Conditioning

GeoComput & ML

28 Apr. 2022

Transition

Transition

Transition

- Independent Thinking
- Innovative Solutions

Disruption

Logistics

who am I

- fellowship
- perspectives
- self-enrichment

Logistics

Interactions

- voice yourself
- in-class hours
- Matera times

Logistics

Class structure

- begins at sharp hours
- duration : 45~50 min
- two breaks

Logistics

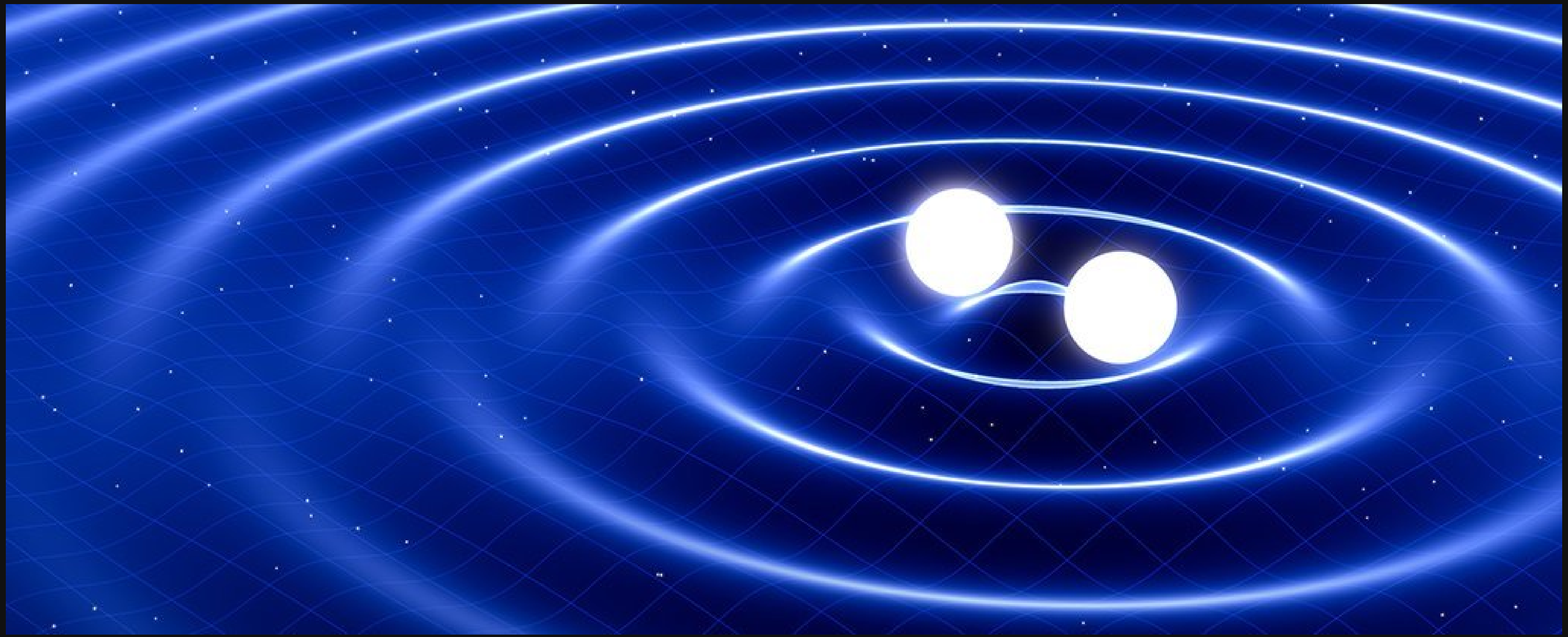
Questions

- in lecture notes
- respond to the interesting
- in class activity
- l.shen@spatial-ecology.net

Modelling

Motivation

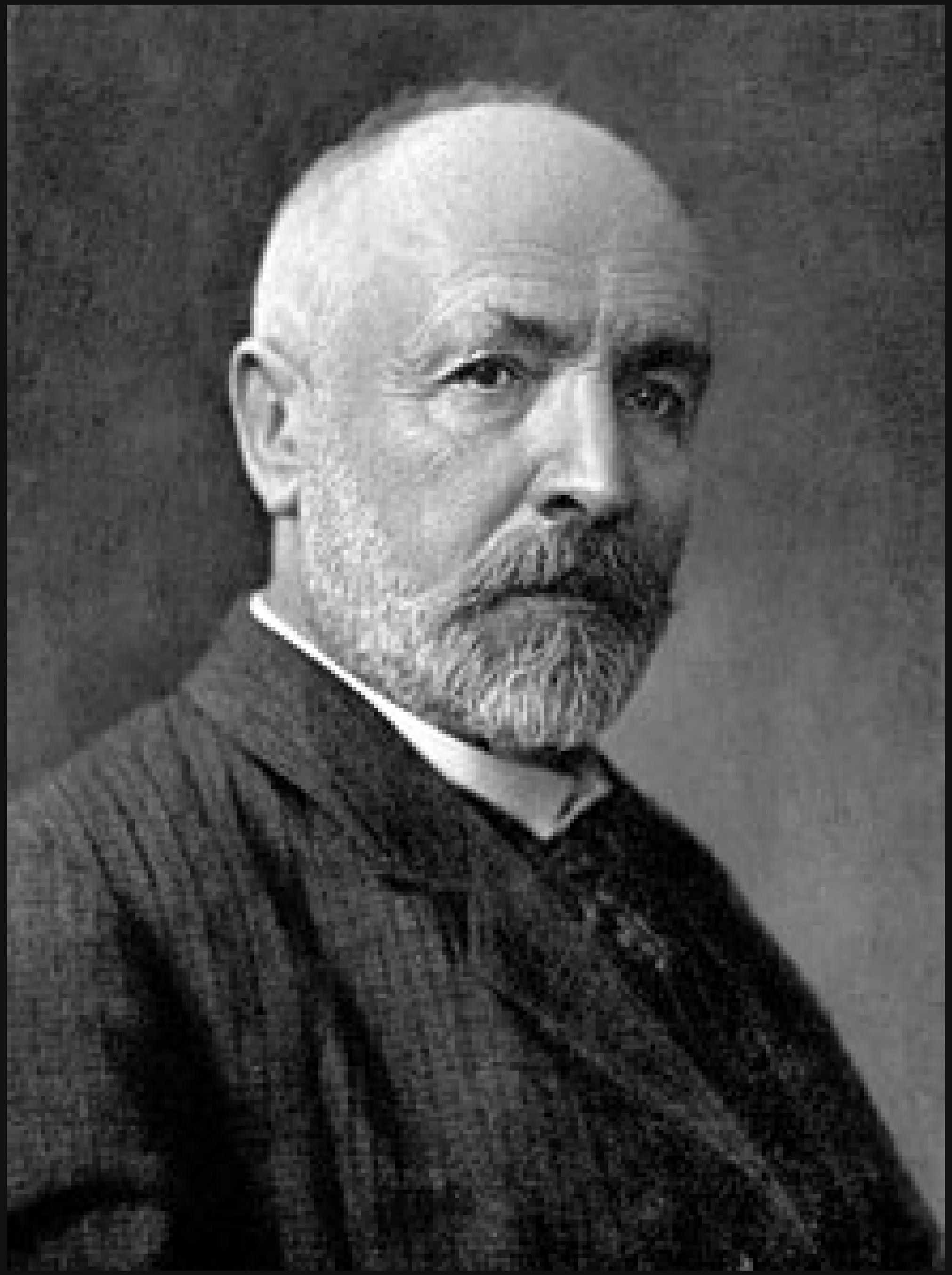
- do the impossible



Pillars

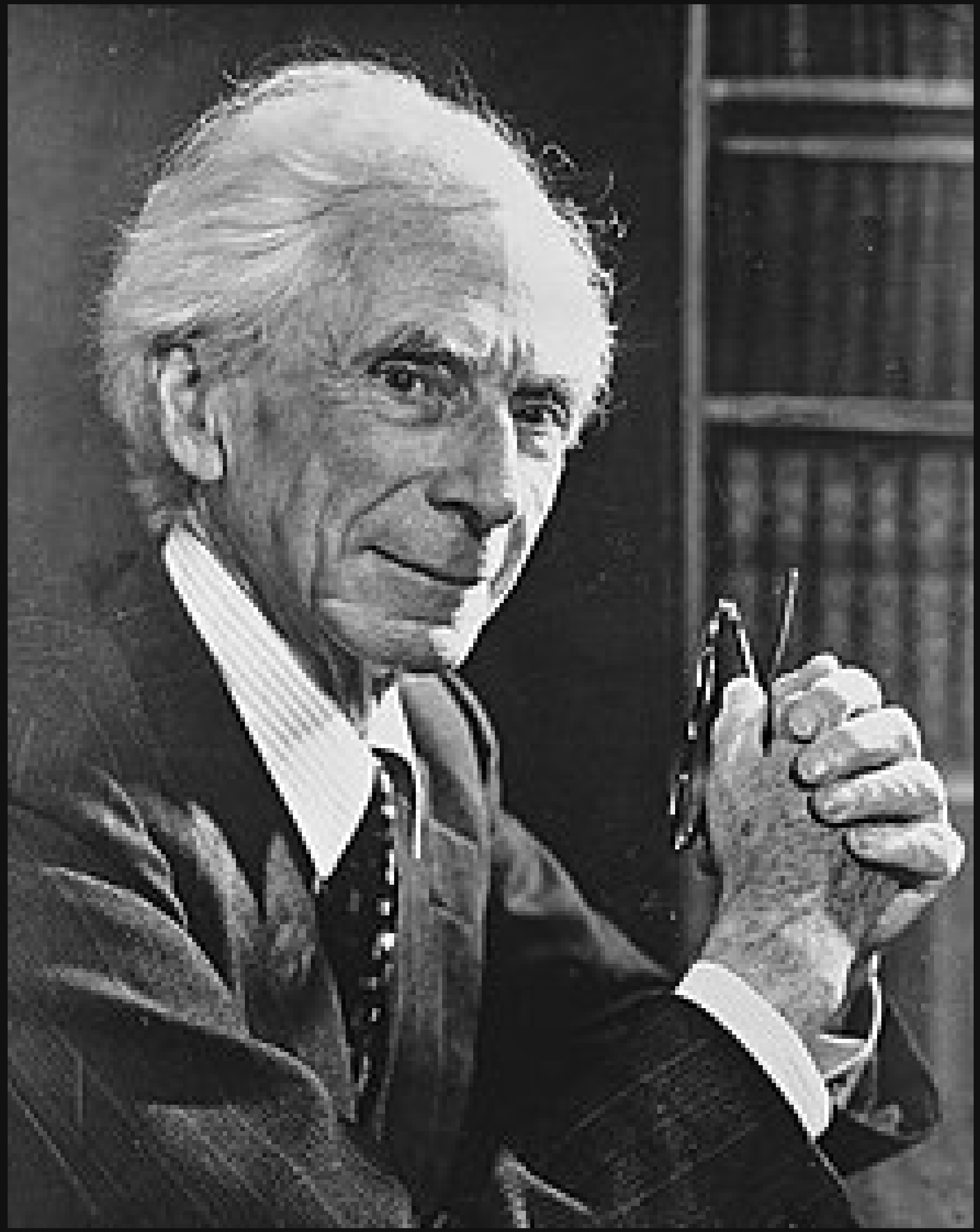
- Domain Knowledge
- Mathematics
- Scientific Computing

Set Theory



Georg Cantor

Set Theory



Bertrand Russell

Set Theory

A barber shaves those who only do NOT shave themselves

Incompleteness Theorem

Kurt Gödel

Computing

- Arithmetic
- Algorithms
- Analytics

Arithmetic

Definition

$$x = \pm \left(d_0 + \frac{d_1}{\beta^1} + \frac{d_2}{\beta^2} + \ldots + \frac{d_{p-1}}{\beta^{p-1}} \right) \beta^E$$

β : base

p : precision

$[L, U]$: exponent range

$$0 \leq d_i \leq \beta - 1$$

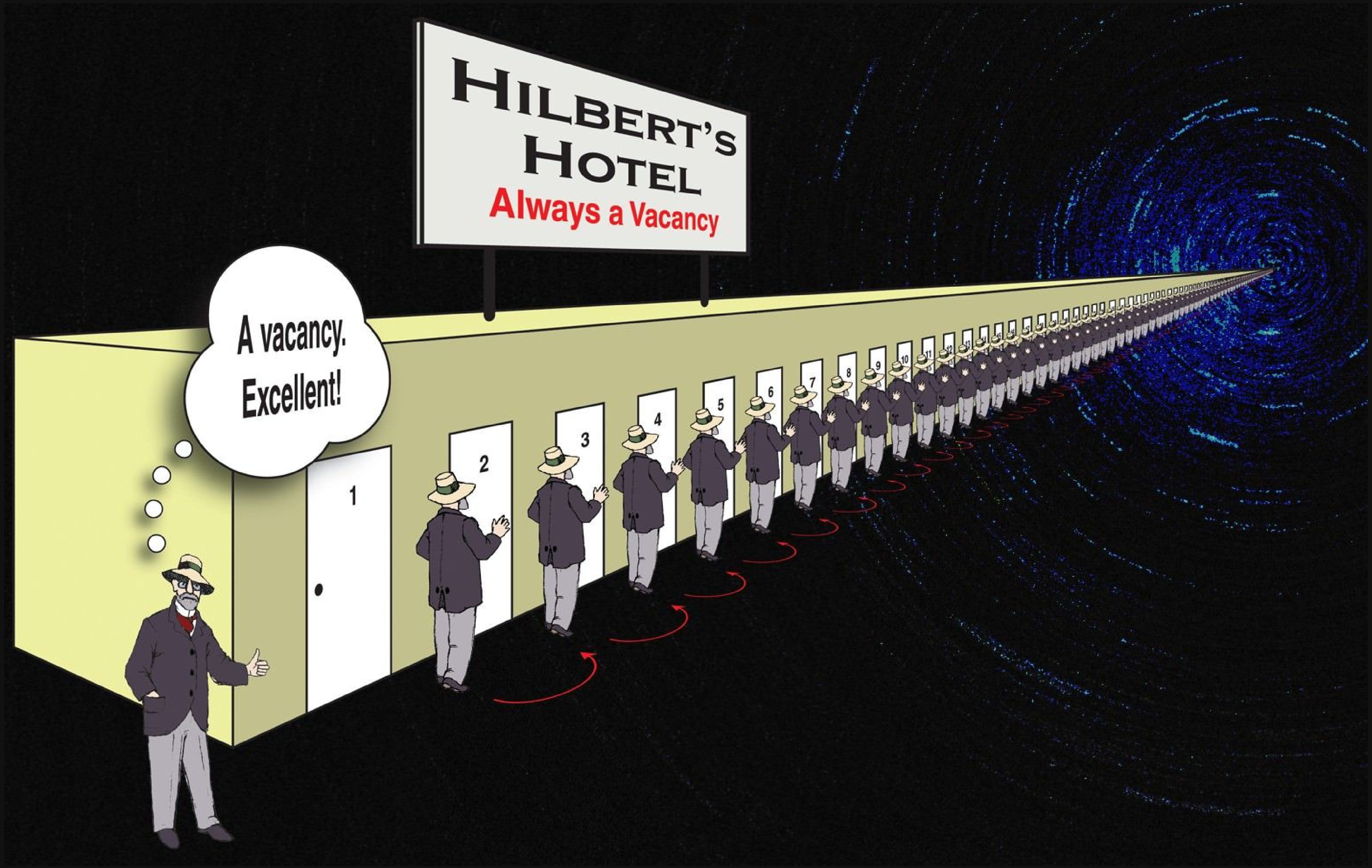
$$i = 0, \ldots, p - 1$$

$$E \in [L, U]$$

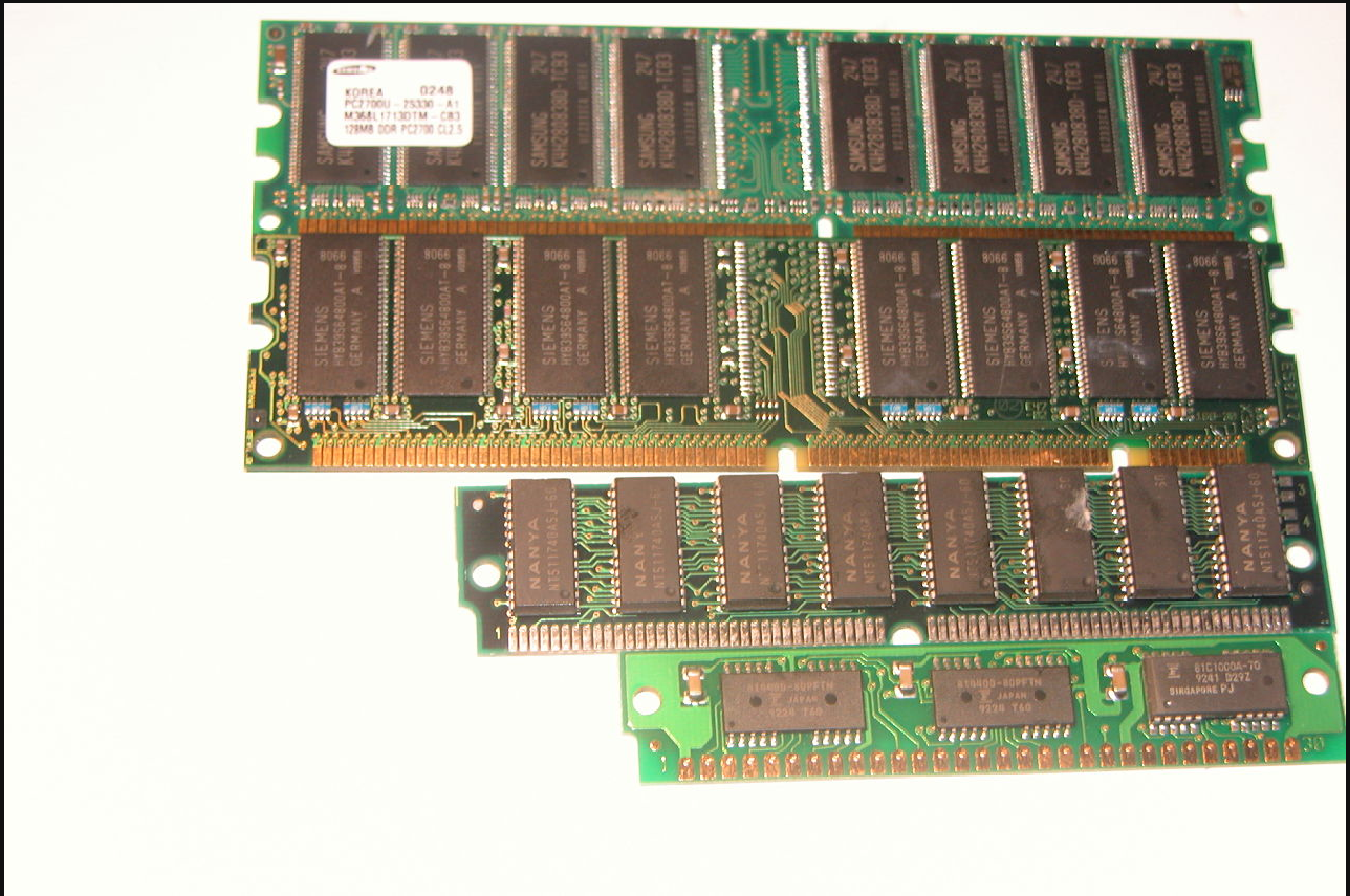
Machine Precision

finite and discrete

Machine Precision



Machine Precision



Machine Precision

let $x = 1/n,\ n \in \mathbb{Z}$, show $(n+1)x - 1 = x$

```
for n in range(1 , 11) :
  x = 1/n
  xin = x
  for k in range (30) :
    x = (n + 1)*x - 1
  print(n,xin,x)
```

```
1 1.0 1.0
2 0.5 0.5
3 0.3333333333333333 -21.0
4 0.25 0.25
5 0.2 6545103.021815777
6 0.16666666666666666 -476641800.7969146
7 0.14285714285714285 -9817068105.0
8 0.125 0.125
9 0.1111111111111111 4934324553889.695
10 0.1 140892568471739.25
```

Machine Precision

$$\left(d_0 + \frac{d_1}{\beta^1} + \frac{d_2}{\beta^2} + \ldots + \frac{d_{p-1}}{\beta^{p-1}} \right) \beta^E$$

$$\in [\beta^E, \beta^{(E+1)}]$$

Machine Precision

relative error

$$\in \left[\frac{(\beta/2)\beta^{-p}\beta^{E}}{\beta^{(E+1)}}, \frac{(\beta/2)\beta^{-p}\beta^{E}}{\beta^{E}} \right]$$

$$\in [(1/2)\beta^{-p}, (\beta/2)\beta^{-p}]$$

Machine Precision

therefore

$$\boxed{\epsilon_{mach} = \beta^{1-p}/2}$$

Operations

$$\texttt{fl}(x \ \texttt{op} \ y) = (x \ \texttt{op} \ y)(1 + \delta)$$

where $|\delta| \leq \epsilon_{mach}$,

$\texttt{fl}$ denotes floating representation and

$\texttt{op}$ denotes any elementary arithmetic operations, +, -, x and /.

Operations

Example

$$
\begin{aligned}
\texttt{fl}(x(y+z)) &= \texttt{fl}((x+(y+z)(1+\delta_1))(1+\delta_2)) \\
&= x(y+z)(1+\delta_1+\delta_2+\delta_1\delta_2) \\
&\approx x(y+z)(1+\delta_1+\delta_2) \\
&\leq x(y+z)(2\epsilon_{mach})
\end{aligned}
$$

Operations

Catastrophic Cancellation

```
import math
def funexp(x,order) :
  ex = 1
  for i in range(1 , order + 1):
    ex = ex + math.pow(x,i)/math.factorial(i)
  return (ex)
ex = funexp(-4,10)
print(ex)
print(math.pow(math.e,-4))
```

```
0.09671957671957698
0.018315638888734186
```

Operations

Computing Residuals

Suppose we obtained the solution $\hat{x}$ for a linear system $ax = b$.
We are to compute the residual $r = b - a\hat{x}$

$$\texttt{fl}(a\hat{x}) = a\hat{x}(1 + \delta_1)$$

$$\begin{aligned}
\texttt{fl}(b - a\hat{x}) &= (b - a\hat{x})(1 + \delta_1)(1 + \delta_2) \\
&= (r - a\hat{x}\delta_1)(1 + \delta_2) \\
&= r(1 + \delta_2) - a\hat{x}\delta_1 - a\hat{x}\delta_1\delta_2 \\
&\approx r(1 + \delta_2) - b\delta_1
\end{aligned}$$

Conditioning

Question

well-posed, if its solution

- exists
- unique
- depends continuously on the data

Question

algorithm : stable

solution : well-conditioned

Errors

$$\begin{aligned}\text{total errors} &= \hat{f}(\hat{x}) - f(x) \\ &= (\hat{f}(\hat{x}) - f(\hat{x})) + (f(\hat{x}) - f(x)) \\ &= \text{computation error} + \text{data error}\end{aligned}$$

Errors

forward error : $\Delta y = \hat{y} - y$

backward error : $\Delta x = \hat{x} - x$, where $f(\hat{x}) = \hat{y}$

Errors

Example :

$$cos(x) = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} \dots$$

$$\hat{y} = \hat{f}\,(x) = 1 - \frac{x^2}{2}$$

for $x = 1$, we have

$$\left.\begin{array}{l} y = f(1) \approx 0.5403 \\ \hat{y} = \hat{f}\,(1) = 0.5 \end{array}\right\} \Rightarrow \Delta y = \hat{y} - y = -0.0403$$

$$\Delta x = \hat{x} - x = arccos(\hat{y}) - x = 0.0472$$

Condition number

a measure on the effects on the solution incurred by data perturbation

$$\left|\frac{\Delta y/y}{\Delta x/x}\right| \approx \left|\frac{xf'(x)}{f(x)}\right|$$

Condition number

Question :

what is the condition number for the inverse function?

$$g(y) = f^{-1}(y)$$

Linear System

$$\boldsymbol{Ax} = \boldsymbol{b}$$

cond($\boldsymbol{A}$) = $\|\boldsymbol{A}\| \, \|\boldsymbol{A}\|^{-1}$

Linear System

induced matrix norm

$$\|\boldsymbol{A}\| = \max_{\boldsymbol{x} \neq \boldsymbol{0}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|}$$

Linear System

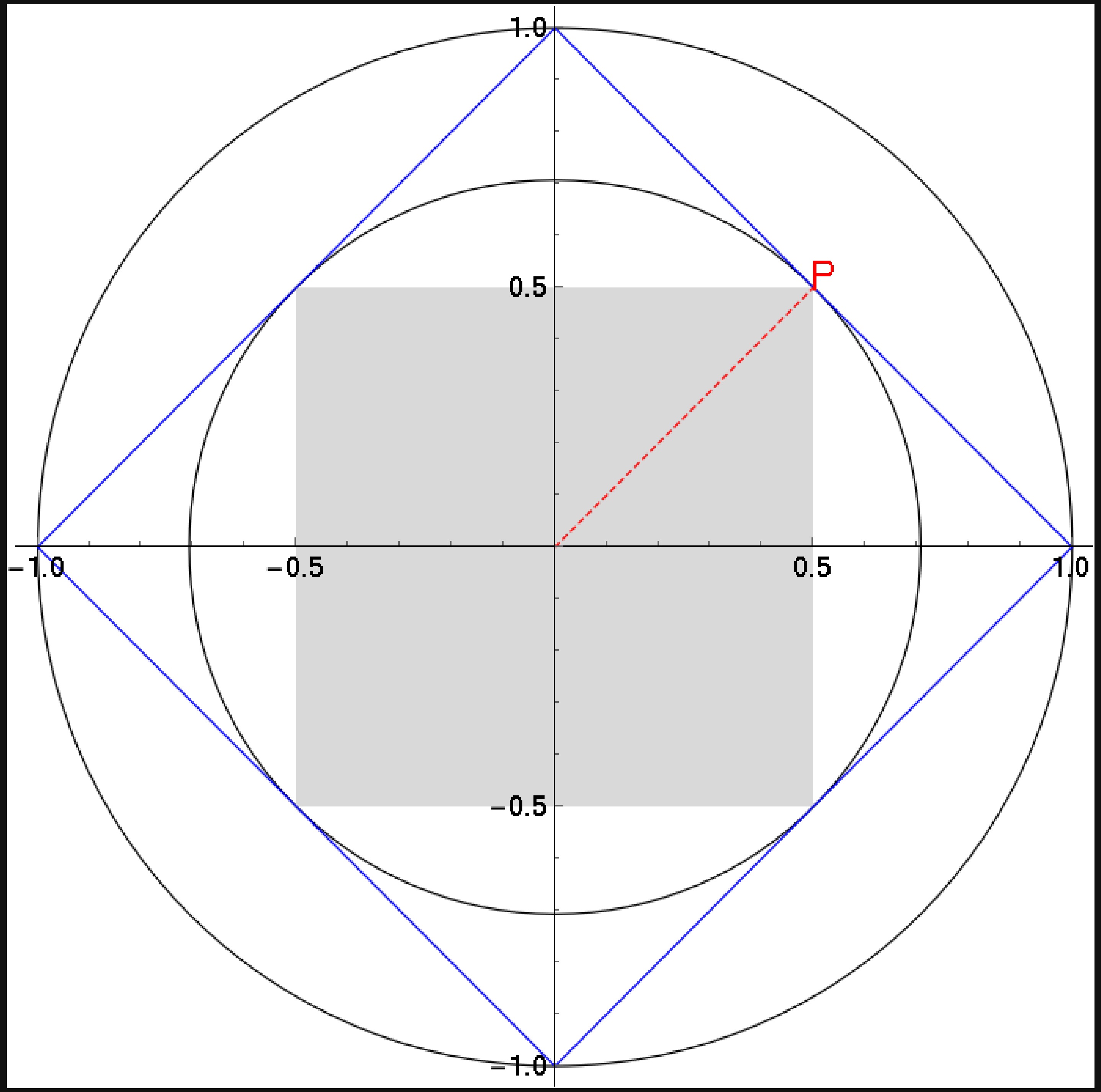
vector norms

$$\| \boldsymbol{x} \|_1 = \sum_{i}^{n} |x_i|$$

$$\| \boldsymbol{x} \|_2 = \left(\sum_{i}^{n} x_i^2 \right)^{1/2}$$

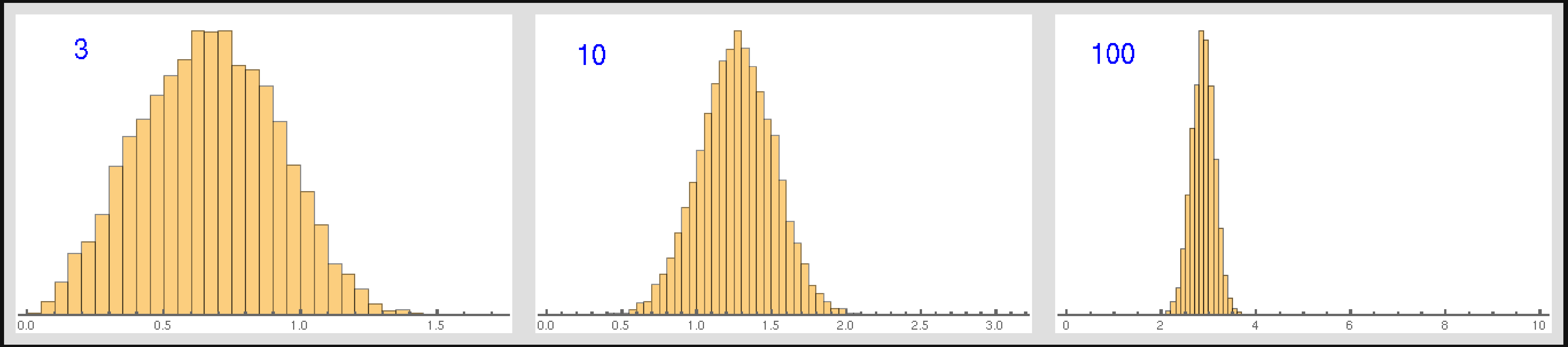
$$\| \boldsymbol{x} \|_\infty = \max_{1 \le i \le n} |x_i|$$

Linear System



Linear System

Euclidean distance between two random points



Linear System

linear system : $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$

residual : $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}$

$$
\begin{aligned}
\|\Delta x\| &= \| \hat{\boldsymbol{x}} - \boldsymbol{x} \| \\
&= \| \boldsymbol{A}^{-1}(\boldsymbol{A}\hat{\boldsymbol{x}} - \boldsymbol{b}) \| \\
&= \| \boldsymbol{A}^{-1}\boldsymbol{r} \| \\
&\leq \| \boldsymbol{A}^{-1} \| \| \boldsymbol{r} \|
\end{aligned}
$$

$$
\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \mathrm{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{r}\|}{\|\boldsymbol{A}\| \| \hat{\boldsymbol{x}} \|}
$$

Least Square

$$\boldsymbol{A}\boldsymbol{x} \simeq \boldsymbol{b}$$

Least Square

Normal equation

$$\begin{aligned}\phi(\boldsymbol{x}) &= (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x})^T(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}) \\ &= \boldsymbol{b}^T\boldsymbol{b} - 2\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{b} + \boldsymbol{x}^T\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x}\end{aligned}$$

$$\mathbf{0} = \nabla\phi(\boldsymbol{x}) = 2\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} - 2\boldsymbol{A}\boldsymbol{b}$$

$$\boxed{\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{b}}$$

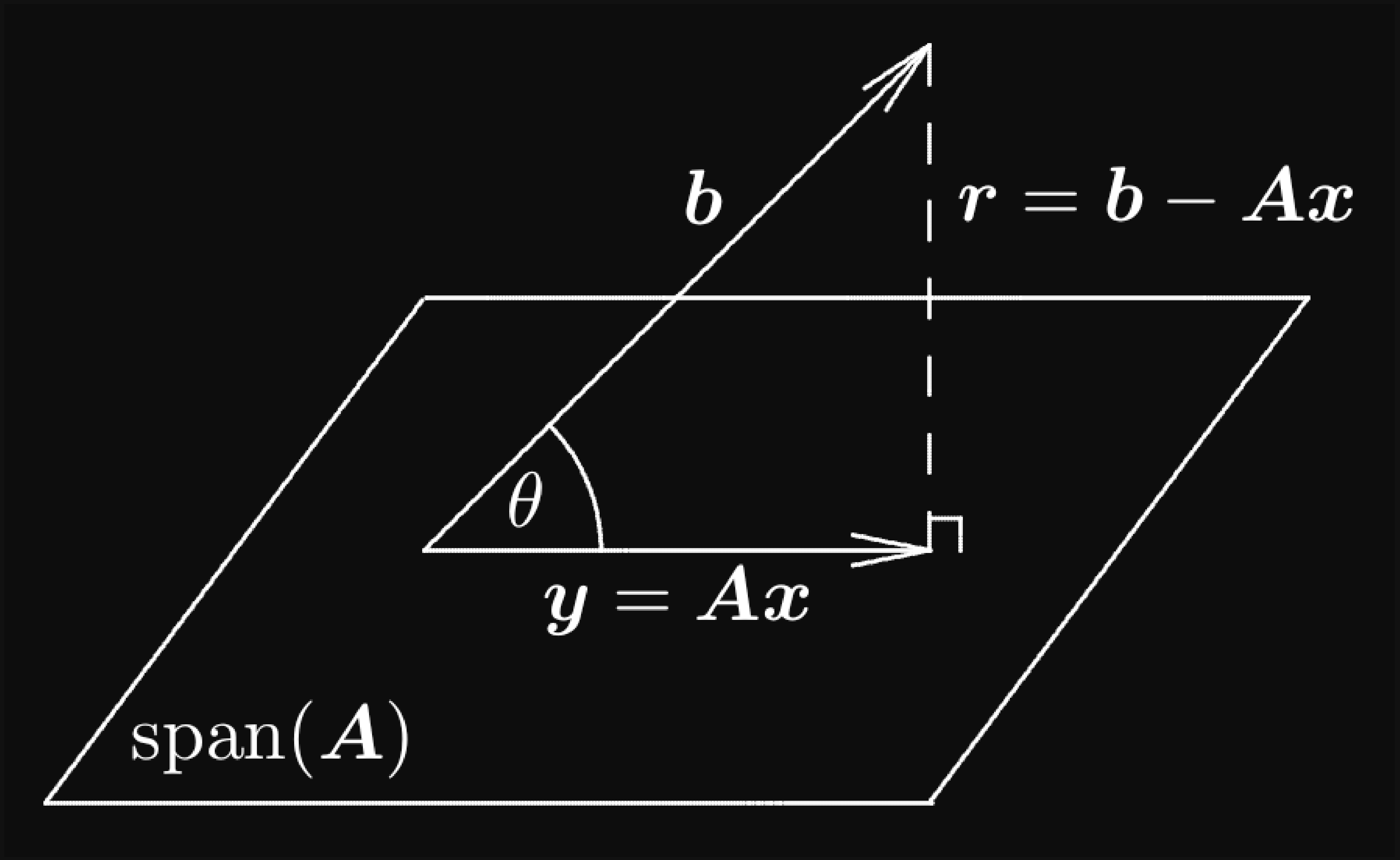
Least Square

Geometrical interpretation

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} \ \in \ \mathrm{span}(\boldsymbol{A})$$

orthogonal projection $\boldsymbol{b}$ onto the span(A)

Least Square



Least Square

Projector matrix : idempotent

$$\boldsymbol{P}^2 = \boldsymbol{P}$$

Orthogonal projector :

$$\boldsymbol{P}^T = \boldsymbol{P}$$

$$\boldsymbol{P}_\perp = \boldsymbol{I} - \boldsymbol{P}$$

$$\boldsymbol{v} = (\boldsymbol{P} + (\boldsymbol{I} - \boldsymbol{P})\boldsymbol{v}) = \boldsymbol{P}\boldsymbol{v} + \boldsymbol{P}_\perp \boldsymbol{v}$$

Least Square

$$\begin{aligned}\|\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x}\| &= \| \boldsymbol{P}(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x})+\boldsymbol{P}_{\perp}(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x})\|^2 \\ &= \| \boldsymbol{P}(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x}) \|^2 + \| \boldsymbol{P}_{\perp}(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x})\|^2 \\ &= \| \boldsymbol{P}\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x} \|^2 + \| \boldsymbol{P}_{\perp}\boldsymbol{b}\|^2\end{aligned}$$

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{P}\boldsymbol{b}$$

Least Square

$$\boldsymbol{A}^T\boldsymbol{P} = \boldsymbol{A}^T\boldsymbol{P}^T = (\boldsymbol{P}\boldsymbol{A})^T = \boldsymbol{A}^T$$

$$\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$$

$$\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$$

Least Square

Question :

Can you show P is indeed a projection matrix?

Can P be an identity matrix?

Least Square

pseudo inverse : $\boldsymbol{A}^{+} = (\boldsymbol{A}^{T}\boldsymbol{A})^{-1}\boldsymbol{A}^{T}$

$$\operatorname{cond}(\boldsymbol{A}) = \| \boldsymbol{A} \|_2 \| \boldsymbol{A}^{+} \|_2$$

Least Square

perturbation : $\boldsymbol{b} + \Delta \boldsymbol{b}$

$$\boldsymbol{A}^T \boldsymbol{A} \Delta \boldsymbol{x} = \boldsymbol{A}^T \boldsymbol{b}$$

$$\Delta \boldsymbol{x} = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \Delta \boldsymbol{b} = \boldsymbol{A}^+ \Delta \boldsymbol{b}$$

$$\begin{aligned}
\|\Delta \boldsymbol{x}\|_2 &\leq \| \boldsymbol{A}^+ \|_2 + \| \Delta \boldsymbol{b}\|_2 \\
\frac{\|\Delta \boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} &\leq \| \boldsymbol{A}^+ \|_2 + \frac{\|\Delta \boldsymbol{b}\|_2}{\|\boldsymbol{x}\|_2} \\
&= \mathrm{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{b}\|_2}{\| \boldsymbol{A} \|_2 \| \boldsymbol{x}\|_2} \frac{\|\Delta \boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2} \\
&\leq \mathrm{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{b}\|_2}{\|\boldsymbol{A}\boldsymbol{x}\|_2} \frac{\|\Delta \boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2} \\
&= \mathrm{cond}(\boldsymbol{A}) \frac{1}{cos(\theta)} \frac{\|\Delta \boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2}
\end{aligned}$$

Least Square

Example

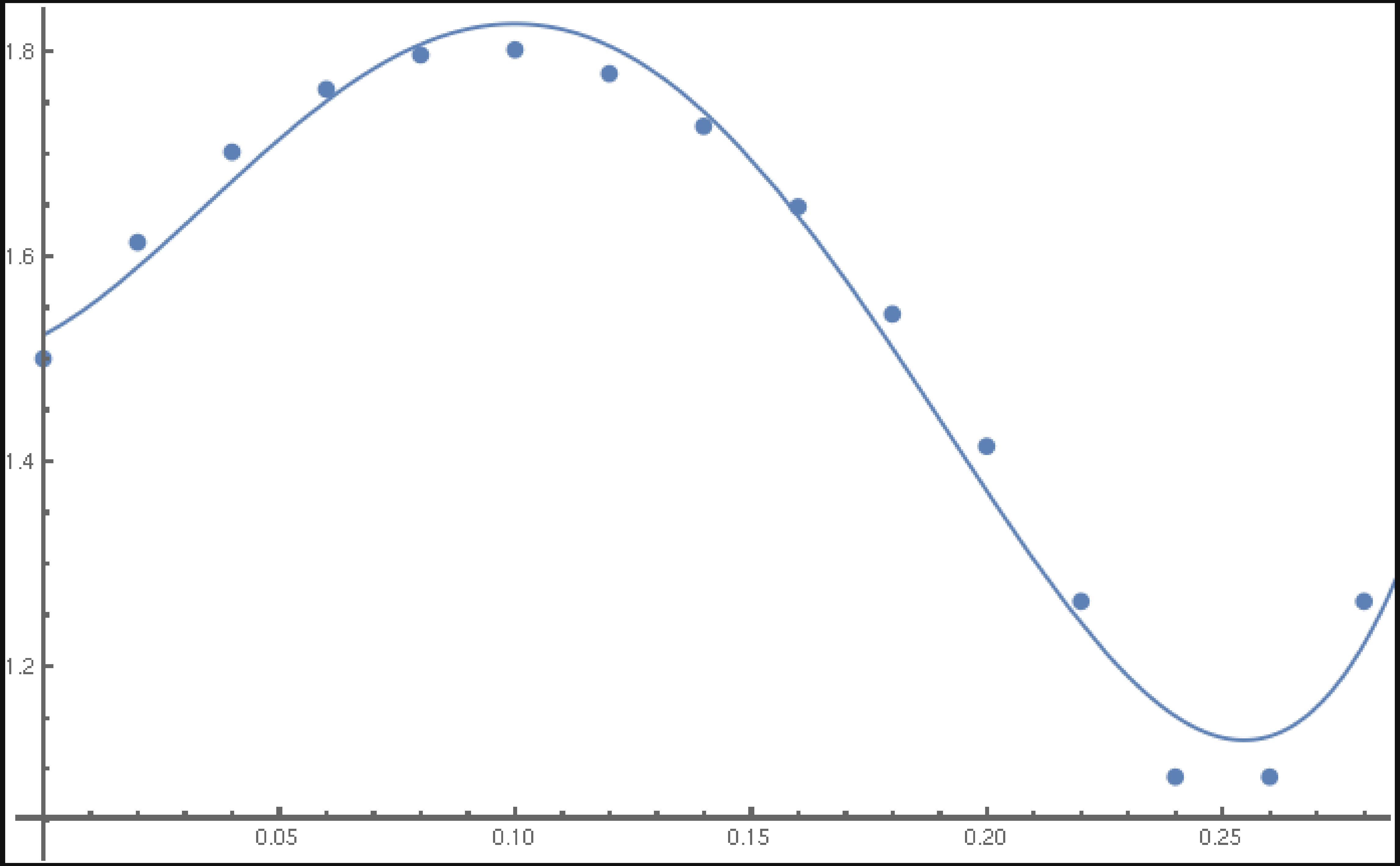
A 4th order polynomial fit

$$\begin{pmatrix} 0. & 1.5 \\ 0.02 & 1.61351 \\ 0.04 & 1.70156 \\ 0.06 & 1.76279 \\ 0.08 & 1.79621 \\ 0.1 & 1.80131 \\ 0.12 & 1.778 \\ 0.14 & 1.72665 \\ 0.16 & 1.64807 \\ 0.18 & 1.5435 \\ 0.2 & 1.41458 \\ 0.22 & 1.26336 \\ 0.24 & 1.09221 \\ 0.26 & 1.09221 \\ 0.28 & 1.26336 \end{pmatrix}$$

Least Square

$$\begin{pmatrix}
1 & 0. & 0. & 0. & 0. \\
1 & 0.02 & 0.0004 & 8.\times 10^{-6} & 1.6\times 10^{-7} \\
1 & 0.04 & 0.0016 & 0.000064 & 2.56\times 10^{-6} \\
1 & 0.06 & 0.0036 & 0.000216 & 0.00001296 \\
1 & 0.08 & 0.0064 & 0.000512 & 0.00004096 \\
1 & 0.1 & 0.01 & 0.001 & 0.0001 \\
1 & 0.12 & 0.0144 & 0.001728 & 0.00020736 \\
1 & 0.14 & 0.0196 & 0.002744 & 0.00038416 \\
1 & 0.16 & 0.0256 & 0.004096 & 0.00065536 \\
1 & 0.18 & 0.0324 & 0.005832 & 0.00104976 \\
1 & 0.2 & 0.04 & 0.008 & 0.0016 \\
1 & 0.22 & 0.0484 & 0.010648 & 0.00234256 \\
1 & 0.24 & 0.0576 & 0.013824 & 0.00331776 \\
1 & 0.26 & 0.0676 & 0.017576 & 0.00456976 \\
1 & 0.28 & 0.0784 & 0.021952 & 0.00614656
\end{pmatrix}$$

Least Square



Least Square

$$\mathrm{cond}(\boldsymbol{A}) = 7.6 \times 10^5$$

$$\cos(\theta) = \frac{\|\boldsymbol{Ax}\|_2}{\|\boldsymbol{b}\|_2} \approx 0.99$$

Take-home

Reading Assignment

What Role Does Hydrological Science Play in the Age of Machine Learning?

Grey S. Nearing[1,2], Frederik Kratzert[3], Alden Keefe Sampson[1], Craig S. Pelissier[4], Daniel Klotz[3], Jonathan M. Frame[2], Cristina Prieto[5], Hoshin V. Gupta[6]

Acknowledgement

Thanks for Your Attention

References

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- https://en.wikipedia.org/wiki/Bertrand_Russell
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