x*y	y-a*x-b	(y-a*x-b)^2	x-xsr	y-ysr
	1	-2	1	-2	-0.4	0.16	-4	18
	3	-10	9	-30	0.8	0.64	-2	10
	5	-20	25	-100	0	0	0	0
	7	-30	49	-210	-0.8	0.64	2	-10
	9	-38	81	-342	0.4	0.16	4	-18
Sum:	**25**	**-100**	**165**	**-684**	**0.00**	**1.6**	**0**	**0**

a=	-4.6 kg/km				
b=	3 kg				
s^2=	0.5333	kg^2	s=	0.7303 kg	
sa^2=	0.0133		sa=	0.1155	kg/km
sb^2=	0.44		sb=	0.6633	kg
xsr=	5		cov(x,y)=	-36.8000	
ysr=	-20		var(x)=	8.0000	
			var(y)=	169.6000	
			r(x,y)=	-0.9991	

More about regression - quadrants



Quadrants:

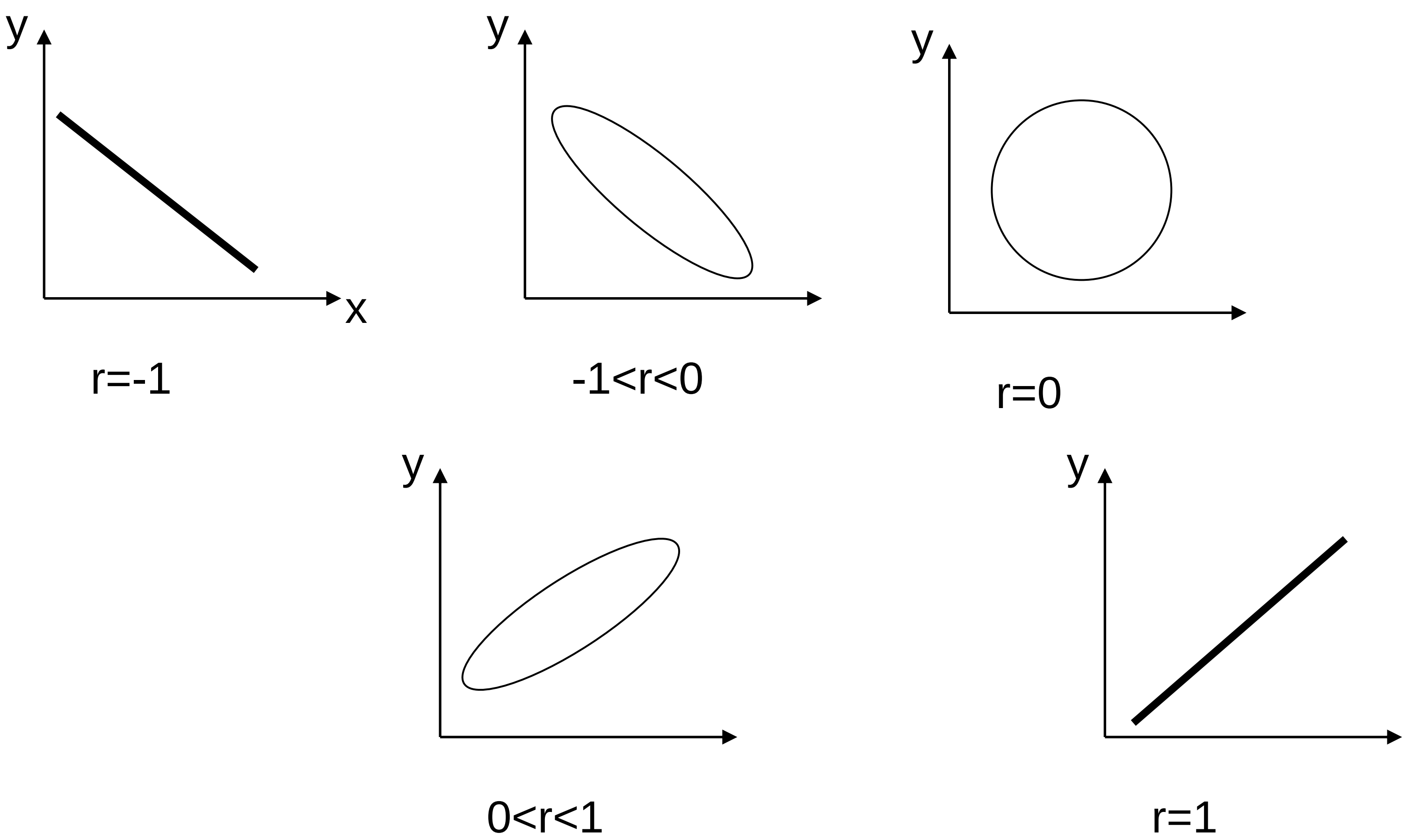
I	$x-\mu_x<0$	$y-\mu_y<0$	$(x-\mu_x)(y-\mu_y)>0$
II	$x-\mu_x>0$	$y-\mu_y<0$	$(x-\mu_x)(y-\mu_y)<0$
III	$x-\mu_x>0$	$y-\mu_y>0$	$(x-\mu_x)(y-\mu_y)>0$
IV	$x-\mu_x<0$	$y-\mu_y>0$	$(x-\mu_x)(y-\mu_y)<0$

$$cov(x,y) = \frac{\sum (x_i - \mu_x)(y_i - \mu_y)}{n}$$

$$-\infty < cov(x,y) < \infty$$

Linear regression coefficient

$$r = \frac{cov(x_i, y_i)}{\sqrt{var(x_i)var(y_i)}} = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}}$$



Excess system of linear equations

$$[\mathbf{y}-\mathbf{J}\mathbf{a}]=\boldsymbol{\varepsilon}$$

$$\sum_{i=1}^{n}\varepsilon_i^2=[\varepsilon_1 \quad \varepsilon_2 \quad \ldots \quad \varepsilon_n]\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \ldots\\ \varepsilon_n\end{bmatrix}=\boldsymbol{\varepsilon}^{\mathbf{T}}\boldsymbol{\varepsilon}=[\mathbf{y}-\mathbf{J}\mathbf{a}]^{\mathbf{T}}[\mathbf{y}-\mathbf{J}\mathbf{a}]$$

We search for a solution **a**, where the value of $\boldsymbol{\varepsilon}^{\mathbf{T}}\boldsymbol{\varepsilon}$ is minimal.

$$[\mathbf{y}-\mathbf{J}\mathbf{a}]^{\mathbf{T}}[\mathbf{y}-\mathbf{J}\mathbf{a}]=[\mathbf{y}^{\mathbf{T}}-\mathbf{a}^{\mathbf{T}}\mathbf{J}^{\mathbf{T}}][\mathbf{y}-\mathbf{J}\mathbf{a}]=$$

$$=\mathbf{y}^{\mathbf{T}}\mathbf{y}+\mathbf{a}^{\mathbf{T}}\mathbf{J}^{\mathbf{T}}\mathbf{J}\mathbf{a}-\mathbf{a}^{\mathbf{T}}\mathbf{J}^{\mathbf{T}}\mathbf{y}-\mathbf{y}^{\mathbf{T}}\mathbf{J}\mathbf{a}=\mathbf{y}^{\mathbf{T}}\mathbf{y}+\mathbf{a}^{\mathbf{T}}\mathbf{J}^{\mathbf{T}}\mathbf{J}\mathbf{a}-2\mathbf{a}^{\mathbf{T}}\mathbf{J}^{\mathbf{T}}\mathbf{y}$$

$$\frac{\partial\boldsymbol{\varepsilon}^{\mathbf{T}}\boldsymbol{\varepsilon}}{\partial\mathbf{a}}=2\mathbf{J}^{\mathbf{T}}\mathbf{J}\mathbf{a}-2\mathbf{J}^{\mathbf{T}}\mathbf{y}=\mathbf{0}$$

$$\mathbf{J}^{\mathbf{T}}\mathbf{J}\mathbf{a}=\mathbf{J}^{\mathbf{T}}\mathbf{y}$$

$$\boxed{\mathbf{a}=\left(\mathbf{J}^{\mathbf{T}}\mathbf{J}\right)^{-1}\mathbf{J}^{\mathbf{T}}\mathbf{y}}$$

The optinal values of parameters **a** which minimize the sum of squares

Example of the matrix representation

$$\mathbf{y} = \begin{bmatrix} 21 \\ 28 \\ 40 \\ 51 \end{bmatrix} \qquad \mathbf{J} = \begin{bmatrix} 2 & 1 \\ 4 & 1 \\ 6 & 1 \\ 8 & 1 \end{bmatrix} \qquad \mathbf{a} = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$\mathbf{J}^{\mathbf{T}}\mathbf{J} = \begin{bmatrix} 2 & 4 & 6 & 8 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 4 & 1 \\ 6 & 1 \\ 8 & 1 \end{bmatrix} = \begin{bmatrix} 120 & 20 \\ 20 & 4 \end{bmatrix} \qquad \det \mathbf{J}^{\mathbf{T}}\mathbf{J} = 120 * 4 - 20^2 = 80$$

$$\left(\mathbf{J}^{\mathbf{T}}\mathbf{J}\right)^{-\mathbf{1}} = \begin{bmatrix} \frac{4}{80} & -\frac{20}{80} \\ -\frac{20}{80} & \frac{120}{80} \end{bmatrix} \qquad \mathbf{J}^{\mathbf{T}}\mathbf{y} = \begin{bmatrix} 2 & 4 & 6 & 8 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 21 \\ 28 \\ 40 \\ 51 \end{bmatrix} = \begin{bmatrix} 802 \\ 140 \end{bmatrix}$$

$$\mathbf{a} = \begin{bmatrix} \frac{4}{80} & -\frac{20}{80} \\ -\frac{20}{80} & \frac{120}{80} \end{bmatrix} \begin{bmatrix} 802 \\ 140 \end{bmatrix} = \begin{bmatrix} 5{,}1 \\ 9{,}5 \end{bmatrix}$$

Variance

Variance of the variable y

$$s_y^2 = \frac{\boldsymbol{\varepsilon}^{\mathbf{T}}\boldsymbol{\varepsilon}}{n-2}$$

$$\boldsymbol{\varepsilon} = \mathbf{y} - \mathbf{Ja} = \begin{bmatrix} 21 \\ 28 \\ 40 \\ 51 \end{bmatrix} - \begin{bmatrix} 2 & 1 \\ 4 & 1 \\ 6 & 1 \\ 8 & 1 \end{bmatrix} \begin{bmatrix} 5{,}1 \\ 9{,}5 \end{bmatrix} = \begin{bmatrix} 1{,}3 \\ -1{,}9 \\ -0{,}1 \\ 0{,}7 \end{bmatrix}$$

$$s_y^2 = \frac{1}{4-2} \begin{bmatrix} 1{,}3 & -1{,}9 & -0{,}1 & 0{,}7 \end{bmatrix} \begin{bmatrix} 1{,}3 \\ -1{,}9 \\ -0{,}1 \\ 0{,}7 \end{bmatrix} = \frac{5{,}8}{2} = 2{,}9$$

Variances and covariance

$$\begin{bmatrix} s_a^2 & \operatorname{cov}(a,b) \\ \operatorname{cov}(a,b) & s_b^2 \end{bmatrix} = s_y^2 \left(\mathbf{J}^{\mathbf{T}}\mathbf{J}\right)^{-1} = 2{,}9 * \begin{bmatrix} \frac{4}{80} & -\frac{20}{80} \\ -\frac{20}{80} & \frac{120}{80} \end{bmatrix} = \begin{bmatrix} \frac{11{,}6}{80} & -\frac{58}{80} \\ -\frac{58}{80} & \frac{348}{80} \end{bmatrix}$$

Linear regression coefficient

$$r(a,b) = \frac{\operatorname{cov}(a,b)}{\sqrt{s_a^2 s_b^2}} = \frac{-58}{\sqrt{11{,}6 * 348}} = -0{,}91$$

Jacobian

The model function in the linear regression $y = a*x + b$.
Jacobian is a matrix of derivatives over parameters a, b in all points of data
i = 1,2,...,n

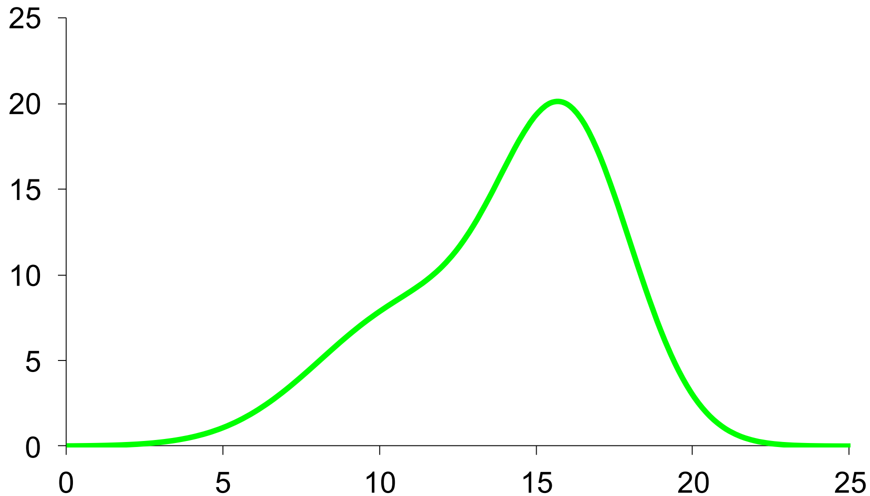
$$\mathbf{J} = \begin{bmatrix} \left(\frac{\partial y}{\partial a}\right)_1 & \left(\frac{\partial y}{\partial b}\right)_1 \\ \left(\frac{\partial y}{\partial a}\right)_2 & \left(\frac{\partial y}{\partial b}\right)_2 \\ \dots & \dots \\ \left(\frac{\partial y}{\partial a}\right)_n & \left(\frac{\partial y}{\partial b}\right)_n \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \dots & \dots \\ x_n & 1 \end{bmatrix}$$

When fitting the data to the polynomial of the 2nd order
$y = a_0 + a_1*x + a_2*x^2$, then the Jacobian takes a form of:

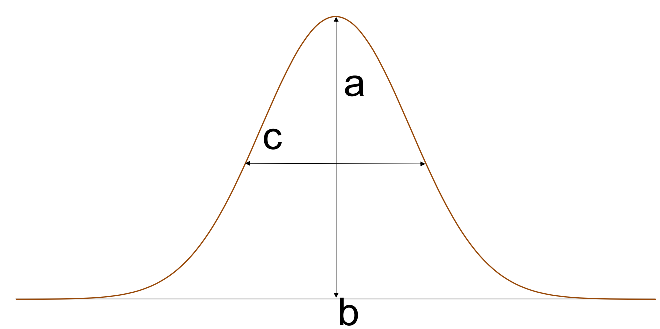
$$\mathbf{J} = \begin{bmatrix} \left(\frac{\partial y}{\partial a_0}\right)_1 & \left(\frac{\partial y}{\partial a_1}\right)_1 & \left(\frac{\partial y}{\partial a_2}\right)_1 \\ \left(\frac{\partial y}{\partial a_0}\right)_2 & \left(\frac{\partial y}{\partial a_1}\right)_2 & \left(\frac{\partial y}{\partial a_2}\right)_2 \\ \dots & \dots & \dots \\ \left(\frac{\partial y}{\partial a_0}\right)_n & \left(\frac{\partial y}{\partial a_1}\right)_n & \left(\frac{\partial y}{\partial a_2}\right)_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \dots & \dots & \dots \\ 1 & x_n & x_n^2 \end{bmatrix}$$

Deconvolution of a complex band

Experimental band



The band should be expressed as a sum of Gaussian curves



$$P_k(x) = a_k e^{-\frac{(x-b_k)^2}{2c_k^2}}$$

a - height
b - position
c - width

The least squares method

$\{a_k\}$, k=1:M , M fitted parameters

The error function (sum over n points):

$\Phi\{a_k\} = \Sigma_j\ [y_j(\text{exp}) - y_j(\{a_k\}]^2$

Problem

To minimize Φ through modification of $\{a_k\}$ using the starting values of parameters $\{a_k\}_0$

The error function and Jacobian

$$P_k(x) = a_k e^{-\frac{(x-b_k)^2}{2c_k^2}}$$

$$P(x) = \sum_{k=1}^{N} P_k(x)$$

Decomposition over N bands

Elements of the Jacobian

$$\frac{\partial P_k}{\partial a_k} = e^{-\frac{(x-b_k)^2}{2c_k^2}}$$

$$\frac{\partial P_k}{\partial b_k} = a_k \frac{(x-b_k)}{c_k^2} e^{-\frac{(x-b_k)^2}{2c_k^2}}$$

$$\frac{\partial P_k}{\partial c_k} = a_k \frac{(x-b_k)^2}{c_k^3} e^{-\frac{(x-b_k)^2}{2c_k^2}}$$

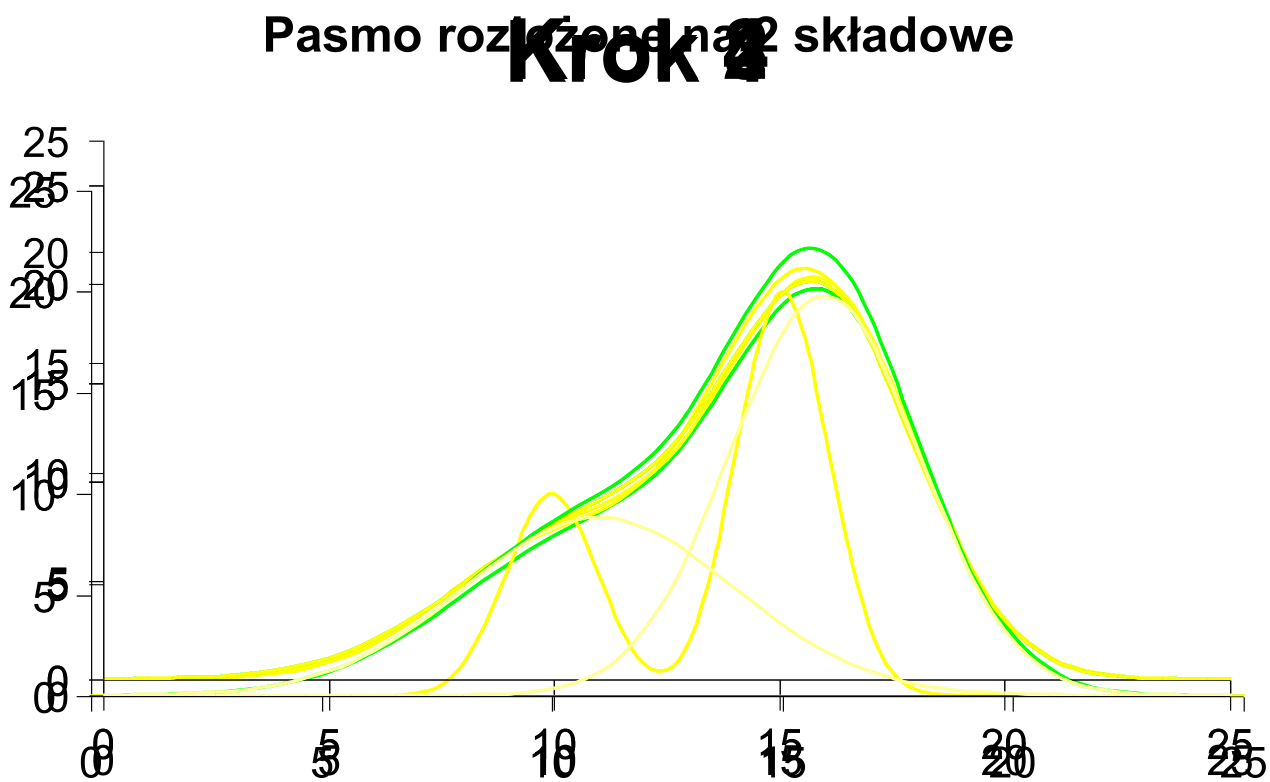
Algorythm

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix} \qquad J = \begin{bmatrix} \left(\frac{\partial P}{\partial a_1}\right)_1 & \left(\frac{\partial P}{\partial b_1}\right)_1 & \left(\frac{\partial P}{\partial c_1}\right)_1 & \left(\frac{\partial P}{\partial a_2}\right)_1 & \dots \\ \left(\frac{\partial P}{\partial a_1}\right)_2 & \left(\frac{\partial P}{\partial b_1}\right)_2 & \dots & \dots & \\ \dots & \dots & \dots & \dots & \\ \left(\frac{\partial P}{\partial a_1}\right)_n & \left(\frac{\partial P}{\partial b_1}\right)_n & \dots & \dots & \end{bmatrix} \qquad \Delta a = \begin{bmatrix} \Delta a_1 \\ \Delta b_1 \\ \Delta c_1 \\ \Delta a_2 \\ \Delta b_2 \\ \Delta c_2 \end{bmatrix}$$

Corrections to the values of parameters $\{a_k\}$

$$\Delta a = \left(J^T J\right)^{-1} J^T Y$$

The least squares method



Matrices

Set of linear equations

$a_1 x + b_1 y = c_1$
$a_2 x + b_2 y = c_2$

$a_1, b_1, c_1, a_2, b_2, c_2$ - constants
x, y - variables (unknown)

$a_1 b_2 x + b_1 b_2 y = c_1 b_2$ multiplying by b_2
$b_1 a_2 x + b_1 b_2 y = b_1 c_2$ multiplying by b_1

$(a_1 b_2 - b_1 a_2) x = c_1 b_2 - b_1 c_2$ subtrackting on both sides
$(a_1 b_2 - b_1 a_2) y = a_1 c_2 - c_1 a_2$ similarily as for x

$$x = \frac{c_1 b_2 - b_1 c_2}{a_1 b_2 - b_1 a_2} \qquad y = \frac{a_1 c_2 - c_1 a_2}{a_1 b_2 - b_1 a_2}$$

$$D = \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} = a_1 b_2 - b_1 a_2$$ determinat

$$D_1 = \begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix} \qquad D_2 = \begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix} \qquad x = \frac{D_1}{D} \qquad y = \frac{D_2}{D}$$

Cramer's rule

Solve a set of equations

3 x - 4 y = 1
2 x + y = 8

$$D = \begin{vmatrix} 3 & -4 \\ 2 & 1 \end{vmatrix} = 3 * 1 - 2(-4) = 11$$

$$D_1 = \begin{vmatrix} 1 & -4 \\ 8 & 1 \end{vmatrix} = 1 * 1 - 8 * (-4) = 33$$

$$D_2 = \begin{vmatrix} 3 & 1 \\ 2 & 8 \end{vmatrix} = 3 * 8 - 1 * 2 = 22$$

$$x = \frac{D_1}{D} = \frac{33}{11} = 3 \qquad y = \frac{D_2}{D} = \frac{22}{11} = 2$$

Determinant of the 3rd order

$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$
$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$
$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$

a_{ij} i – numer wiersza
j – numer kolumny

Calculate the determinants:

$$D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = (-1)^{1+1} a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} + (-1)^{1+2} a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + (-1)^{1+3} a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} =$$

$$= a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31}$$

$$D_1 = \begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix} \qquad D_2 = \begin{vmatrix} a_{11} & b_1 & a_{13} \\ a_{21} & b_2 & a_{23} \\ a_{31} & b_3 & a_{33} \end{vmatrix} \qquad D_3 = \begin{vmatrix} a_{11} & a_{12} & b_1 \\ a_{21} & a_{22} & b_2 \\ a_{31} & a_{32} & b_3 \end{vmatrix}$$

$$x_1 = \frac{D_1}{D} \qquad x_2 = \frac{D_2}{D} \qquad x_3 = \frac{D_3}{D}$$

If the right sides are not equal to 0, then the set of equations has a solution, if the determinat $D \neq 0$.

If $b_1 = b_2 = b_3 = 0$, then $D_1 = D_2 = D_3 = 0$ and the trivial solution is $x_1 = x_2 = x_3 = 0$, and nontrivial solution requires the determinant $D = 0$.

Determinat of the n^{th} order

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{32} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{vmatrix} = (-1)^{1+1}a_{11}M_{11} + (-1)^{1+2}a_{12}M_{12} + (-1)^{1+3}a_{13}M_{13} + \dots + (-1)^{1+n}a_{1n}M_{1n}$$

Minors

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{32} & \dots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \dots & a_{3n} \\ \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{vmatrix} \Rightarrow \begin{vmatrix} a_{22} & a_{32} & \dots & a_{2n} \\ a_{32} & a_{33} & \dots & a_{3n} \\ \dots & \dots & \dots & \dots \\ a_{n2} & a_{n3} & \dots & a_{nn} \end{vmatrix} = M_{11}$$

Algebraic adjugate of the element a_{ij} : $A_{ij} = (-1)^{i+j} M_{ij}$

Properties of determinants 1

1. Transposition does not change the value

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix}$$

2. Multiplication with a constant

$$D = \begin{vmatrix} \lambda a_1 & \lambda b_1 & \lambda c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = \lambda \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

If λ=0, then the value of determinat = 0

3. Permutation of rows or columns

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = - \begin{vmatrix} a_2 & b_2 & c_2 \\ a_1 & b_1 & c_1 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = - \begin{vmatrix} b_1 & a_1 & c_1 \\ b_2 & a_2 & c_2 \\ b_3 & a_3 & c_3 \end{vmatrix}$$

Properties of determinants 2

4. Sum of determinants differing in one row or column

$$\begin{vmatrix} a_1 + d_1 & b_1 & c_1 \\ a_2 + d_2 & b_2 & c_2 \\ a_3 + d_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} + \begin{vmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d_3 & b_3 & c_3 \end{vmatrix}$$

5. Equality or proportionality of two rows or columns

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ \lambda a_1 & \lambda b_1 & \lambda c_1 \\ a_3 & b_3 & c_3 \end{vmatrix} = 0 \qquad \begin{vmatrix} a_1 & \lambda a_1 & c_1 \\ a_2 & \lambda a_2 & c_2 \\ a_3 & \lambda a_3 & c_3 \end{vmatrix} = 0$$

6. Adding rows or columns premultiplied with a constant

$$\begin{vmatrix} a_1 + \lambda b_1 & b_1 & c_1 \\ a_2 + \lambda b_2 & b_2 & c_2 \\ a_3 + \lambda b_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} + \begin{vmatrix} \lambda b_1 & b_1 & c_1 \\ \lambda b_2 & b_2 & c_2 \\ \lambda b_3 & b_3 & c_3 \end{vmatrix} = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

Solving a set of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

$$\mathbf{A}^{-1}\mathbf{A}\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

Example

$x_1+2x_2+3x_3=1$

$2x_1+3x_2+4x_3=1$

$3x_1+4x_2+ x_3=1$

Matrix notation

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \mathbf{A}^{-1} = \begin{bmatrix} -\frac{13}{4} & \frac{10}{4} & -\frac{1}{4} \\ \frac{10}{4} & -\frac{8}{4} & \frac{2}{4} \\ -\frac{1}{4} & \frac{2}{4} & -\frac{1}{4} \end{bmatrix}$$

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \qquad \Rightarrow \qquad \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -\frac{13}{4} & \frac{10}{4} & -\frac{1}{4} \\ \frac{10}{4} & -\frac{8}{4} & \frac{2}{4} \\ -\frac{1}{4} & \frac{2}{4} & -\frac{1}{4} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$

$x_1=-1$

$x_2=1$

$x_3=0$

Types of matricies

Rectangular n×m

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \ldots & a_{1m} \\ a_{21} & a_{22} & a_{32} & \ldots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \ldots & a_{3m} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & a_{n3} & \ldots & a_{nm} \end{bmatrix}$$

Square n×n

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \ldots & a_{1n} \\ a_{21} & a_{22} & a_{32} & \ldots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \ldots & a_{3n} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ a_{n1} & a_{n2} & a_{n3} & \ldots & a_{nn} \end{bmatrix}$$

Column matrix

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \ldots \\ b_n \end{bmatrix}$$

Row matrix

$$\begin{bmatrix} b_1 & b_2 & b_3 & \ldots & b_n \end{bmatrix}$$

Unity matrix

$$\boldsymbol{I} = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 1 \end{bmatrix}$$

Matrix algebra

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \qquad \boldsymbol{B} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix}$$

Equality of matrices

$\boldsymbol{A} = \boldsymbol{B}$, gdy $a_{11}=b_{11}$, $a_{12}=b_{12}$, $a_{13}=b_{13}$, $a_{21}=b_{21}$, $a_{22}=b_{22}$, $a_{23}=b_{23}$

Multiplying with a constant

$$c\boldsymbol{A} = c\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} = \begin{bmatrix} ca_{11} & ca_{12} & ca_{13} \\ ca_{21} & ca_{22} & ca_{23} \end{bmatrix}$$

Addition of matricies

$$\boldsymbol{A} + \boldsymbol{B} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix} = \begin{bmatrix} a_{11} + b_{11} & a_{12} + b_{12} & a_{13} + b_{13} \\ a_{21} + b_{21} & a_{22} + b_{22} & a_{23} + b_{23} \end{bmatrix}$$

Comment: to add both matrices must have the same dimensions

Multiplication of matricies

$$\boldsymbol{a} = \begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} \qquad \boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$\boldsymbol{ab} = \begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = a_1 b_1 + a_2 b_2 + a_3 b_3$$

Necessary condition: the number of rows in the second matrix must be the same as the number of rows of the first matrix

$$\boldsymbol{C} = \boldsymbol{AB} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix} =$$

$$= \begin{bmatrix} a_{11} b_{11} + a_{12} b_{21} & a_{11} b_{12} + a_{12} b_{22} & a_{11} b_{13} + a_{12} b_{23} \\ a_{21} b_{11} + a_{22} b_{21} & a_{21} b_{12} + a_{22} b_{22} & a_{21} b_{13} + a_{22} b_{23} \end{bmatrix}$$

If the matric ***C*** (m×p) is a result of the multiplication of ***A***(m×n) and ***B*** (n×p)

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

i=1 to m , *j*=1 to p

Properties of matrix multiplication

Associativity $\boldsymbol{A(BC)} = \boldsymbol{(AB)C} = \boldsymbol{ABC}$

Distributivity $\boldsymbol{A(B+C)} = \boldsymbol{AB} + \boldsymbol{AC}$

Non commutativity $\boldsymbol{AB} \neq \boldsymbol{BA}$

$\boldsymbol{A} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ $\boldsymbol{B} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$

$$\boldsymbol{AB} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\boldsymbol{BA} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$$

Inverse matrix n×n

Procedure

Square matrix

Matrix of algebraic complements

Matrix of algebraic complements transposed

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} \xrightarrow{replace\ with} \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix} \xrightarrow{transpose} \begin{bmatrix} A_{11} & \cdots & A_{n1} \\ \vdots & \ddots & \vdots \\ A_{1n} & \cdots & A_{nn} \end{bmatrix} = \widetilde{\boldsymbol{A}}$$

Adjugate matrix

Algebraic adjugate of the element a_{ij}: $A_{ij} = (-1)^{i+j} M_{ij}$ M_{ij} - minor

Inverse matrix $$\boldsymbol{A}^{-1} = \frac{\widetilde{\boldsymbol{A}}}{\det \boldsymbol{A}}$$ $$\boldsymbol{A}\,\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\,\boldsymbol{A} = \boldsymbol{I}$$

Exists if the determinant $|\boldsymbol{A}| \equiv \det \boldsymbol{A}$ is not equal 0

Solving a set of linear equations

$$\mathbf{Ax} = \mathbf{b}$$
$$\mathbf{A}^{-1}\mathbf{Ax} = \mathbf{A}^{-1}\mathbf{b}$$
$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

Example:

$x_1+2x_2+3x_3=1$
$2x_1+3x_2+4x_3=1$
$3x_1+4x_2+x_3=1$

det $\boldsymbol{A}$ = 4

$$\boldsymbol{A} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 1 \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \boldsymbol{A}^{-1} = \begin{bmatrix} -\frac{13}{4} & \frac{10}{4} & -\frac{1}{4} \\ \frac{10}{4} & -\frac{8}{4} & \frac{2}{4} \\ -\frac{1}{4} & \frac{2}{4} & -\frac{1}{4} \end{bmatrix}$$

Test of the inverse matrix

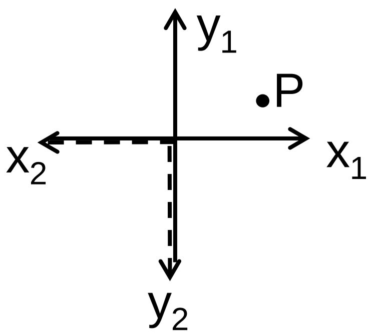
$$\boldsymbol{A}^{-1}\boldsymbol{A} = \begin{bmatrix} -\frac{13}{4} & \frac{10}{4} & -\frac{1}{4} \\ \frac{10}{4} & -\frac{8}{4} & \frac{2}{4} \\ -\frac{1}{4} & \frac{2}{4} & -\frac{1}{4} \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Identity matrix

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \quad \Rightarrow \quad \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -\frac{13}{4} & \frac{10}{4} & -\frac{1}{4} \\ \frac{10}{4} & -\frac{8}{4} & \frac{2}{4} \\ -\frac{1}{4} & \frac{2}{4} & -\frac{1}{4} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$

$x_1=-1$
$x_2=1$
$x_3=0$

Matrices and geometrical transformations

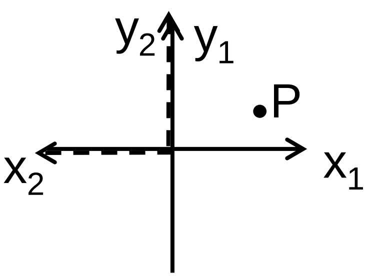


inversion

$$\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mathbf{Q}^{-1}\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

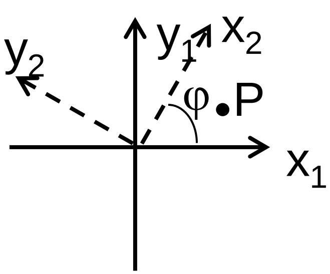


mirror reflection

$$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{Q}^{-1}\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



rotation

$$\begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix} = \begin{bmatrix} x_2 \\ y_2 \end{bmatrix}$$

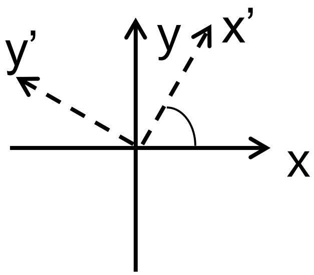
$$\mathbf{Q} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix}$$

$$\mathbf{Q}^{-1}\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \begin{bmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{bmatrix} \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Transformation matrices are orthogonal

Similarity transformation of matrices

Mapping **A**, transforms **x** → **y:** $\mathbf{Ax} = \mathbf{y}$



If vectors **x'** and **y'** are transformed to vectors **x** i **y** through a mapping **Q**, what is a mapping of vector **x'** into vector **y'** ?

If $\mathbf{x} = \mathbf{Qx'}$, $\mathbf{y} = \mathbf{Qy'}$ and $\mathbf{Ax} = \mathbf{y}$, than $\mathbf{AQx'} = \mathbf{Qy'}$

If the matrix **Q** is not singular, than $\mathbf{Q}^{-1}\mathbf{Qy'} = \mathbf{Q}^{-1}\mathbf{AQx'}$

thus $\mathbf{y'} = \mathbf{Q}^{-1}\mathbf{AQx'} = \mathbf{Bx'}$

The matrices **A** i **B** are two matrices transformed through a similarity transformation

$$\mathbf{B} = \mathbf{Q}^{-1}\mathbf{AQ}$$

Example

$$\begin{aligned} x_1 + x_2 &= y_1 \\ x_1 - x_2 &= y_2 \end{aligned}$$

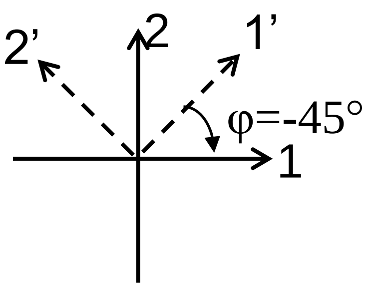
$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{bmatrix}$$

$$\begin{aligned} x_1 &= \tfrac{1}{\sqrt{2}} x_1' + \tfrac{1}{\sqrt{2}} x_2' \\ x_2 &= -\tfrac{1}{\sqrt{2}} x_1' + \tfrac{1}{\sqrt{2}} x_2' \end{aligned}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} y_1' \\ y_2' \end{bmatrix}$$



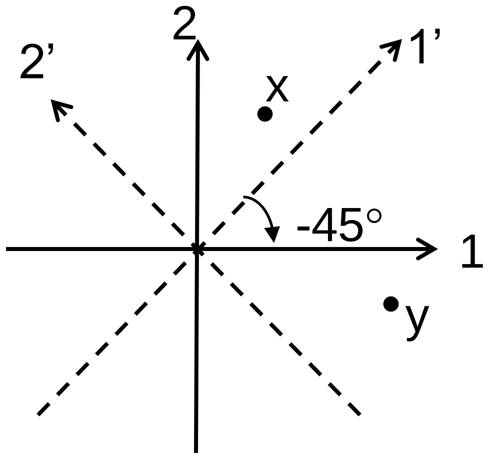
$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} y_1' \\ y_2' \end{bmatrix}$$

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}$$

$$\begin{aligned} x_1' - x_2' &= y_1' \\ -x_1' - x_2' &= y_2' \end{aligned}$$

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{2} & 0 \\ 0 & -\sqrt{2} \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} x_1' \\ x_2' \end{bmatrix}$$

Example



$$\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\begin{bmatrix}1\\2\end{bmatrix}=\begin{bmatrix}3\\-1\end{bmatrix}$$

$$\begin{bmatrix}1\\2\end{bmatrix}=\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\frac{3}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$$

$$\begin{bmatrix}3\\-1\end{bmatrix}=\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\sqrt{2}\\-2\sqrt{2}\end{bmatrix}$$

$(x_1,x_2)=(1,2)$
$(y_1,y_2)=(3,-1)$

$$\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}x_1'\\x_2'\end{bmatrix}=\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}y_1'\\y_2'\end{bmatrix}$$

1+2=3 $\qquad x_1+x_2=y_1$
1-2=-1 $\qquad x_1-x_2=y_2$

$$\begin{bmatrix}y_1'\\y_2'\end{bmatrix}=\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}x_1'\\x_2'\end{bmatrix}$$

$$\begin{bmatrix}y_1'\\y_2'\end{bmatrix}=\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\sqrt{2} & 0\\0 & -\sqrt{2}\end{bmatrix}\begin{bmatrix}x_1'\\x_2'\end{bmatrix}=\begin{bmatrix}1 & -1\\-1 & -1\end{bmatrix}\begin{bmatrix}x_1'\\x_2'\end{bmatrix}$$

$(x'_1,x'_2)=\left(\frac{3}{\sqrt{2}},\frac{1}{\sqrt{2}}\right)$
$(y'_1,y'_2)=\left(\sqrt{2},2\sqrt{2}\right)$

$\frac{3}{\sqrt{2}}-\frac{1}{\sqrt{2}}=\sqrt{2}$ $\qquad x_1'-x_2'=y_1'$

$-\frac{3}{\sqrt{2}}-\frac{1}{\sqrt{2}}=-2\sqrt{2}$ $\qquad -x_1'-x_2'=y_2'$

Characteristic equation

λ – scalar , $\mathbf{A}(n\times n)$ $\mathbf{I}(n\times n)$ $\mathbf{K}(n\times n)$

$\mathbf{K} = \mathbf{A} - \lambda\mathbf{I}$ characteristic matrix of matrix **A**

$\det\mathbf{K} = K(\lambda) = \det(\mathbf{A} - \lambda\mathbf{I}) = |\mathbf{A} - \lambda\mathbf{I}| = 0$ characteristic equation

$K(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + a_{n-2}\lambda^{n-2} + \ldots + a_1\lambda + a_0 = 0$

The roots of the polynomial $K(\lambda)$: $\lambda_1, \lambda_2, \ldots, \lambda_{n-1}, \lambda_n$ are called eigenvalues of matrix **A**.

If $\mathbf{B} = \mathbf{Q}^{-1}\mathbf{A}\mathbf{Q}$, than the characteristic equation for **B**

$\mathbf{K} = \mathbf{B} - \lambda\mathbf{I} = \mathbf{Q}^{-1}\mathbf{A}\mathbf{Q} - \lambda\mathbf{Q}^{-1}\mathbf{I}\mathbf{Q} = \mathbf{Q}^{-1}(\mathbf{A} - \lambda\mathbf{I})\mathbf{Q}$, and the determinant

$\det\mathbf{K} = |\mathbf{B} - \lambda\mathbf{I}| = |\mathbf{Q}^{-1}|\ |\mathbf{A} - \lambda\mathbf{I}|\ |\mathbf{Q}| = |\mathbf{A} - \lambda\mathbf{I}| = 0$

Two matrices related to each other through a similarity transformation have the same set of eigenvalues.

Eigenvalues

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix}$$

$$\det(\mathbf{A} - \lambda\mathbf{I}) = \begin{vmatrix} 1-\lambda & 1 \\ 1 & -1-\lambda \end{vmatrix} = 0$$

$$(1-\lambda)(-1-\lambda) - 1 = 0 \qquad \lambda^2 - 1 - 1 = 0 \qquad \lambda^2 = 2 \qquad \lambda_1 = \sqrt{2},\ \lambda_2 = -\sqrt{2}$$

$$\det(B - \lambda\mathbf{I}) = \begin{vmatrix} 1-\lambda & -1 \\ -1 & -1-\lambda \end{vmatrix} = 0$$

$$(1-\lambda)(-1-\lambda) - 1 = 0 \qquad \lambda^2 - 1 - 1 = 0 \qquad \lambda^2 = 2 \qquad \lambda_1 = \sqrt{2},\ \lambda_2 = -\sqrt{2}$$

Diagonal matrix

$$\mathbf{D} = \begin{bmatrix} d_1 & 0 & 0 & \ldots & 0 \\ 0 & d_2 & 0 & \ldots & 0 \\ 0 & 0 & d_3 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & d_n \end{bmatrix} \qquad \mathbf{D} - \lambda\mathbf{I} = \begin{bmatrix} d_1 - \lambda & 0 & 0 & \ldots & 0 \\ 0 & d_2 - \lambda & 0 & \ldots & 0 \\ 0 & 0 & d_3 - \lambda & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & d_n - \lambda \end{bmatrix}$$

$$\left|\mathbf{D} - \lambda\mathbf{I}\right| = (d_1 - \lambda)(d_2 - \lambda)(d_3 - \lambda)\ldots(d_n - \lambda) = 0$$

$$\lambda_1 = d_1,\ \lambda_2 = d_2,\ \lambda_3 = d_3, \ldots,\ \lambda_n = d_n$$

Can we transform a given quadratic matrix **A** to a diagonal matrix **D** through a similarity transformation?

Diagonalization

$$\mathbf{Q}=\begin{bmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{bmatrix} \qquad \mathbf{A}=\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

$$\mathbf{Q}^{-1}\mathbf{A}\mathbf{Q}=\begin{bmatrix}\cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi\end{bmatrix}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{bmatrix}=\begin{bmatrix}\cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi\end{bmatrix}\begin{bmatrix}\cos\varphi-\sin\varphi & \cos\varphi+\sin\varphi\\ \cos\varphi+\sin\varphi & -\cos\varphi+\sin\varphi\end{bmatrix}=$$

$$=\begin{bmatrix}\cos^2\varphi-2\sin\varphi\cos\varphi-\sin^2\varphi & \cos^2\varphi+2\sin\varphi\cos\varphi-\sin^2\varphi\\ \cos^2\varphi+2\sin\varphi\cos\varphi-\sin^2\varphi & -\cos^2\varphi+2\sin\varphi\cos\varphi+\sin^2\varphi\end{bmatrix}=$$

$$=\begin{bmatrix}\cos 2\varphi-\sin 2\varphi & \cos 2\varphi+\sin 2\varphi\\ \cos 2\varphi+\sin 2\varphi & -\cos 2\varphi+\sin 2\varphi\end{bmatrix}$$

Now we set the nondiagonal elements to zero:

$$\cos 2\varphi+\sin 2\varphi=0 \qquad \sin 2\varphi=-\cos 2\varphi \qquad \tan 2\varphi=-1 \qquad 2\varphi=-\frac{\pi}{4} \qquad \varphi=-\frac{\pi}{8}$$

After the transformation:

$$\begin{bmatrix}\cos\frac{\pi}{4}+\sin\frac{\pi}{4} & 0\\ 0 & -\cos\frac{\pi}{4}-\sin\frac{\pi}{4}\end{bmatrix}=\begin{bmatrix}\sqrt{2} & 0\\ 0 & -\sqrt{2}\end{bmatrix} \qquad \lambda_1=\sqrt{2},\ \lambda_2=-\sqrt{2}$$

Eigenvalues and eigenvectors

$\mathbf{C^{-1}AC}$ is a similarity transformation which diagonalizes the matrix **A.**

Columns of the matrix **C** contain eigenvectors.

If the matrix **C** is orthogonal, than $\mathbf{C^{-1}=C^T}$, and $\mathbf{C^{-1}AC} = \mathbf{C^TAC}$.

$$\mathbf{C} = \begin{bmatrix} \cos\left(-\frac{\pi}{8}\right) & \sin\left(-\frac{\pi}{8}\right) \\ -\sin\left(-\frac{\pi}{8}\right) & \cos\left(-\frac{\pi}{8}\right) \end{bmatrix} = \begin{bmatrix} \cos\left(\frac{\pi}{8}\right) & -\sin\left(\frac{\pi}{8}\right) \\ \sin\left(\frac{\pi}{8}\right) & \cos\left(\frac{\pi}{8}\right) \end{bmatrix}$$

Multiplication of the matrix **A** on both sides by the eigenvector produces a respective eigenvalue:

$$\begin{bmatrix} \cos\left(\frac{\pi}{8}\right) & \sin\left(\frac{\pi}{8}\right) \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \cos\left(\frac{\pi}{8}\right) \\ \sin\left(\frac{\pi}{8}\right) \end{bmatrix} = \begin{bmatrix} \cos\left(\frac{\pi}{8}\right) & \sin\left(\frac{\pi}{8}\right) \end{bmatrix} \begin{bmatrix} \cos\left(\frac{\pi}{8}\right) + \sin\left(\frac{\pi}{8}\right) \\ \cos\left(\frac{\pi}{8}\right) - \sin\left(\frac{\pi}{8}\right) \end{bmatrix} =$$

$$= \cos^2\left(\frac{\pi}{8}\right) + \cos\left(\frac{\pi}{8}\right)\sin\left(\frac{\pi}{8}\right) + \sin\left(\frac{\pi}{8}\right)\cos\left(\frac{\pi}{8}\right) - \sin^2\left(\frac{\pi}{8}\right) = \cos\left(\frac{\pi}{4}\right) + \sin\left(\frac{\pi}{4}\right) = \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} = \sqrt{2}$$

In general:

$$\mathbf{c_k^T A c_k} = \lambda_k \qquad\qquad k = 1, 2, \ldots, n$$

Jacobi diagonalization 1

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}$$

Matrix A symmetric

Search for the largest nondiagonal element, e.g. $\rightarrow a_{23}$

$$\boldsymbol{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi_1 & \sin\varphi_1 \\ 0 & -\sin\varphi_1 & \cos\varphi_1 \end{bmatrix}$$

Calculation

$$\boldsymbol{C^T A C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi_1 & -\sin\varphi_1 \\ 0 & \sin\varphi_1 & \cos\varphi_1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi_1 & \sin\varphi_1 \\ 0 & -\sin\varphi_1 & \cos\varphi_1 \end{bmatrix} =$$

$$= \begin{bmatrix} a_{11} & ca_{12} - sa_{13} & sa_{12} + ca_{13} \\ ca_{12} - sa_{13} & c^2a_{22} - 2sca_{23} + s^2a_{33} & (c^2 - s^2)a_{23} + sc(a_{22} - a_{33}) \\ sa_{12} + ca_{13} & (c^2 - s^2)a_{23} + sc(a_{22} - a_{33}) & s^2a_{22} + 2sca_{23} + c^2a_{33} \end{bmatrix}$$

where $\mathrm{s} = \sin\varphi_1$ $c = \cos\varphi_1$

Jacobi diagonalization 2

Remove the largest nondiagonal element in position 23

$$(c^2 - s^2)a_{23} + sc(a_{22} - a_{33}) = 0$$

$$\cos(2\varphi_1)\, a_{23} + \frac{1}{2}\sin(2\varphi_1)\,(a_{22} - a_{33}) = 0 \quad / \cos(2\varphi_1)$$

$$a_{23} + \frac{1}{2}\tan(2\varphi_1)\,(a_{22} - a_{33}) = 0$$

$$\tan(2\varphi_1) = \frac{2a_{23}}{a_{33} - a_{22}}$$

$$\boldsymbol{C^T A C} == \begin{bmatrix} a_{11} & ca_{12} - sa_{13} & sa_{12} + ca_{13} \\ ca_{12} - sa_{13} & c^2 a_{22} - 2sca_{23} + s^2 a_{33} & 0 \\ sa_{12} + ca_{13} & 0 & s^2 a_{22} + 2sca_{23} + c^2 a_{33} \end{bmatrix}$$

Traces of the matrices:

Initial

$$a_{11} + a_{22} + a_{33}$$

After the transformation

$$a_{11} + c^2 a_{22} - 2sca_{23} + s^2 a_{33} + s^2 a_{22} + 2sca_{23} + c^2 a_{33}$$
$$= a_{11} + a_{22}(c^2 + s^2) + a_{33}(s^2 + c^2)$$
$$= a_{11} + a_{22} + a_{33}$$

Jacobi diagonalization 3

Sum of squares of nondiagonal elements

Initial $SS_0 = a_{12}^2 + a_{13}^2 + a_{23}^2$

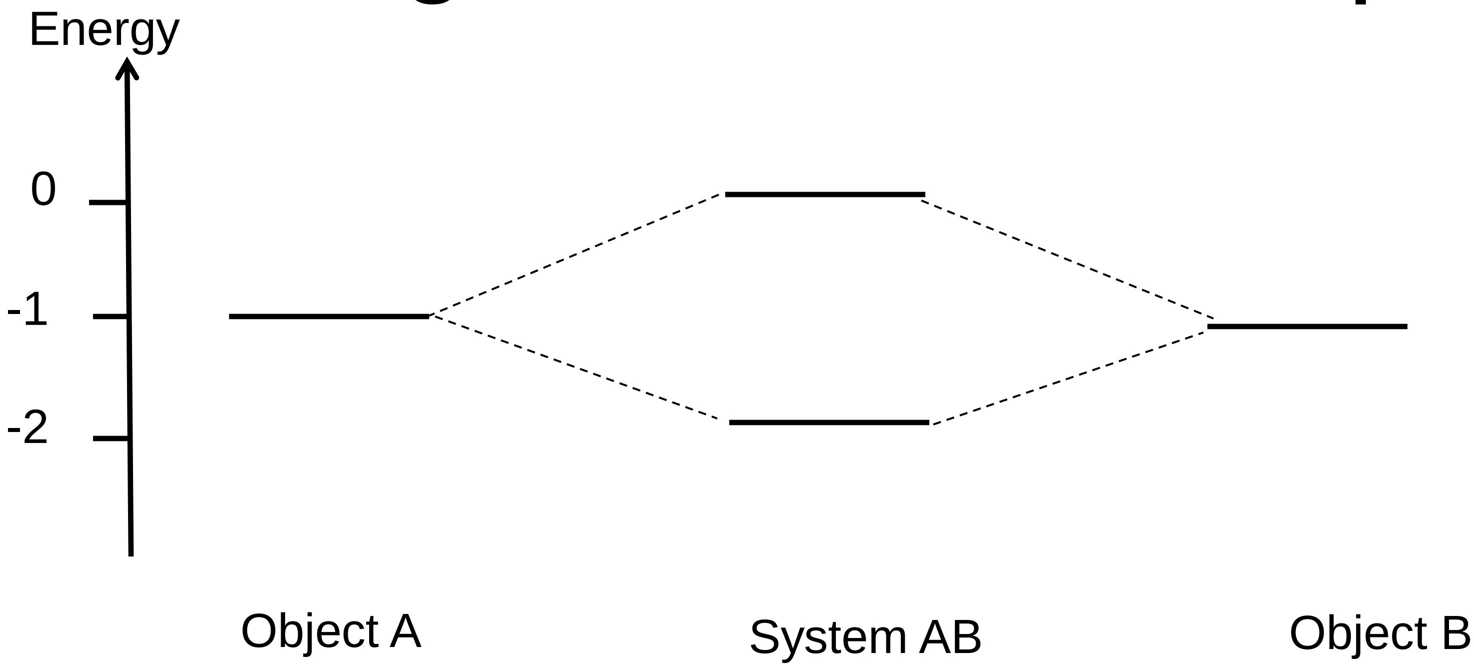
After transformation

$$SS_1 = (ca_{12} - sa_{13})^2 + (sa_{12} + ca_{13})^2 + 0$$
$$= c^2 a_{12}^2 + s^2 a_{13}^2 - 2sca_{12}a_{13} + s^2 a_{12}^2 + c^2 a_{13}^2 + 2sca_{12}a_{13}$$
$$= (c^2 + s^2)a_{12}^2 + (c^2 + s^2)a_{13}^2 = a_{12}^2 + a_{13}^2$$

$$SS_1 < SS_0$$

Next step: selection of the largest nondiagonal element after transformation and repetition of the procedure

Diagonalization example 1



Energy matrix

$$\begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix}$$

Eigenvalues

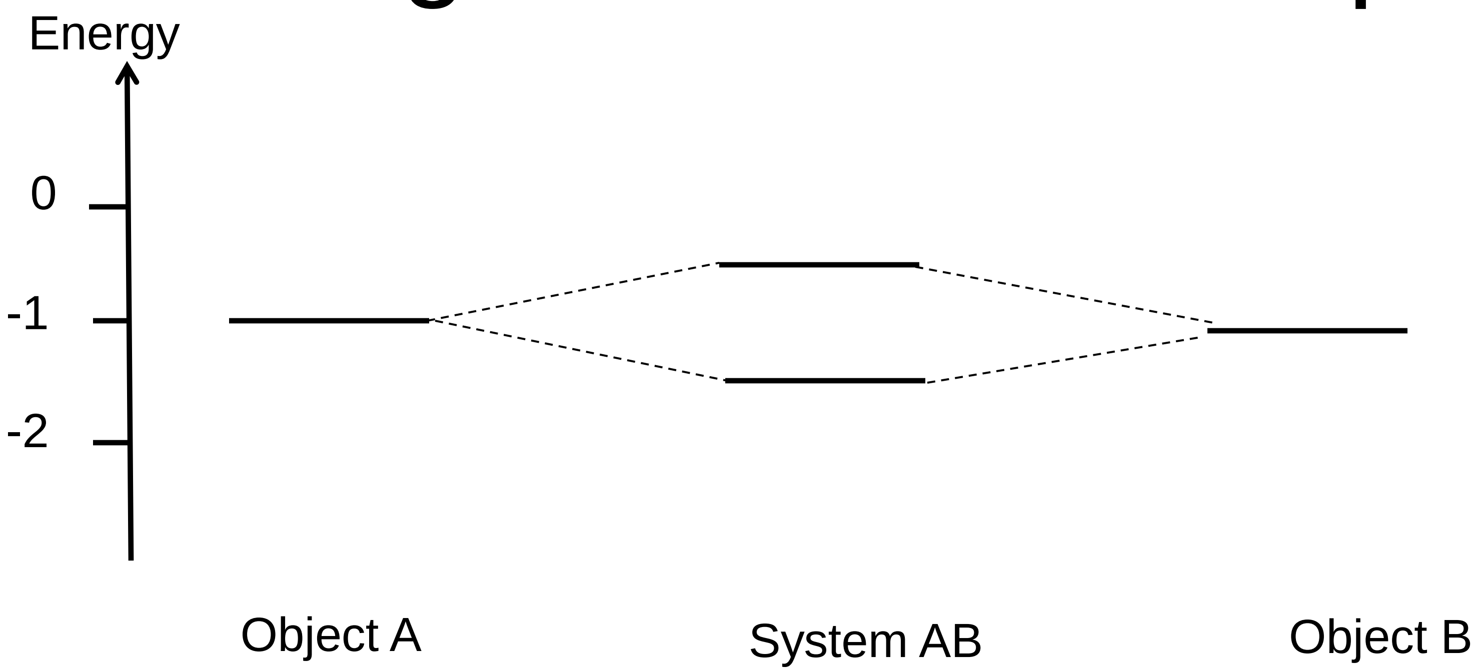
E_1=0
E_2=-2

Eigenvectors

V_1=[0.71 ; -0.71]
V_2=[0.71 ; 0.71]

$$\varphi = 45°$$

Diagonalization example 2



Energy matrix

$$\begin{bmatrix} -1 & -0.5 \\ -0.5 & -1 \end{bmatrix}$$

Eigenvalues

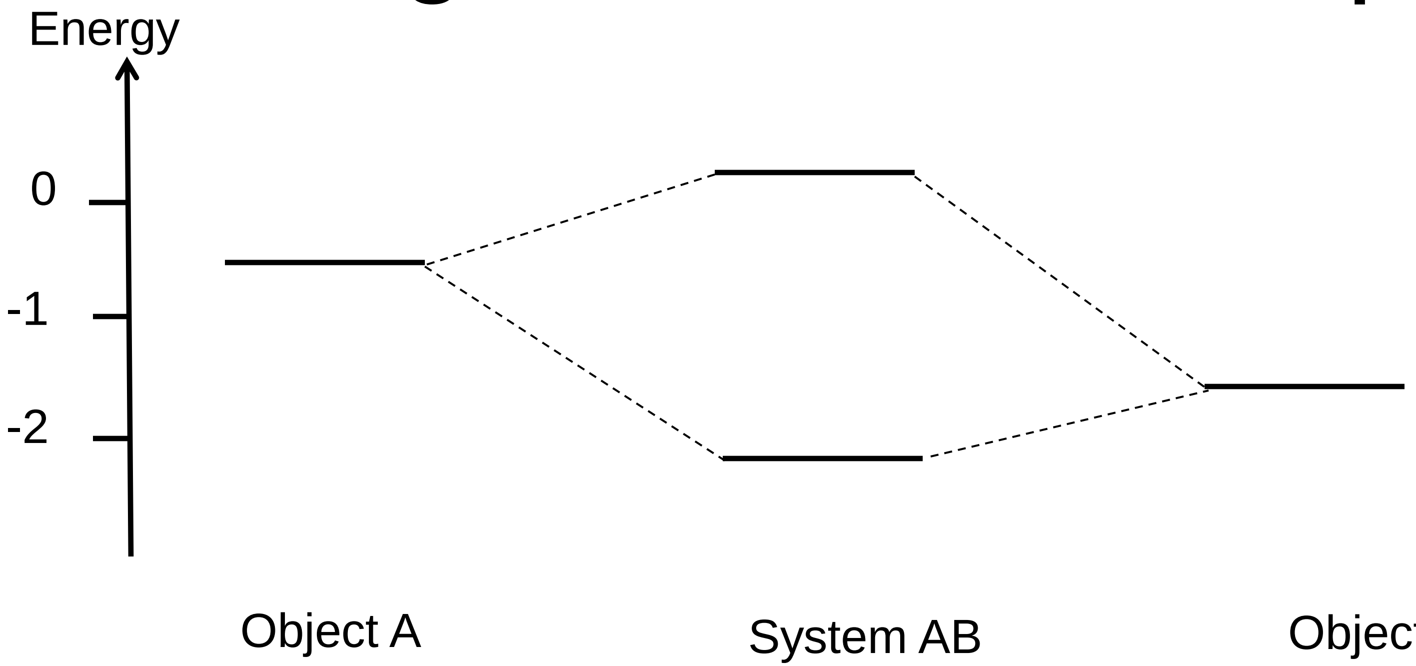
E_1=-0.5
E_2=-1.5

Eigenvectors

V_1=[0.71 ; -0.71]
V_2=[0.71 ; 0.71]

$$\varphi = 45°$$

Diagonalization example 3



Energy matrix

$$\begin{bmatrix} -0.5 & -1 \\ -1 & -1.5 \end{bmatrix}$$

Eigenvalues

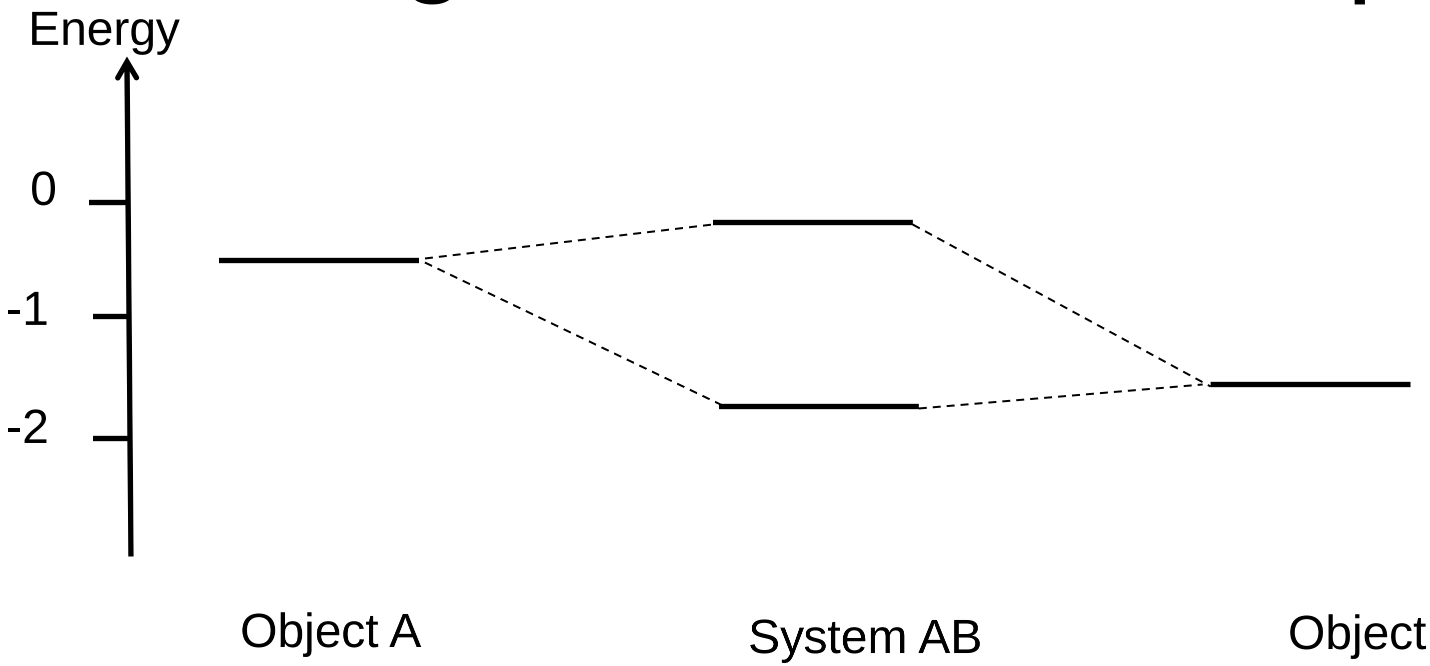
E_1=0.12
E_2=-2.12

Eigenvectors

V_1=[0.85 ; -0.53]
V_2=[0.53 ; 0.85]

$\varphi = 31.7°$

Diagonalization example 4



Energy matrix

$$\begin{bmatrix} -0.5 & -0.5 \\ -0.5 & -1.5 \end{bmatrix}$$

Eigenvalues

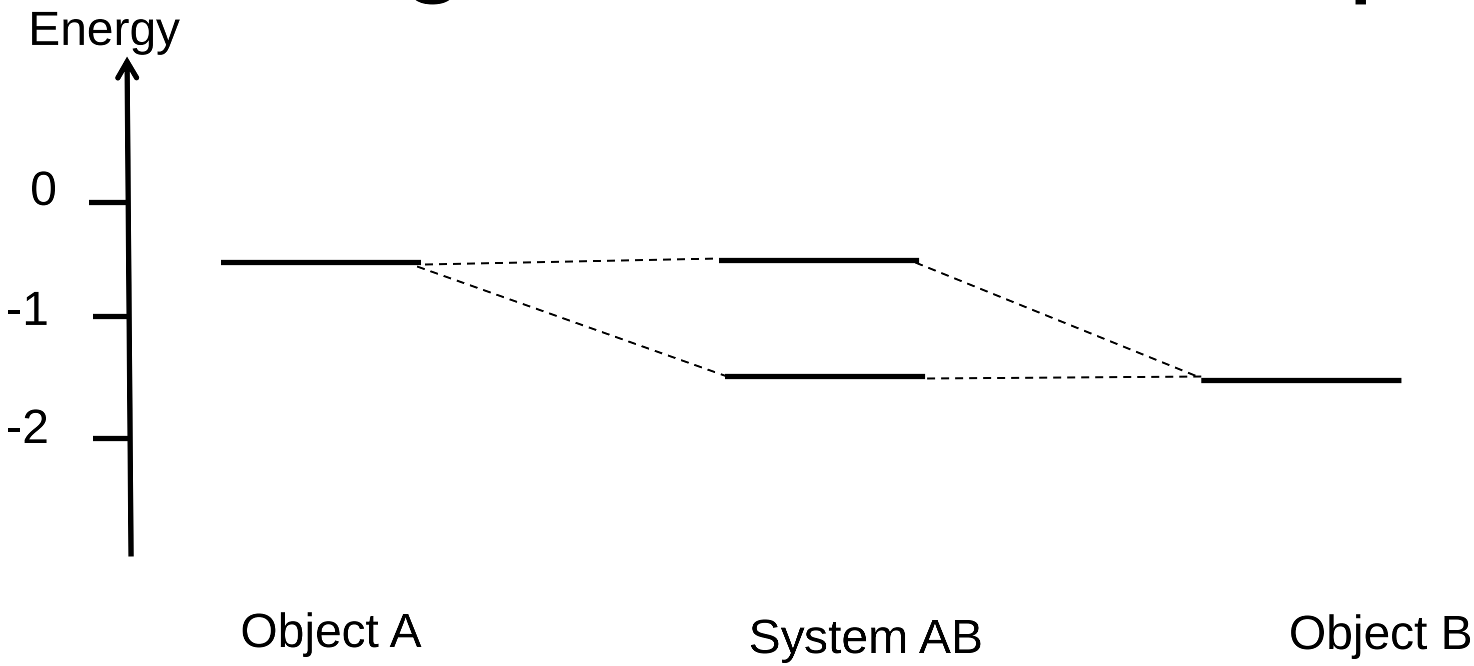
E_1=-0.29
E_2=-1.71

Eigenvectors

V_1=[0.92 ; -0.38]
V_2=[0.38 ; 0.92]

$\varphi = 22.5°$

Diagonalization example 4



Energy matrix

$$\begin{bmatrix} -0.5 & -0.1 \\ -0.1 & -1.5 \end{bmatrix}$$

Eigenvalues

E_1=-0.49
E_2=-1.51

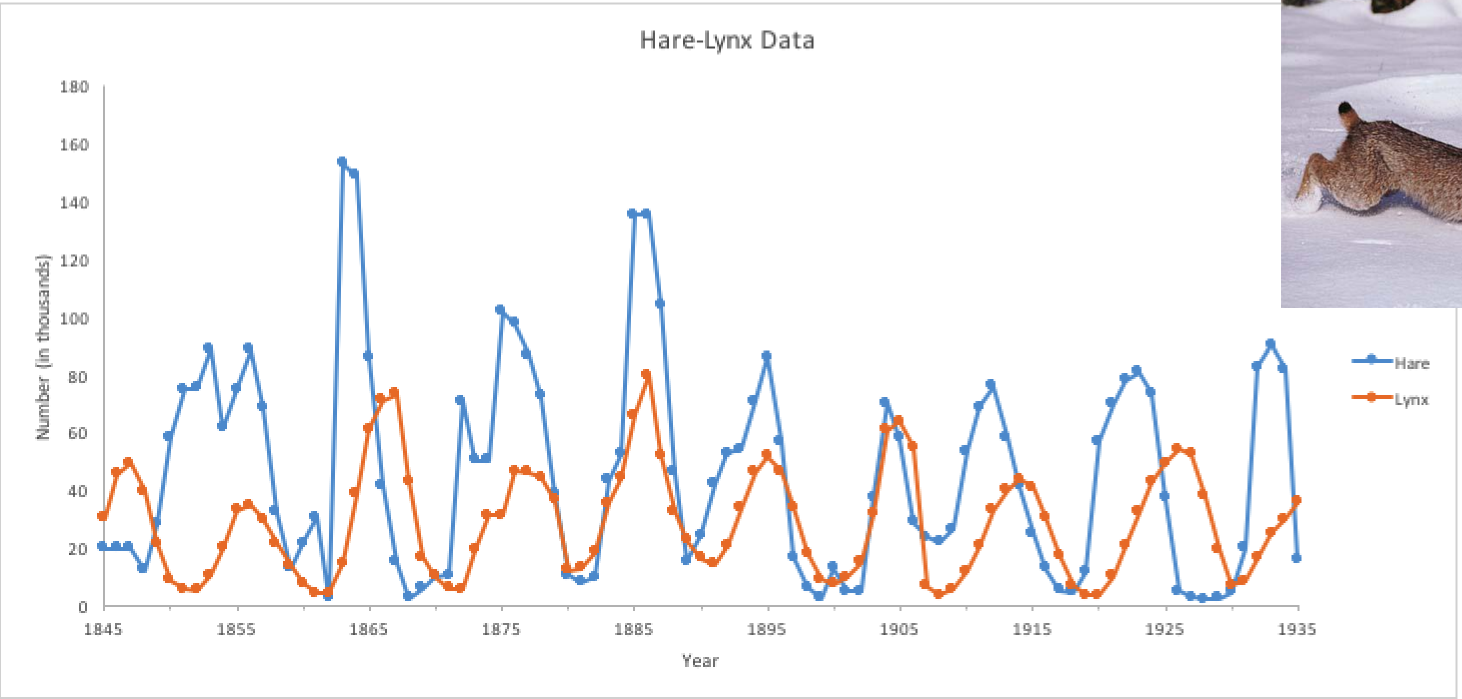
Eigenvectors

V_1=[0.99 ; -0.10]
V_2=[0.10 ; 0.99]

$$\varphi = 5.65°$$

Predator-Prey Interaction

One of the classic studies of predator-prey interactions is the 90-year data set of snowshoe hare and lynx pelts purchased by the Hudson's Bay Company of Canada. While this is an indirect measure of predation, the assumption is that there is a direct relationship between the number of pelts collected and the number of hare and lynx in the wild. As you can see, there does appear to be cycling over time in both hare and lynx number, but it's not as clean as in the simple mathematical models. Life rarely is!



The Lotka-Volterra model

Assumptions:

1. Lynx eat hares only.
2. Hares have unlimited amount of food.
3. The increase of hare population x(t) is proportional (a) to their number.
4. Some meetings of lynx and hares decreases the number of hares with with corfficient (b).
5. If food is not available the decrease of number of lynx is proportional to the total population y(t) and (c) is a coefficient of mortality.
6. The increase of lynx population is proportional to the number of meetings of lynx and hares with a coefficient (p)

$$\frac{dx(t)}{dt} = ax(t) - bx(t)y(t)$$

$$\frac{dy(t)}{dt} = -cy(t) + px(t)y(t)$$

To the Excel sheet