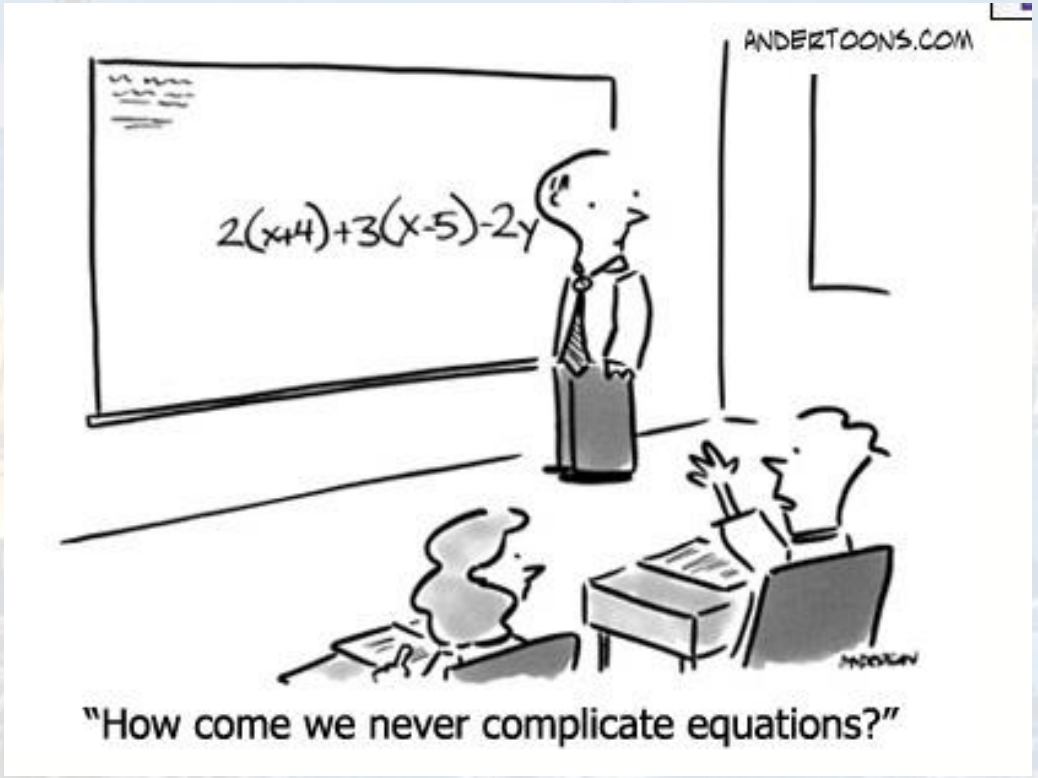
Berkeley
UNIVERSITY OF CALIFORNIA

M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



Introduction to Computational Techniques in Physics: syllabus

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**:

$$y_1 = a_1 x_1 + c_1$$

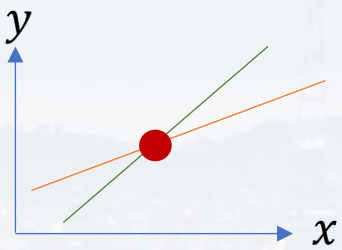
$$y_2 = a_2 x_2 + c_2$$

$$x_1 = x_2 \qquad y_1 = y_2$$

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

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

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



finding the intersection of **three planes**:

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

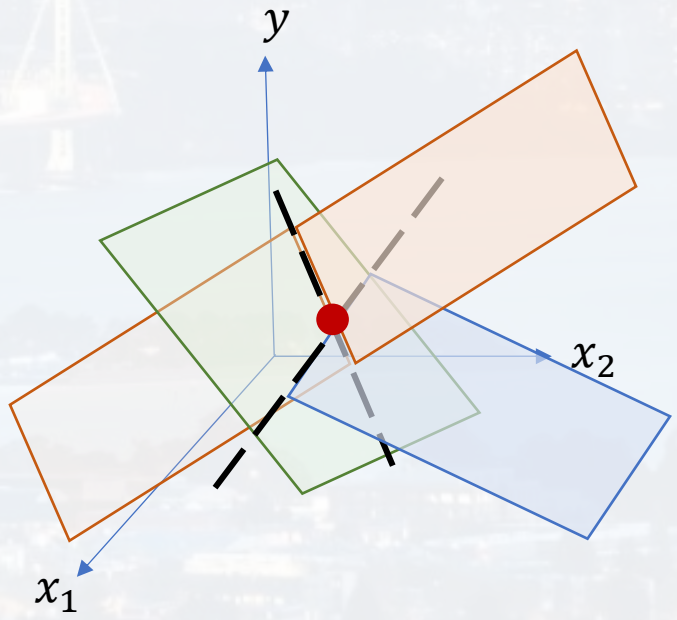
$$y_2 = a_{21} x_{21} + a_{22} x_{22} + c_2$$

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

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

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

$$y_1 = y_2 = y_3 = y$$

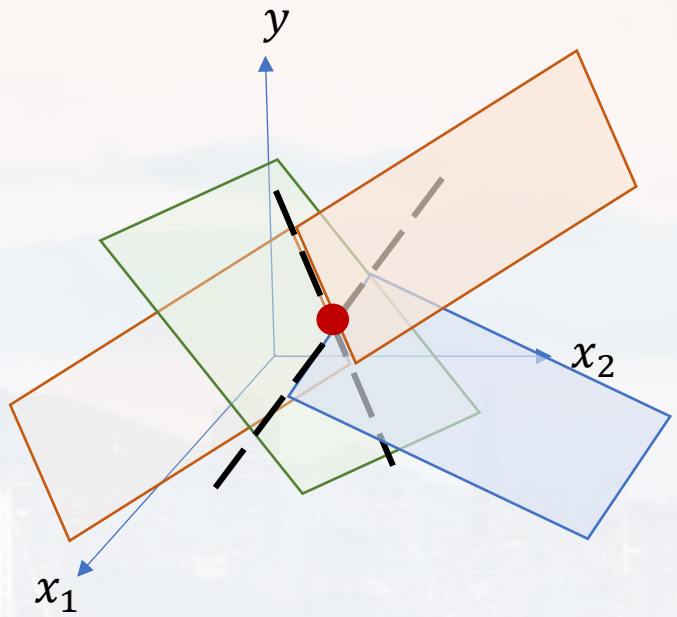


more general:

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

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

$$y_1 = y_2 = y_3 = y$$



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

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

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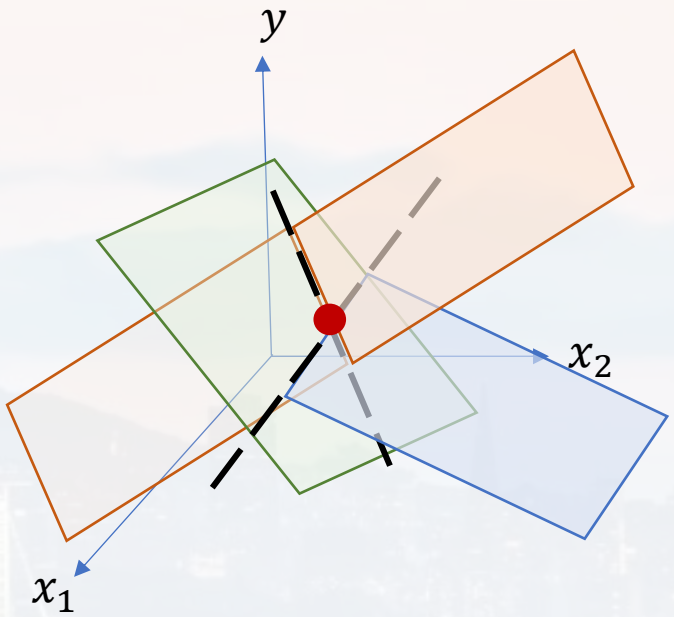
A $\quad \vec{x} \quad \vec{c}$



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

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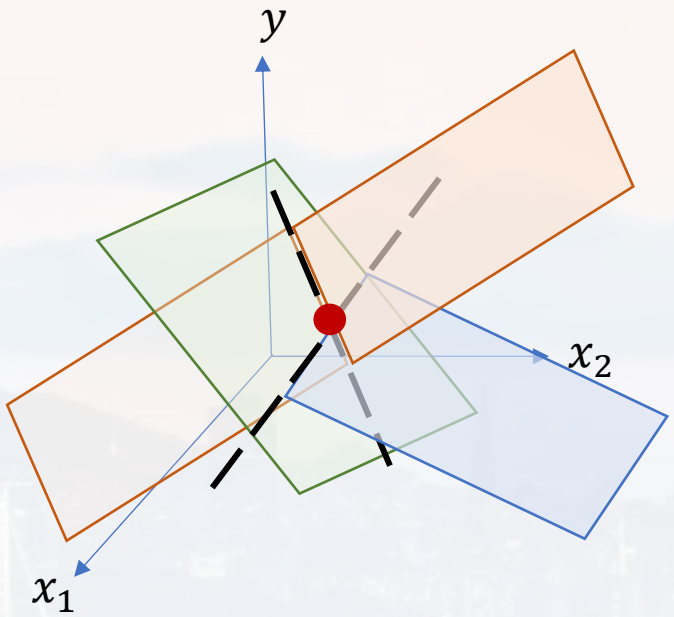

general set of solutions

for n = m → solution is unique: a point

more general:

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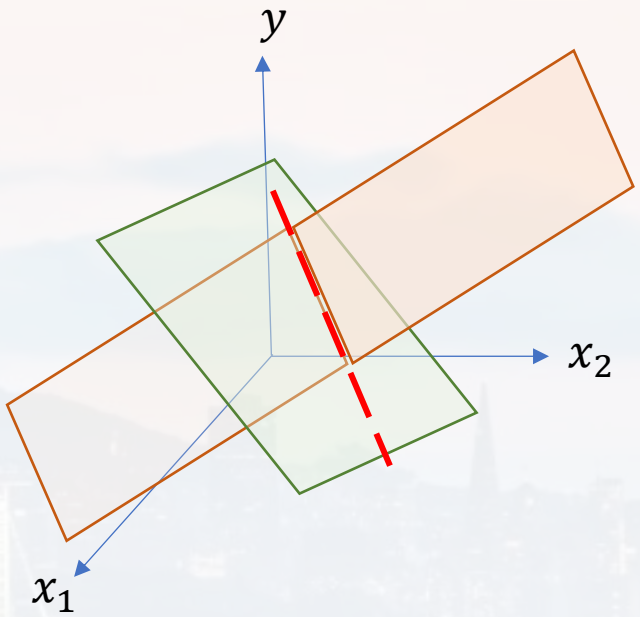

general set of solutions

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

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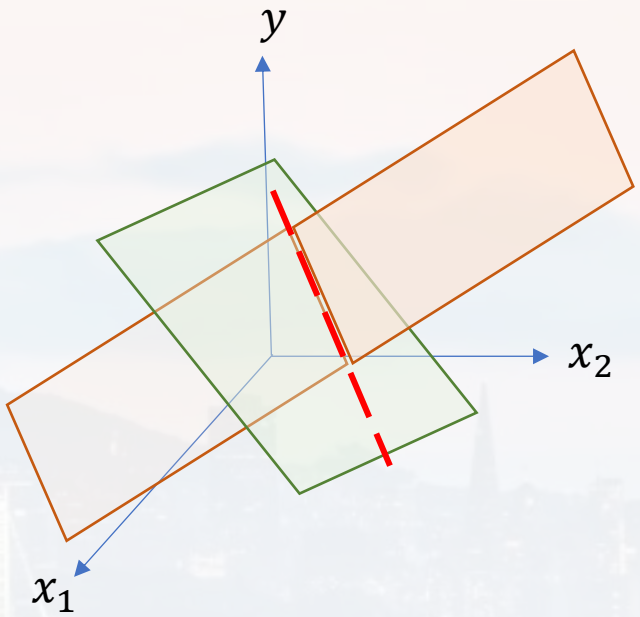

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exceptions!

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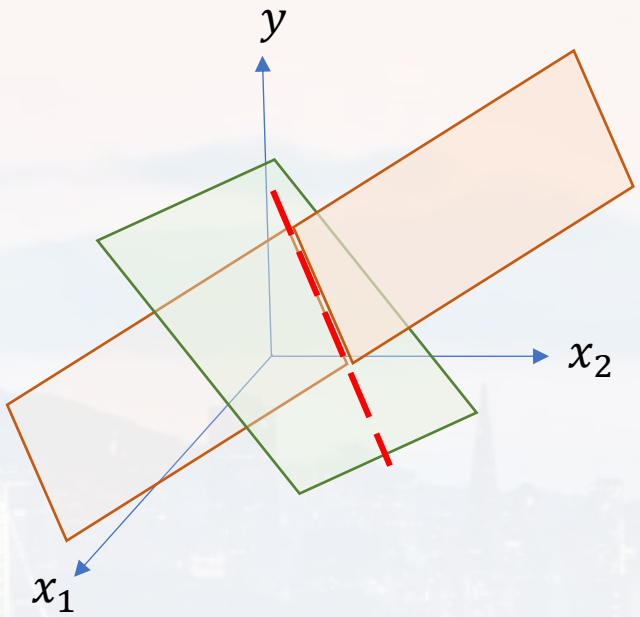

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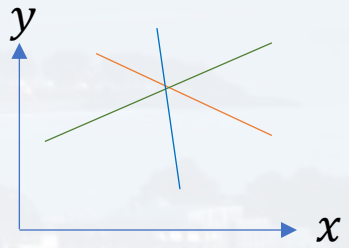

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A $\quad \vec{x} \quad \vec{c}$

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

$\vec{x}$ = ?

for n = m

$$A = [a_{ij}]$$

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

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

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:	$A^+A = AA^+$

Introduction to Computational Techniques in Physics:

solving for x:

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

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

determinant of A, *det(A)*

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

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

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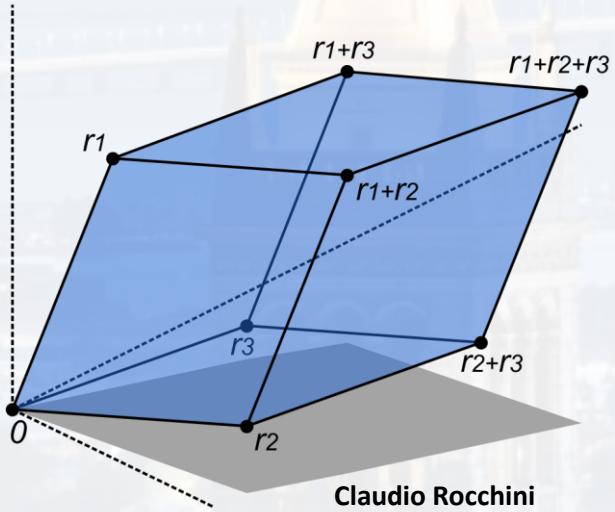
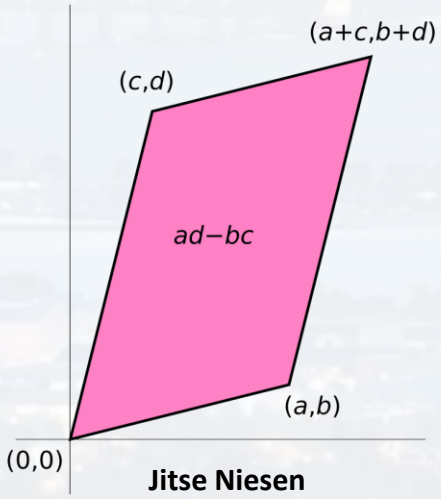


Claudio Rocchini



Jitse Niesen

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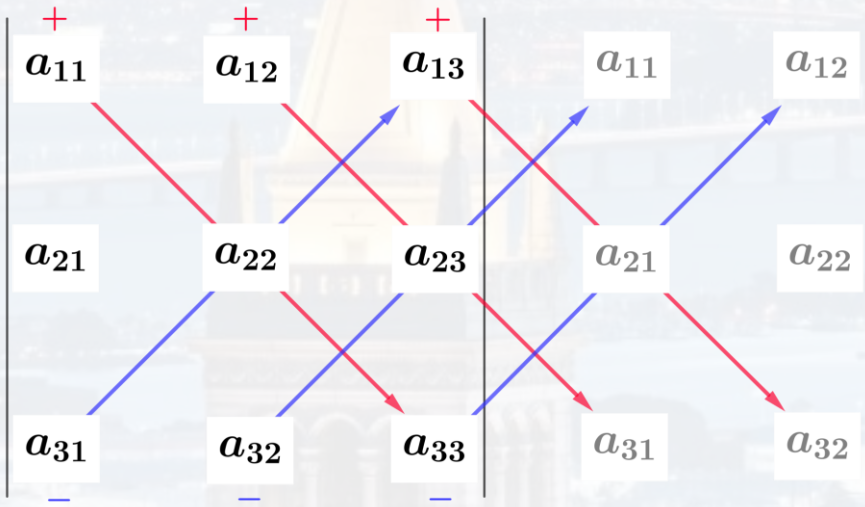

$$\det(A) = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{31}a_{22}a_{13} - a_{32}a_{23}a_{11} - a_{33}a_{21}a_{12}$$

Kmhkmh

solving for x:

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N x N matrix:

$$\det(A) = \sum_{i_1, i_2, \ldots, i_n} \varepsilon_{i_1 \ldots i_n} a_{1,i_1} \ldots a_{n\, i_n} \qquad \text{where} \qquad \varepsilon_{i_1 \ldots i_n} = \prod_{1 \le \mu < \vartheta \le n} \mathrm{sgn}(i_\vartheta - i_\mu)$$

(Levi-Civita symbol)

changing indices does not change |det(A)|

determinant of A, *det(A)*

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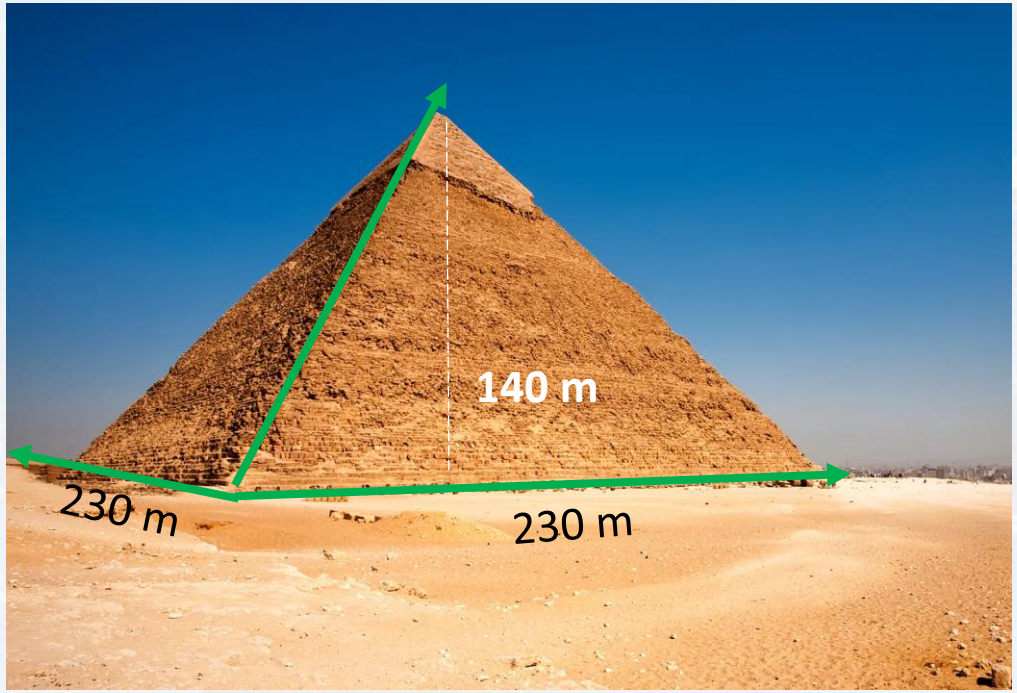


$$\varepsilon_{i_1 \ldots i_n} = \prod_{1 \le \mu < \vartheta \le n} \operatorname{sgn}(i_\vartheta - i_\mu)$$

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

determinant of A, *det(A)*

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

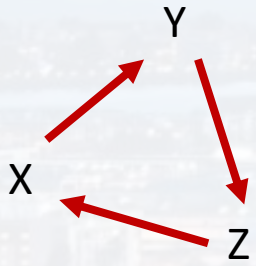
volume does not depend on **where** I put my **coord origin**…

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

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

…or how I **turn** the object!

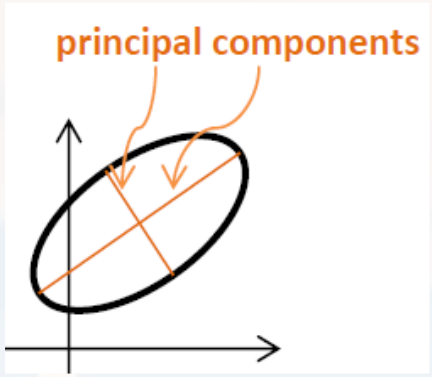
$$V = \left| \det \begin{pmatrix} 115 & 230 & 0 \\ 115 & 0 & 230 \\ 140 & 0 & 0 \end{pmatrix} \right| \frac{1}{3} = \left| \frac{0 + 230 * 230 * 140 + 0 \; - \; 0 - 0 - 0}{3} \right| = 2{,}468{,}666\ m^3$$

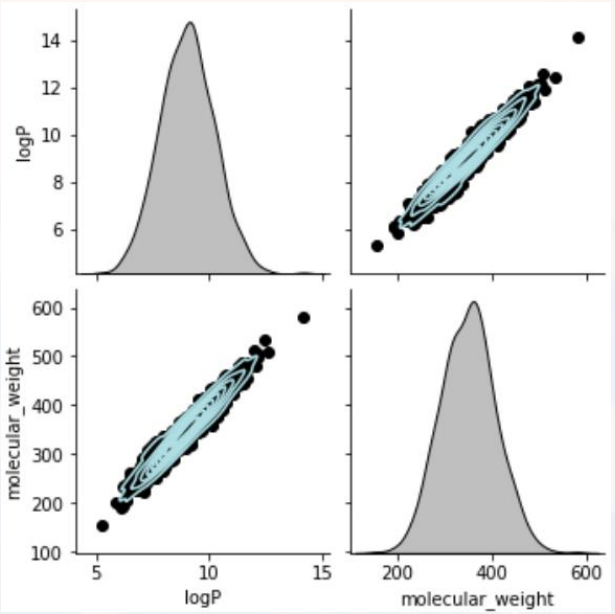


$$V = \left| \det \begin{pmatrix} 140 & 0 & 0 \\ 115 & 230 & 0 \\ 115 & 0 & 230 \end{pmatrix} \right| \frac{1}{3} = \left| \frac{140 * 230 * 230 + 0 + 0 \; - \; 0 - 0 - 0}{3} \right| = 2{,}468{,}666\ m^3$$

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

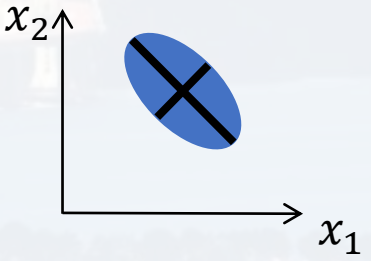
$$A\vec{v}_i = \lambda_i \vec{v}_i$$ **characteristic equation**

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

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

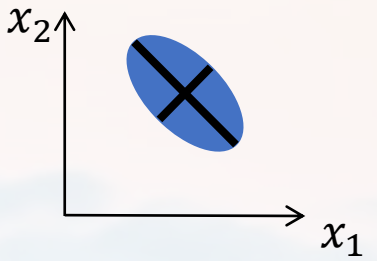
simple example:

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



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

eigen coordinates & eigenvalues



simple example:

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

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

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

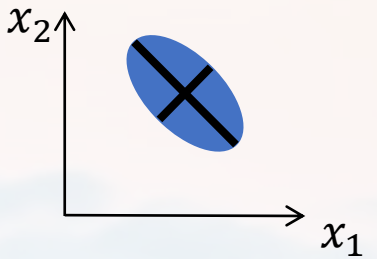
$= \boxed{3 - 4\lambda_i + \lambda_i^{\,2} = 0}$ **characteristic polynomial**

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:

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

$$\lambda_1 = 1 \qquad \lambda_2 = 3$$

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

for λ_1

$$\left[\begin{pmatrix}2 & -1\\-1 & 2\end{pmatrix} - \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\right]\begin{pmatrix}v_{1x}\\v_{1y}\end{pmatrix} = \begin{pmatrix}v_{1x} & -v_{1y}\\-v_{1x} & v_{1y}\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix} \qquad v_{1x} = v_{1y}$$

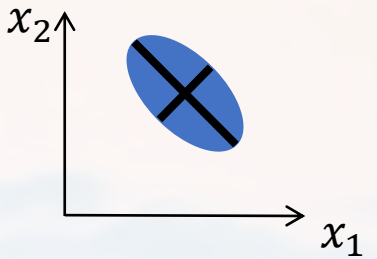
e.g. $\vec{v_1} = \begin{pmatrix}1\\1\end{pmatrix}$

for λ_2

$$\left[\begin{pmatrix}2 & -1\\-1 & 2\end{pmatrix} - \begin{pmatrix}3 & 0\\0 & 3\end{pmatrix}\right]\begin{pmatrix}v_{2x}\\v_{2y}\end{pmatrix} = \begin{pmatrix}-v_{2x} & -v_{2y}\\-v_{2x} & -v_{2y}\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix} \qquad v_{2x} = -v_{2y}$$

e.g. $\vec{v_2} = \begin{pmatrix}1\\-1\end{pmatrix}$

eigen coordinates & eigenvalues



simple example:

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

$\lambda_1 = 1 \qquad \lambda_2 = 3$

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

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 $\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$

$\lambda_2 = 3$

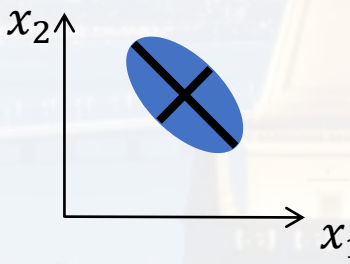
eigen coordinates & eigenvalues

simple example:

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

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

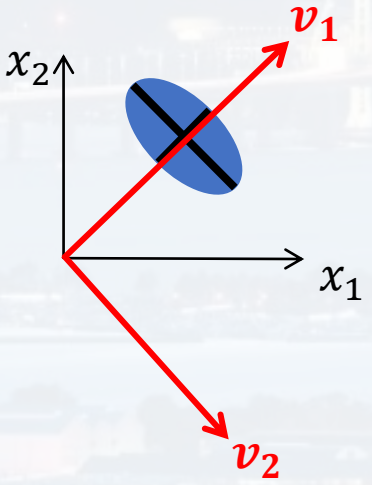
the old coordinates



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

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

the new coordinates

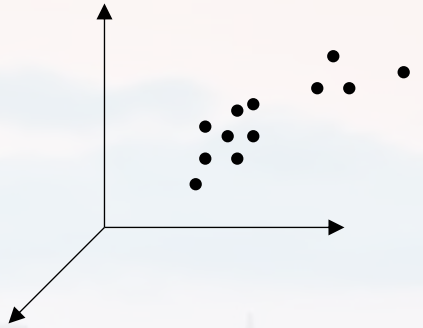


$A_{new} = 2\begin{pmatrix}1 & 0\\0 & 3\end{pmatrix}$

linear regression

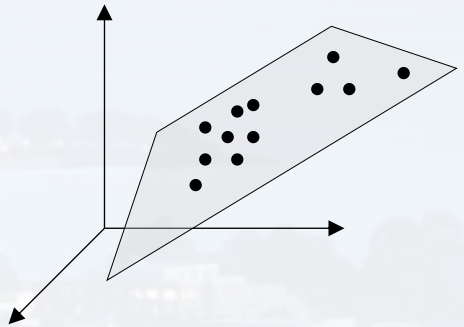
idea: data point y_k in *N* dimensional space

$\rightarrow y_k = f(x_1, \dots x_n, \dots x_N) + \epsilon$ 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.)**



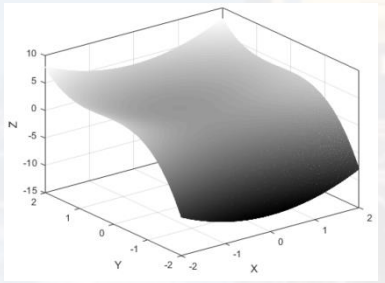
y:	**response**
x:	**regressors**
β:	**factors**
β_0:	**intercept**
ε:	**error**

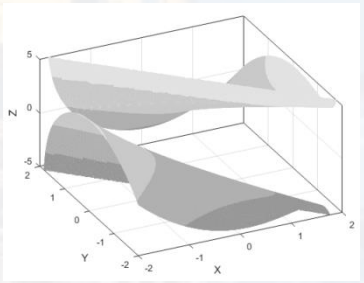
general: linear refers to the **factors**

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

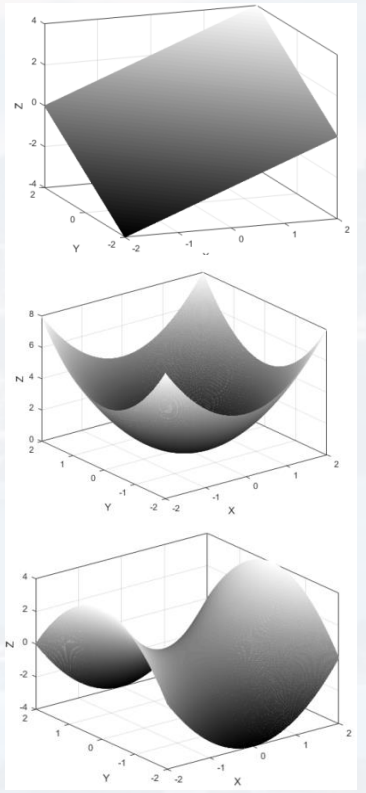
$y_k = \beta_0 + \beta_1 {x_1}^2 + \beta_2 {x_2}^2$ 2*D* parabolic

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





...and many more...

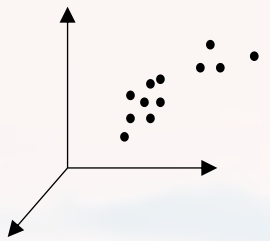


all linear

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

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**
β_0:	**intercept**
ε:	**error**

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

Y X β ε

$$Y = X\beta + \varepsilon$$

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

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

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

the model

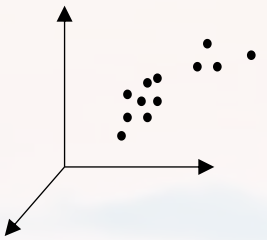
$$\hat{Y} = X\hat{\beta} = X(X^T X)^{-1} X^T Y$$

X and Y are all observables

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

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

$$Y = X\beta + \varepsilon$$



y:	**response**
x:	**regressors**
β:	**factors**
β_0:	**intercept**
ε:	**error**

check out `Walk_Through_LinRegression.ipynb`

predicting **toxicity of molecules** based on their features

Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	toxicity_score
0	341.704	2.65585	3.09407	2	9.11147	80.9281
1	335.951	3.22262	2.89039	7	8.92848	83.4911
2	235.203	2.44115	2.48203	1	6.49731	61.8406
3	246.505	2.76656	2.71547	7	7.45089	57.0538
4	437.939	3.4801	3.59569	3	10.9156	131.326

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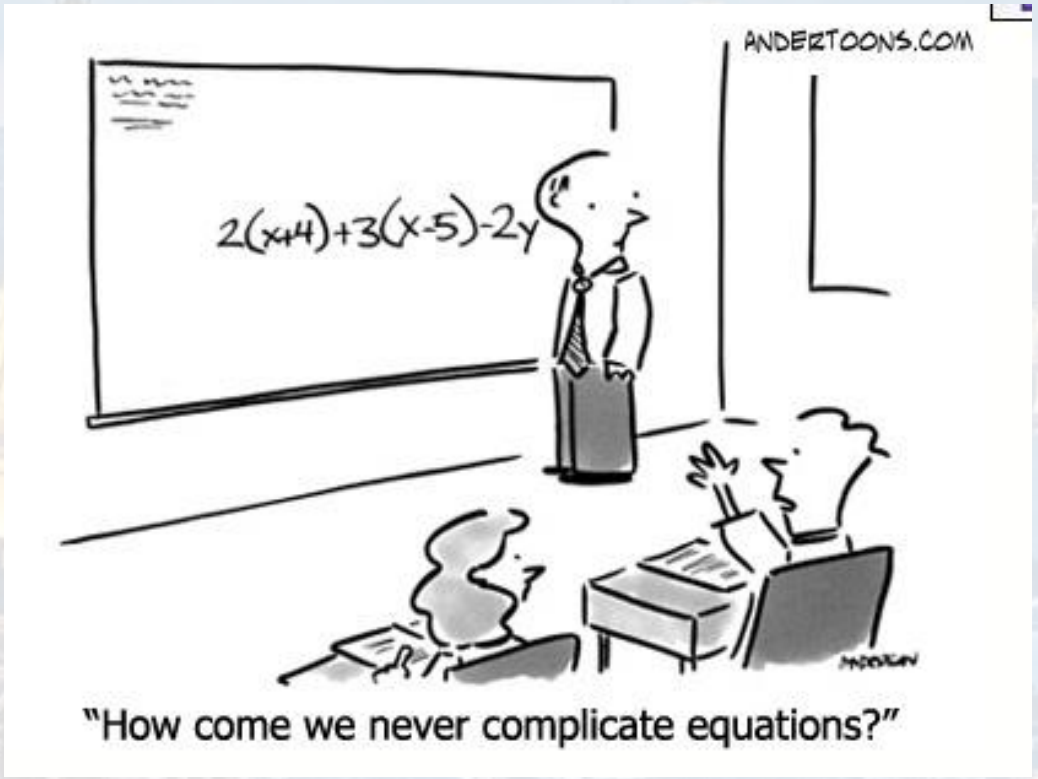
M. Hohle:

Thank you for your attention!