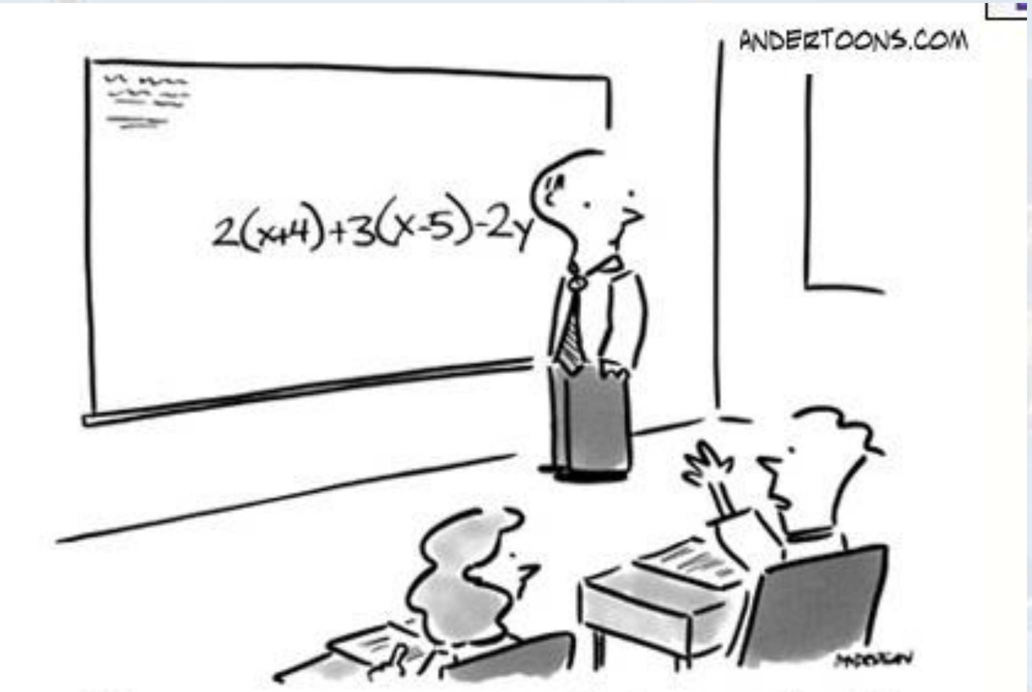
M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



"How come we never complicate equations?"

syllabus:

- Introduction to Unix & Python	(week 1 - 2)
- Functions, Loops, Lists and Arrays	(week 3 - 4)
- Visualization	(week 5)
- Parsing, Data Processing and File I/O	(week 6)
- Statistics and Probability, Interpreting Measurements	(week 7 - 8)
- Random Numbers, Simulation	(week 9)
- Numerical Integration and Differentiation	(week 10)
- Root Finding, Interpolation	(week 11)
- Systems of Linear Equations	**(week 12)**
- Ordinary Differential Equations	(week 13)
- Fourier Transformation and Signal Processing	(week 14)
- Capstone Project Presentations	(week 15)

finding the intersection of **two lines**:

$$y_1 = a_1 x_1 + c_1$$

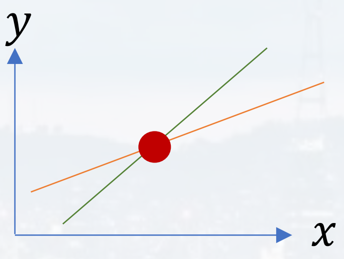
$$y_2 = a_2 x_2 + c_2$$

$$x_1 = x_2$$
$$y_1 = y_2$$

$$a_2 x + c_2 = a_1 x + c_1$$

$$x = \frac{c_2 - c_1}{a_1 - a_2}$$

$$y = a_1 \frac{c_2 - c_1}{a_1 - a_2} + c_1$$



finding the intersection of **three planes**:

$$y_1 = a_{11} x_{11} + a_{12} x_{12} + c_1$$

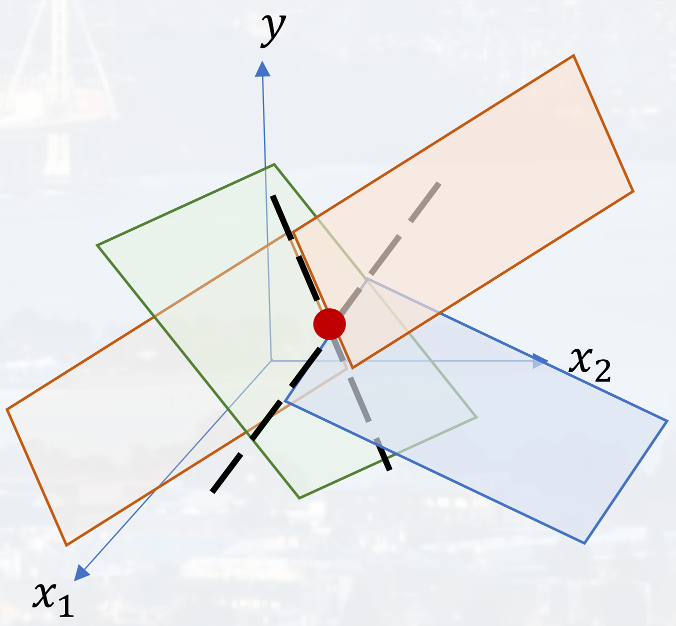
$$y_2 = a_{21} x_{21} + a_{22} x_{22} + c_2$$

$$y_2 = a_{31} x_{31} + a_{32} x_{32} + c_2$$

$$x_{11} = x_{21} = x_{31} = x_1$$

$$x_{12} = x_{22} = x_{32} = x_2$$

$$y_1 = y_2 = y_3 = y$$

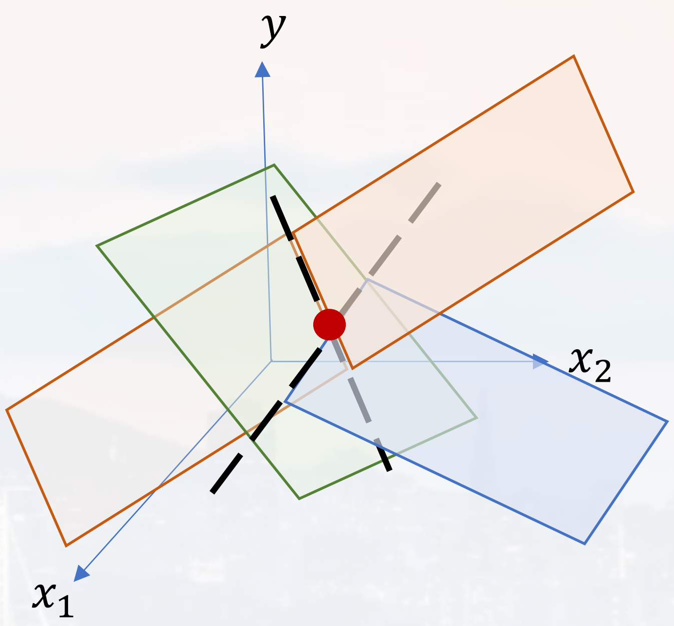


more general:

$$x_{11} = x_{21} = x_{31} = x_1$$

$$x_{12} = x_{22} = x_{32} = x_2$$

$$y_1 = y_2 = y_3 = y$$

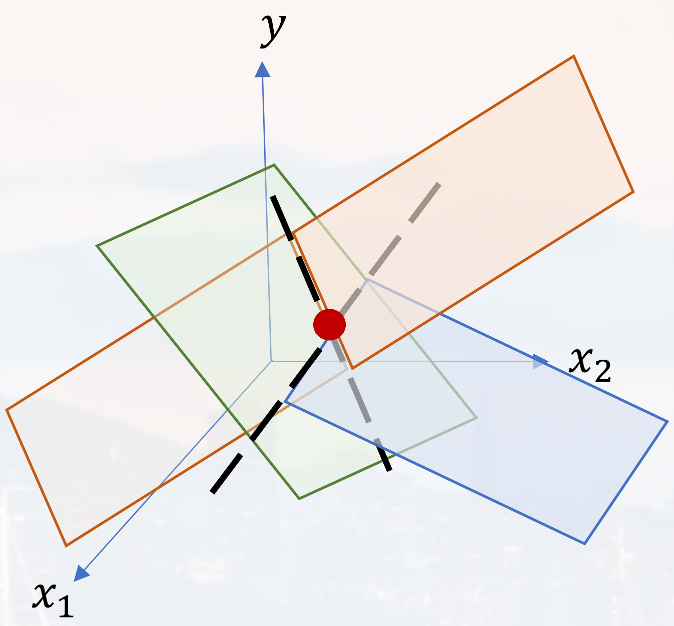


$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = c_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = c_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots + a_{3n}x_n = c_3$$
$$\ldots$$
$$a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \ldots + a_{mn}x_n = c_m$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_m \end{bmatrix}$$

more general:

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_m \end{bmatrix}}_{\vec{c}}$$



$$\boxed{A\vec{x} = \vec{c}}$$

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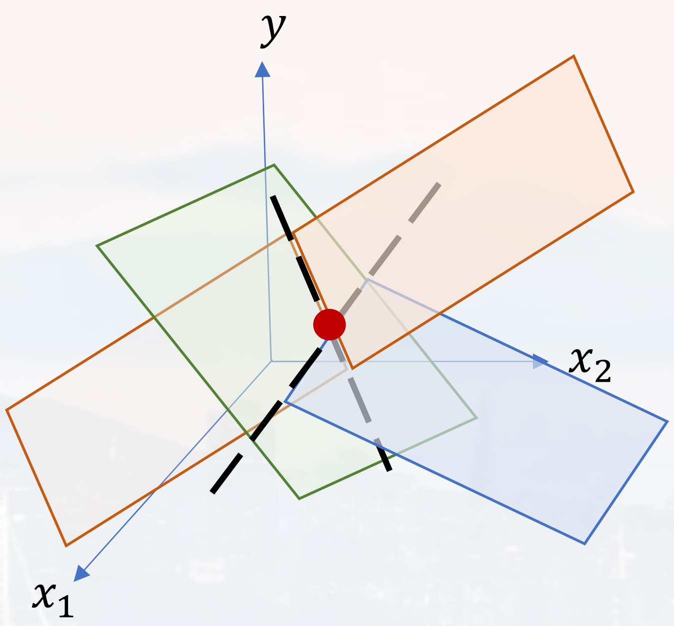

general set of solutions

for n = m → solution is unique: a point

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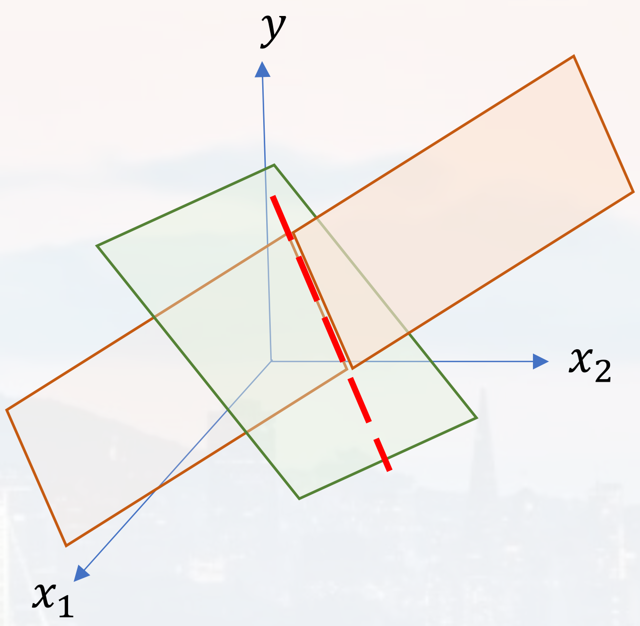

general set of solutions

for n = m → solution is unique: a point

for n > m (more variables than equations)
→ solution is not unique: line, hyperplane

for n < m (more equations than variables)
→ no solution

more general:

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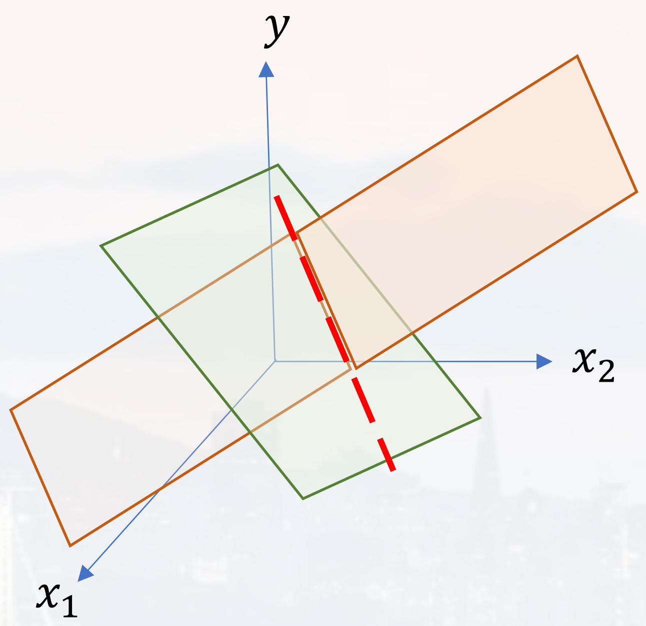

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exceptions!

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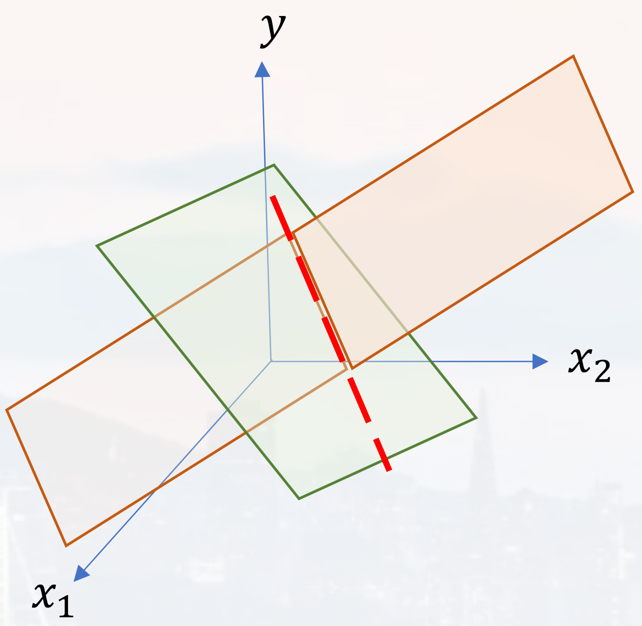

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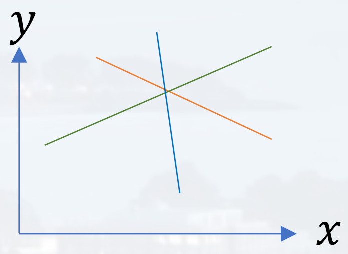

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$$\boxed{A\vec{x} = \vec{c}}$$

$\vec{x}$ = ?

for n = m

$$A^{-1}A\vec{x} = A^{-1}\vec{c}$$

$$\vec{x} = A^{-1}\vec{c}$$

$A = [a_{ij}]$

inverse:	$A^{-1}A = \mathrm{I}$
identity:	$I\ M = M$
transpose:	$[a_{ij}]^T = [a_{ji}]$
symmetry:	$[a_{ij}] = [a_{ji}]$
conjugate transpose:	A^+
unitary:	$A^{-1} = A^+$
idempotency:	$AA = A \rightarrow\ A^n = A$
normal:	$A^+A = AA^+$

solving for x:

$$A\vec{x} = \vec{c}$$

→ need to calculate A^{-1}
→ need to calculate a quantity called

determinant of A, *det(A)*

$$A^{-1} \sim \frac{1}{\det(A)}$$

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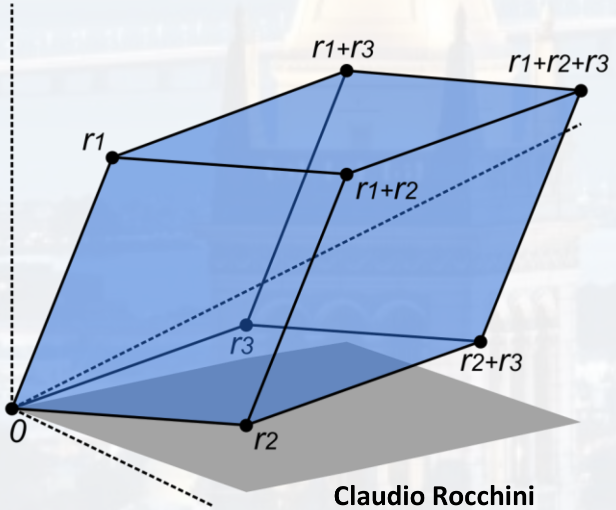
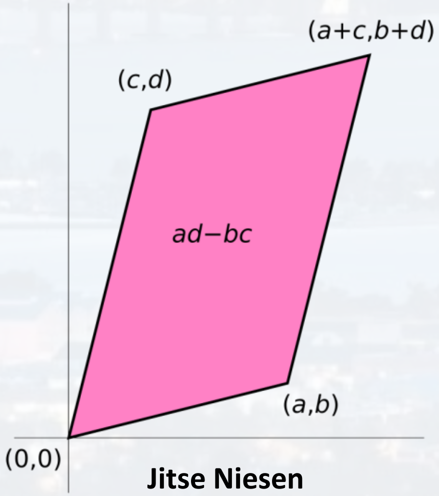
- if *det(A) = 0* → no solution
- |*det(A)*|: volume spanned by the vectors in A



Claudio Rocchini



Jitse Niesen

$$A\vec{x} = \vec{c}$$

solving for x:

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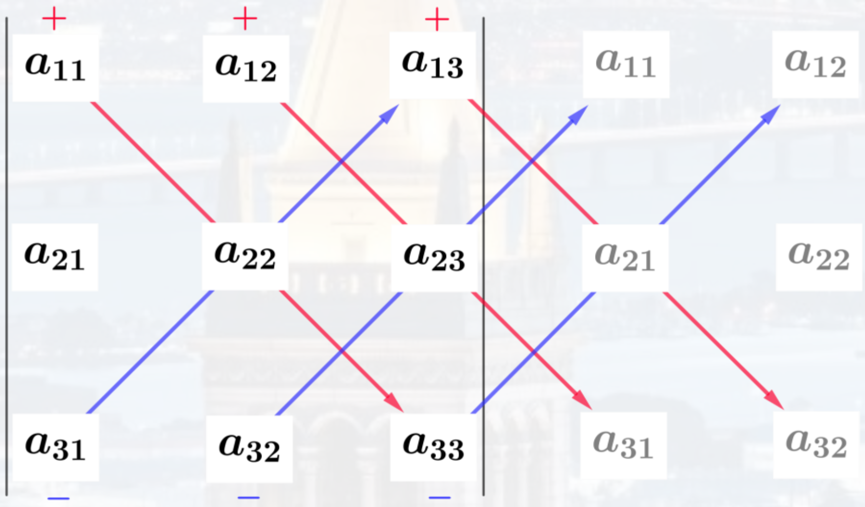

$$\det(A) = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{31}a_{22}a_{13} - a_{32}a_{23}a_{11} - a_{33}a_{21}a_{12}$$

Kmhkmh

solving for x:

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N x N matrix:

$$\det(A) = \sum_{i_1, i_2, \dots, i_n} \varepsilon_{i_1 \dots i_n}\, a_{1,i_1} \dots a_{n\, i_n}$$

where

$$\varepsilon_{i_1 \dots i_n} = \boxed{\prod_{1 \le \mu < \vartheta \le n} \mathrm{sgn}(i_\vartheta - i_\mu)}$$

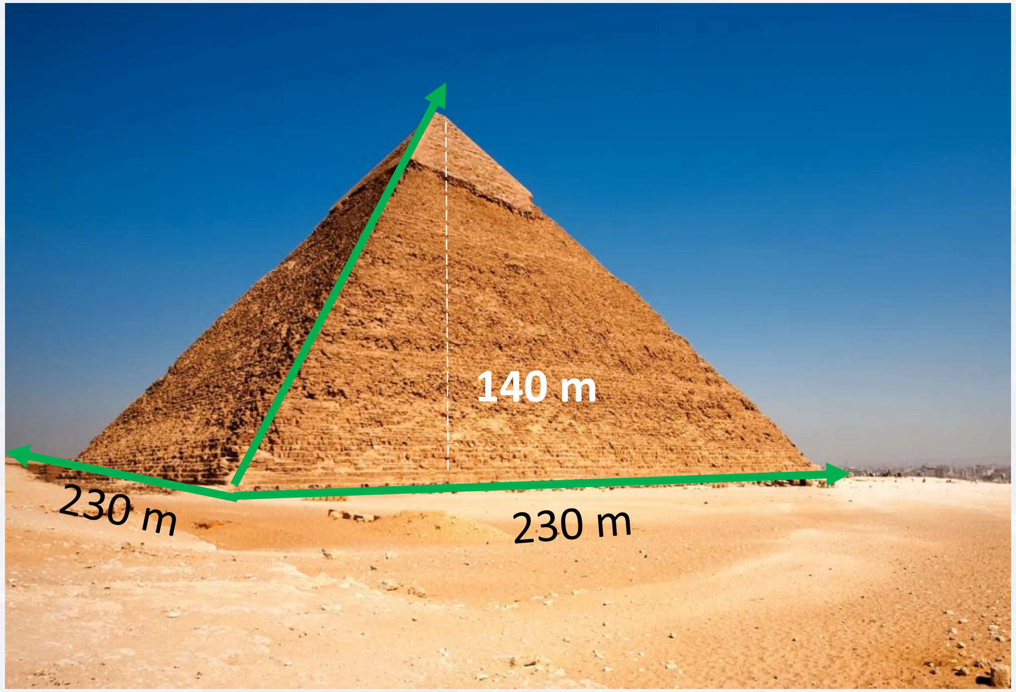
(Levi-Civita symbol)

changing indices does not change |det(A)|

determinant of A, *det(A)*

$$\boxed{A\vec{x} = \vec{c}}$$

inverse:	$A^{-1}A = \mathrm{I}$
identity:	$I\,M = M$
transpose:	$[a_{ij}]^T = [a_{ji}]$
symmetry:	$[a_{ij}] = [a_{ji}]$
conjugate transpose:	A^{+}
unitary:	$A^{-1} = A^{+}$
idempotency:	$AA = A \rightarrow\ A^n = A$
normal:	$A^{+}A = AA^{+}$



$$\varepsilon_{i_1 \ldots i_n} = \prod_{1 \le \mu < \vartheta \le n} \operatorname{sgn}(i_\vartheta - i_\mu)$$

$$V = \left|\det\begin{pmatrix} 230 & 0 & 115 \\ 0 & 230 & 115 \\ 0 & 0 & 140 \end{pmatrix}\right| \frac{1}{3} = \frac{230 * 230 * 140 + 0 + 0\ -\ 0 - 0 - 0}{3} = 2{,}468{,}666\ m^3$$

determinant of A, *det(A)*

$$\varepsilon_{i_1 \dots i_n} = \prod_{1 \le \mu < \vartheta \le n} \operatorname{sgn}(i_\vartheta - i_\mu)$$

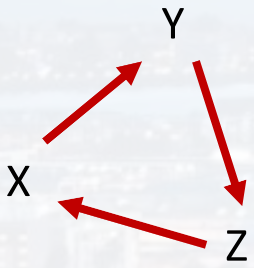
$$V = \left| \det \begin{pmatrix} 230 & 0 & 115 \\ 0 & 230 & 115 \\ 0 & 0 & 140 \end{pmatrix} \right| \frac{1}{3} = \frac{230 * 230 * 140 + 0 + 0 - \;\; 0 - 0 - 0}{3} = 2{,}468{,}666\ m^3$$

volume does not depend on **where** I put my **coord origin**…

$$V = \left| \det \begin{pmatrix} 0 & 230 & 115 \\ 230 & 0 & 115 \\ 0 & 0 & 140 \end{pmatrix} \right| \frac{1}{3} = \left| \frac{0 + 0 + 0 - \;\; 140 * 230 * 230 - 0 - 0}{3} \right| = 2{,}468{,}666\ m^3$$

…or how I **turn** the object!

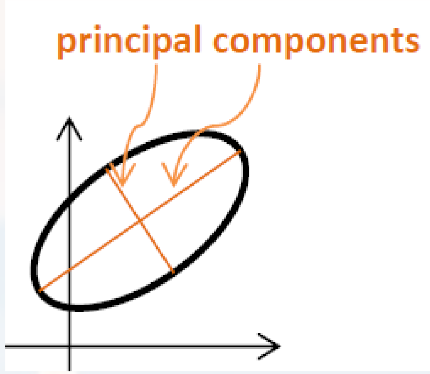
$$V = \left| \det \begin{pmatrix} 115 & 230 & 0 \\ 115 & 0 & 230 \\ 140 & 0 & 0 \end{pmatrix} \right| \frac{1}{3} = \left| \frac{0 + 230 * 230 * 140 + 0 - \;\; 0 - 0 - 0}{3} \right| = 2{,}468{,}666\ m^3$$

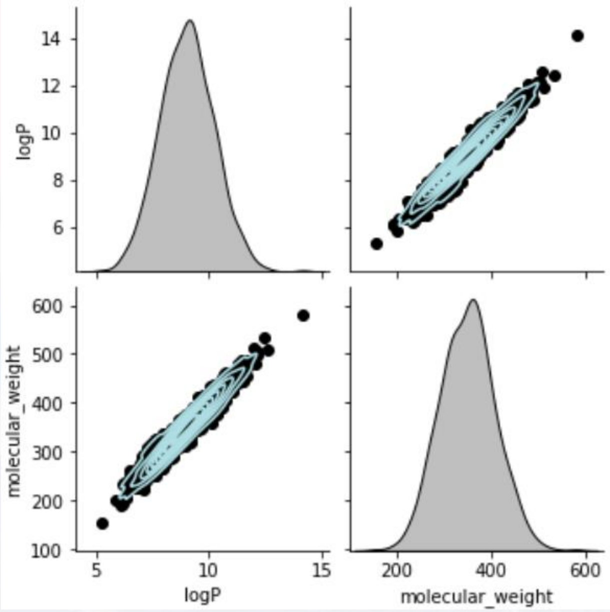


$$V = \left| \det \begin{pmatrix} 140 & 0 & 0 \\ 115 & 230 & 0 \\ 115 & 0 & 230 \end{pmatrix} \right| \frac{1}{3} = \left| \frac{140 * 230 * 230 + 0 + 0 - \;\; 0 - 0 - 0}{3} \right| = 2{,}468{,}666\ m^3$$

eigen coordinates & eigenvalues

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix}$$





A maps *x* to *c*

→ off-diagonal: turns x
→ diagonal: stretches x

→ goal: finding eigenvectors/values of *A*
→ trick: we assume, we have a set of eigenvectors $\vec{v}_i$
→ transforming *A* with *B* = $(\vec{v}_1, \vec{v}_2, \ldots \vec{v}_N)$ should turn *A* into a **diagonal matrix** *D*

$D = B^T AB$

after some algebra: $A\vec{v}_i = \lambda_i \vec{v}_i$ which can be solved with: $\det(A - \lambda_i I) = 0$

eigen coordinates & eigenvalues

$$\boxed{A\vec{v}_i = \lambda_i \vec{v}_i}$$

characteristic equation

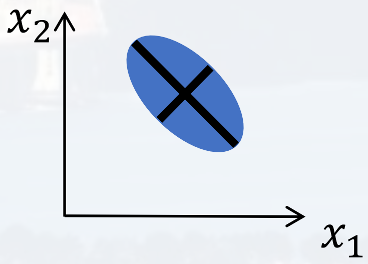
$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix}$$

$\det(A - \lambda_i I) = 0$ solves for eigenvalues λ_i

simple example:

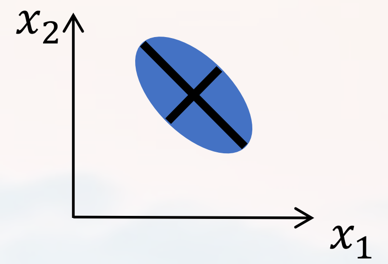
$x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

A= $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$



$$\det(A - \lambda_i I) = 0 = det\left[\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} - \begin{pmatrix} \lambda_i & 0 \\ 0 & \lambda_i \end{pmatrix}\right] = det\left[\begin{pmatrix} 2-\lambda_i & -1 \\ -1 & 2-\lambda_i \end{pmatrix}\right]$$

eigen coordinates & eigenvalues



simple example:

$x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad$ A= $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$

$$\det(M) = \sum_{i_1, i_2, \dots, i_n} \varepsilon_{i_1 \dots i_n} m_{1,i_1} \dots m_{n\, i_n}$$

$\det(A - \lambda_i I)$ = 0 = $det\left[\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}\right.$ - $\left.\begin{pmatrix} \lambda_i & 0 \\ 0 & \lambda_i \end{pmatrix}\right]$ = $det\left[\begin{pmatrix} 2-\lambda_i & -1 \\ -1 & 2-\lambda_i \end{pmatrix}\right]$ = $(2-\lambda_i)^2 - 1$

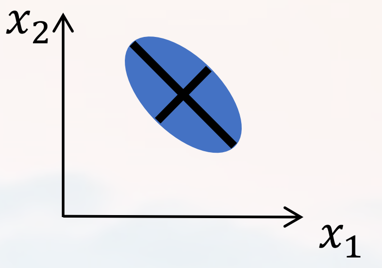
= $\boxed{3 - 4\lambda_i + {\lambda_i}^2 = 0}$ **characteristic polynomial**

N eigenvalues and N eigenvectors for N coordinates

$\boxed{\lambda_1 = 1 \qquad \lambda_2 = 3}$

calculating the eigenvectors: $(A - \lambda_i I)\vec{v_i}$ = 0

eigen coordinates & eigenvalues



simple example:

$x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ A= $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$ $\boxed{\lambda_1 = 1 \qquad \lambda_2 = 3}$

$(A - \lambda_i I)\vec{v_i}$ = 0

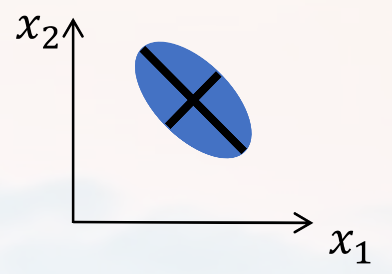
for λ_1

$$\left[\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]\begin{pmatrix} v_{1x} \\ v_{1y} \end{pmatrix} = \begin{pmatrix} v_{1x} & -v_{1y} \\ -v_{1x} & v_{1y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad v_{1x} = v_{1y} \qquad \text{e.g. } \boxed{\vec{v_1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}}$$

for λ_2

$$\left[\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} - \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}\right]\begin{pmatrix} v_{2x} \\ v_{2y} \end{pmatrix} = \begin{pmatrix} -v_{2x} & -v_{2y} \\ -v_{2x} & -v_{2y} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \qquad v_{2x} = -\, v_{2y} \qquad \text{e.g. } \boxed{\vec{v_2} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}}$$

eigen coordinates & eigenvalues



<u>simple example:</u>

$x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad x_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\qquad$ A= $\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$

$\boxed{\lambda_1 = 1 \qquad \lambda_2 = 3}$

$\boxed{\vec{v_1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}}$ $\qquad \boxed{\vec{v_2} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}}$

recall: $B = (\vec{v_1}\ \vec{v_2})$ and D=$B^T \boldsymbol{A} B$

$\lambda_1 = 1$

→A in the new coordinates is $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^T \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ = 2 $\boxed{\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}}$ $\quad \lambda_2 = 3$

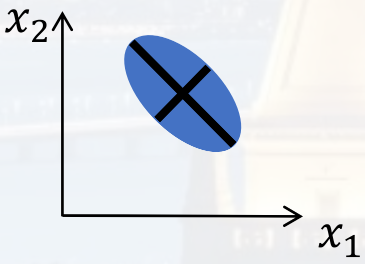
eigen coordinates & eigenvalues

simple example:

$x_1 = \begin{pmatrix}1\\0\end{pmatrix}$ $x_2 = \begin{pmatrix}0\\1\end{pmatrix}$ A= $\begin{pmatrix}2 & -1\\-1 & 2\end{pmatrix}$

$\boxed{\lambda_1 = 1 \qquad \lambda_2 = 3}$ $\boxed{\vec{v_2} = \begin{pmatrix}1\\-1\end{pmatrix}}$ $\boxed{\vec{v_1} = \begin{pmatrix}1\\1\end{pmatrix}}$

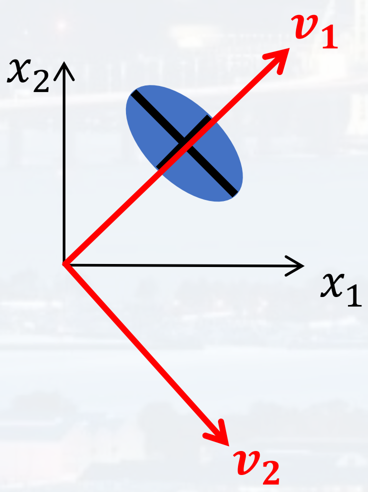
the old coordinates



$A = \begin{pmatrix}2 & -1\\-1 & 2\end{pmatrix}$

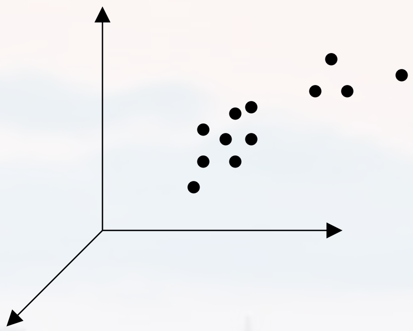
$x_2 = \begin{pmatrix}0\\1\end{pmatrix}$ $x_1 = \begin{pmatrix}1\\0\end{pmatrix}$

the new coordinates



A_{new}= 2 $\begin{pmatrix}1 & 0\\0 & 3\end{pmatrix}$

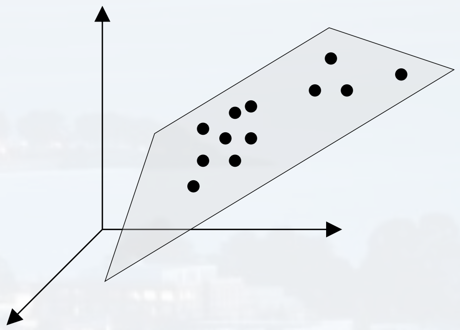
linear regression



idea: data point y_k in N dimensional space

$\rightarrow y_k = f(x_1, \dots x_n, \dots x_N) + \epsilon$ for each data point k

ansatz: $\boxed{y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon}$ ***linear*** combination



y:	response
x:	regressors **(assumed to be independent)**
β:	factors **(how a regressor contributes to the response)**
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

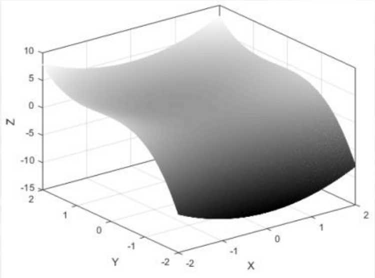
y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

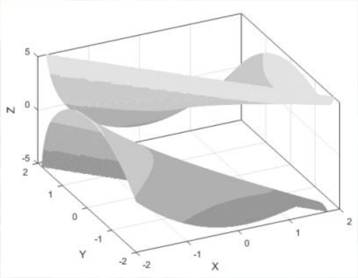
general: linear refers to the **factors**

$y_k = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ 2D plane in 3D space

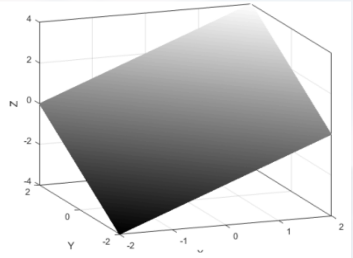
$y_k = \beta_0 + \beta_1 {x_1}^2 + \beta_2 {x_2}^2$ 2D parabolic

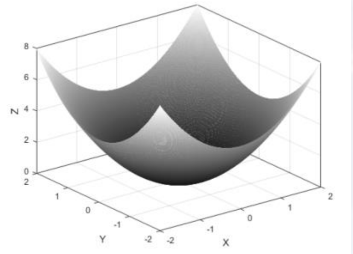
$y_k = \beta_0 + \beta_1 {x_1}^2 - \beta_2 {x_2}^2$ 2D hyperbolic

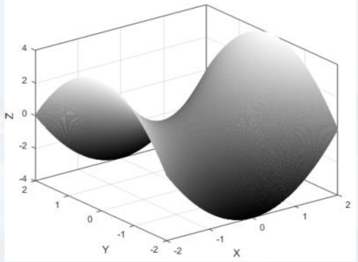




...and many more...





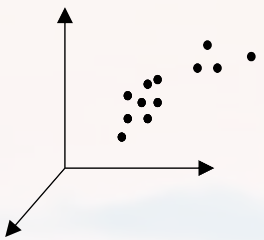


all linear

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

for *K* data points in *N* dimensional space

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

$$\underbrace{\begin{pmatrix} y_1 \\ \dots \\ y_k \\ \dots \\ \dots \\ y_K \end{pmatrix}}_{\text{Y}} = \underbrace{\begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1n} & \dots & x_{1N} \\ \dots & \dots & & & \dots & & \\ 1 & x_{k1} & & & x_{kn} & & \\ 1 & \dots & & & \dots & & \\ 1 & x_{K1} & x_{K2} & \dots & x_{Kn} & \dots & x_{KN} \end{pmatrix}}_{\text{X}} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_n \\ \dots \\ \beta_N \end{pmatrix}}_{\beta} + \underbrace{\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_k \\ \dots \\ \varepsilon_K \end{pmatrix}}_{\varepsilon}$$

$$\boxed{Y = X\beta + \varepsilon}$$

<u>fitting:</u> finding the best β in terms of minimizing the errors

$$(Y - X\beta)^T (Y - X\beta) = \sum_k {\varepsilon_k}^2$$

the model

$$\frac{\partial}{\partial \beta} \sum_k {\varepsilon_k}^2 = 0 \longrightarrow \beta_{best} = \hat{\beta} = (X^T X)^{-1} X^T Y \longrightarrow \boldsymbol{\hat{Y} = X\hat{\beta}} = X(X^T X)^{-1} X^T Y$$

X and Y are all observables

M. Hohle:

Thank you for your attention!