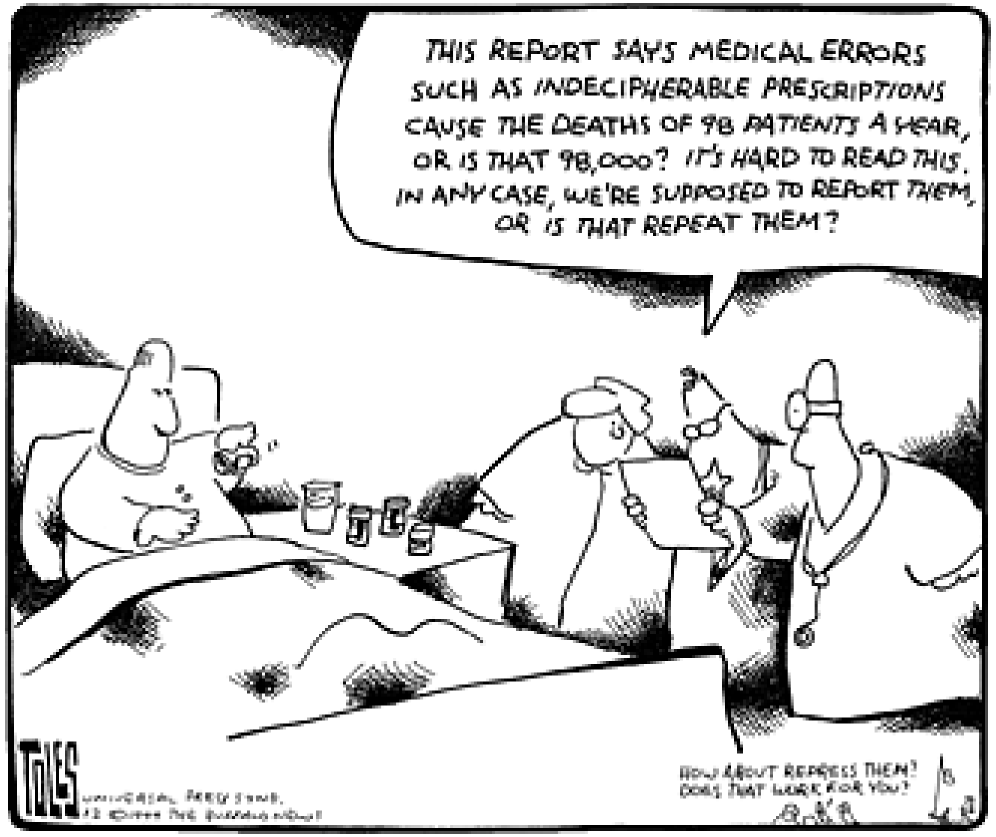


Outline:

Basics

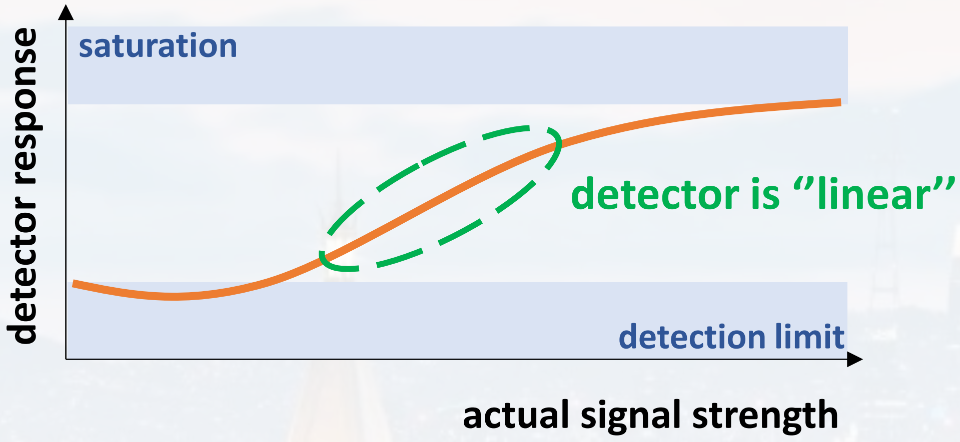
Most Common PDFs

- uniform
- binomial
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics

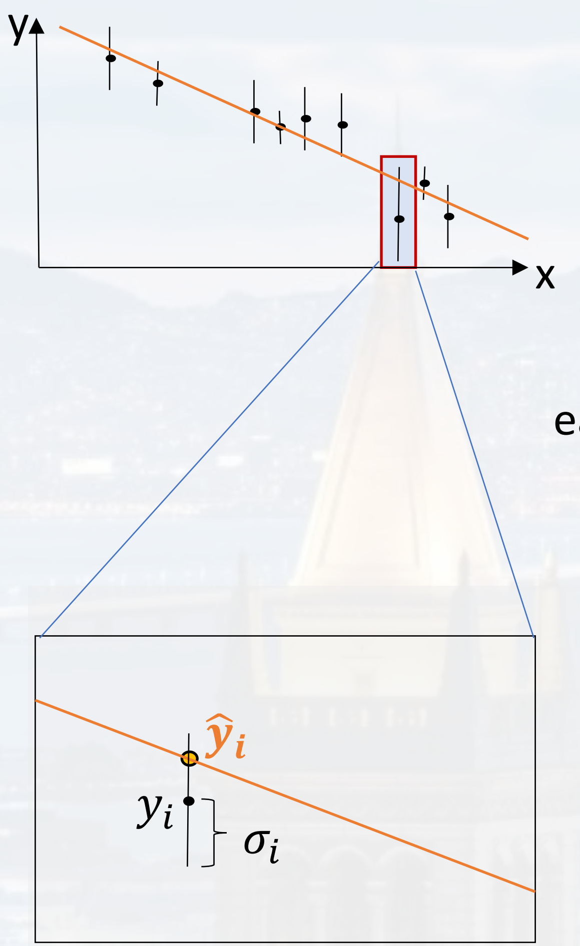
- **<u>systematic errors:</u>** calibration, non-linearity of the detector



- **<u>statistical errors:</u>** limited precision, natural variance of the data
  → spread of the data around **an average value**

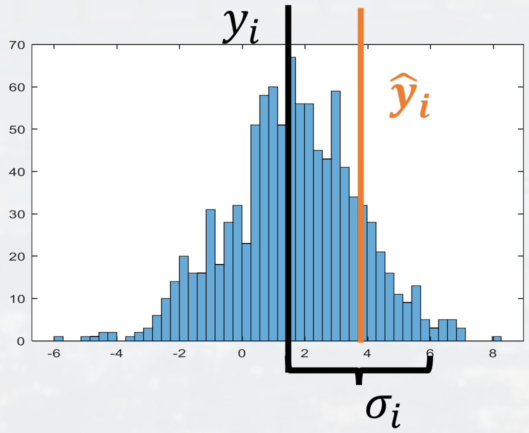
assumption: far from the detection limit and saturation:

the spread follows approximately a **normal distribution.**

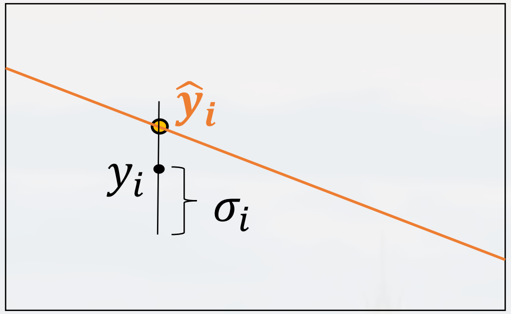


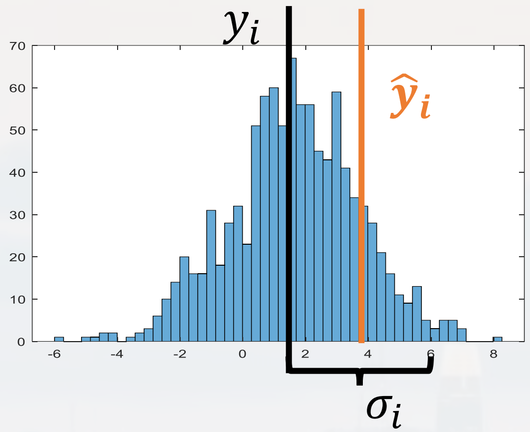
fitting a model ($\hat{y}_i$, orange line) to data points (x_i, y_i) each with an error bar $\boldsymbol{\sigma_i}$

each data point x_i has been drawn from $\boldsymbol{N(\mu_i = y_i, \sigma_i)}$



$$p_i(y_i|\hat{y}_i, \sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i} exp\left[-\frac{1}{2}\frac{(y_i - \hat{y}_i)^2}{\sigma_i^2}\right]$$





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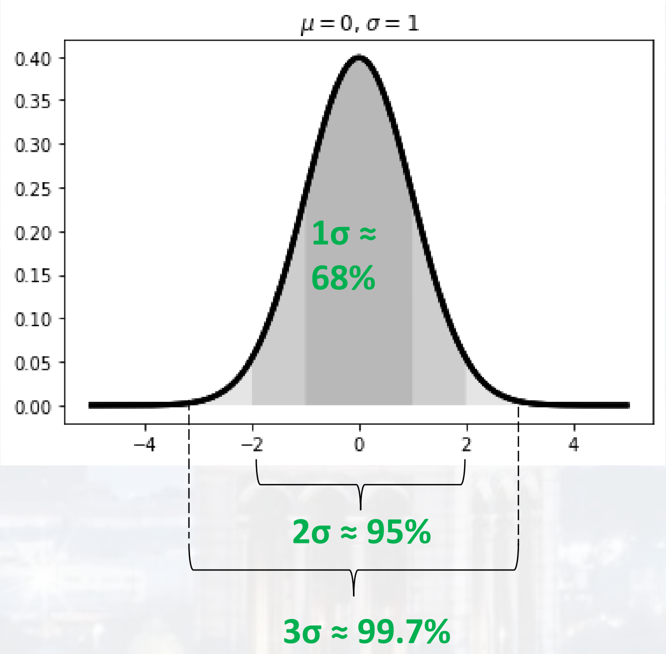

for large **(> 50…100)** N **(number of data points)**:

≈ **2/3** of the data points should be consistent with the model within their **1σ** error bars

≈ **95%** of the data points should be consistent with the model within their **2σ** error bars

≈ **99.7%** of the data points should be consistent with the model within their **3σ** error bars

$$p_i(y_i|\hat{y}_i,\sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i} exp\left[-\frac{1}{2}\frac{(y_i-\hat{y}_i)^2}{\sigma_i^2}\right]$$

based on this model: reduced chi square

$$\boxed{\chi^2_{red} = \frac{1}{df}\sum_{i=1}^{N}\left(\frac{y_i-\hat{y}_i}{\sigma_i}\right)^2}$$

$$df = N - p - 1$$

N : number of data points
p: number of fit parameter (model)

given a fitted model: χ^2_{red} is a **measure of the fit quality**!

$$p_i(y_i|\hat{y}_i, \sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i} exp\left[-\frac{1}{2}\frac{(y_i - \hat{y}_i)^2}{\sigma_i^2}\right]$$

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given a fitted model: χ^2_{red} is a **measure of the fit quality**!

example

good fit: $y_i - \hat{y}_i$ should be within σ_i for 2/3 of all data points, see $\boldsymbol{N(\mu_i = y_i, \sigma_i)}$

therefore $\frac{y_i - \hat{y}_i}{\sigma_i} \approx 1$

therefore $\sum_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{\sigma_i}\right)^2 \approx N$

N should be **much larger** than p, therefore df $\approx N$

hence, $\chi^2_{red} \approx 1$

$$p_i(y_i|\hat{y}_i,\sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i} exp\left[-\frac{1}{2}\frac{(y_i - \hat{y}_i)^2}{\sigma_i^2}\right]$$

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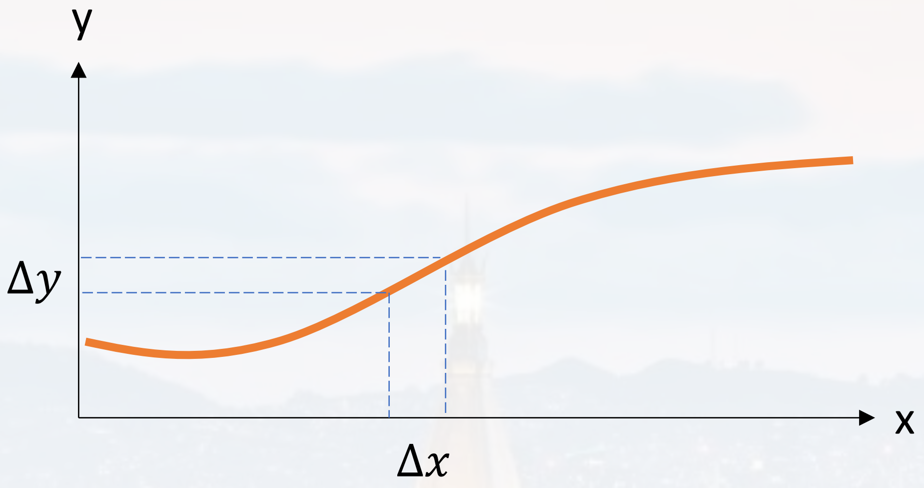
$\chi^2_{red} \approx$

1.0 excellent fit
1.0...1.5 acceptable fit
1.5...1.7 bad fit
>2.0 not acceptable

<<1.0 suspicious, errors are overestimated!

error propagation



$$\frac{dy}{dx} \approx \frac{\Delta y}{\Delta x}$$ for $\Delta x \ll x$

$$\Delta x \left|\frac{dy}{dx}\right| \approx \Delta y$$

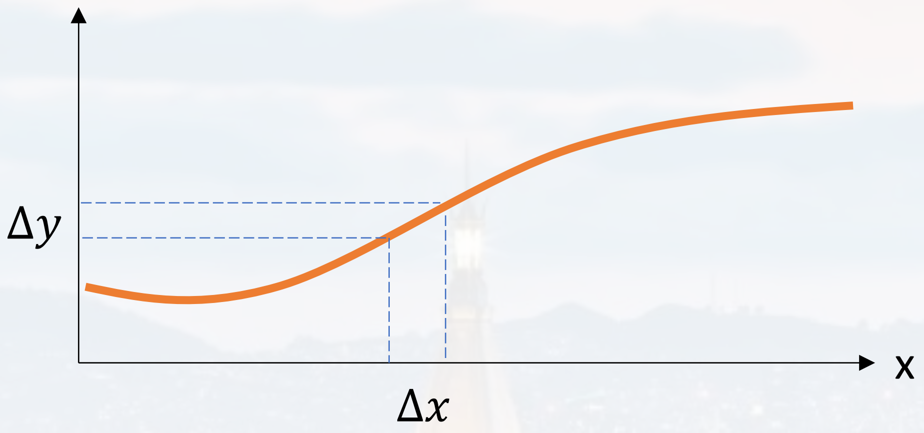
example:

$$V = \frac{4}{3} \pi r^3$$ $\Delta V = ?$ given Δr

$$\Delta V = \frac{dV}{dr} \Delta r = 4 \pi r^2 \Delta r$$

$$\boxed{\frac{\Delta V}{V} = 3 \frac{\Delta r}{r}}$$ $\Delta r, \Delta V \approx 1\sigma$

error propagation



$$\boxed{\frac{\Delta V}{V} = 3\,\frac{\Delta r}{r}}$$

$\Delta r, \Delta V \approx 1\sigma$

$$\Delta V = \frac{dV}{dr}\Delta r = 4\,\pi\,r^2\Delta r$$

radius: r = 1.0µm
Δr = 0.1µm

$$V = \frac{4}{3}\,\pi\,(1.0\mu m)^3 = 4.18879020..\mu m^3$$

$$\Delta V = 4\,\pi\,r^2\Delta r = 4\,\pi\,(1.0\mu m)^2 0.1\mu m$$

$$= 1.2566370614359172\mu m^3$$

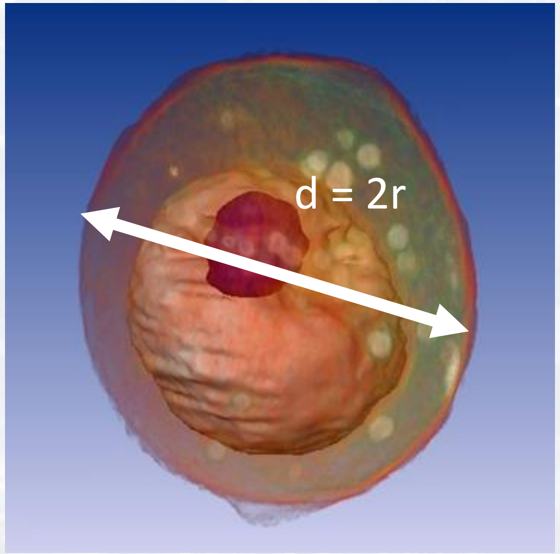
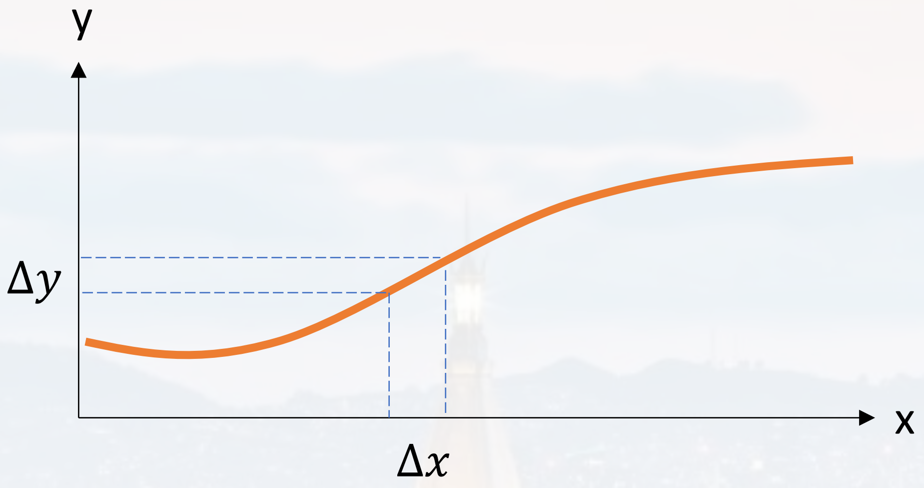


Image: NIH

error propagation



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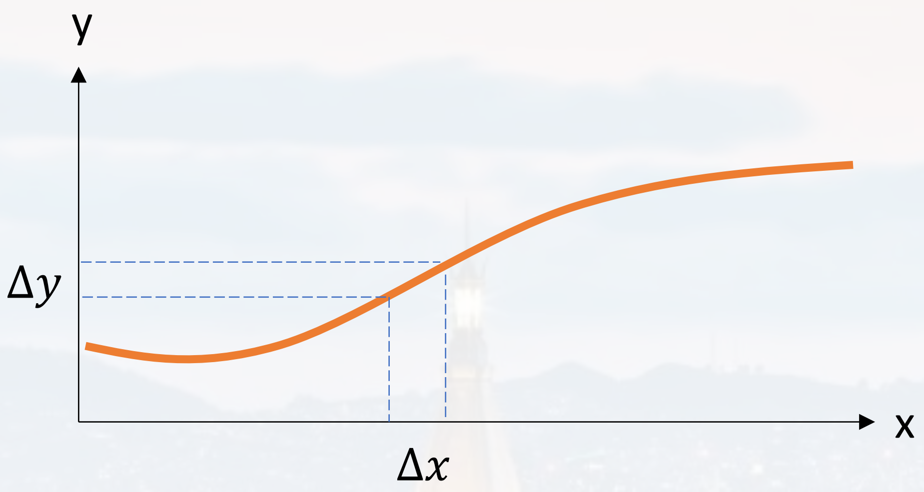
$$= \mathbf{1.25}66370614359172\text{µm}^3$$

$$\boldsymbol{V} = (\mathbf{4.2} \pm \mathbf{1.3})\text{µm}^3$$

error propagation



general:

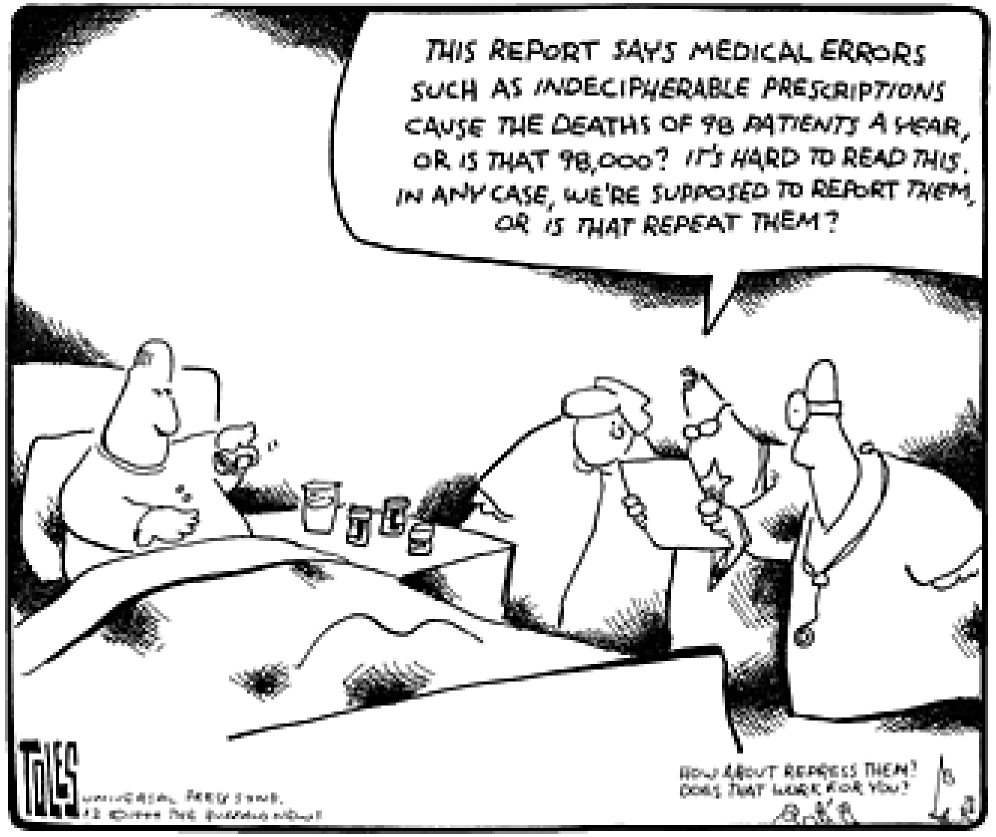
$$\Delta f\,(max) = \sum_{i=1}^{I} \left|\frac{\partial f}{\partial x_i}\right| \Delta x_i$$

maximum error estimation

if x_i do **not correlate**, i. e. are **mutually independent**:

$$\Delta f^2 = \sum_{i=1}^{I} \left|\frac{\partial f}{\partial x_i}\right|^2 (\Delta x_i)^2$$

Note: $\Delta f\,(max)^2 > \Delta f^2$ because of the mixed terms $\left|\frac{\partial f}{\partial x_i}\right| \left|\frac{\partial f}{\partial x_j}\right| \Delta x_i \Delta x_j$ in $\Delta f\,(max)^2$



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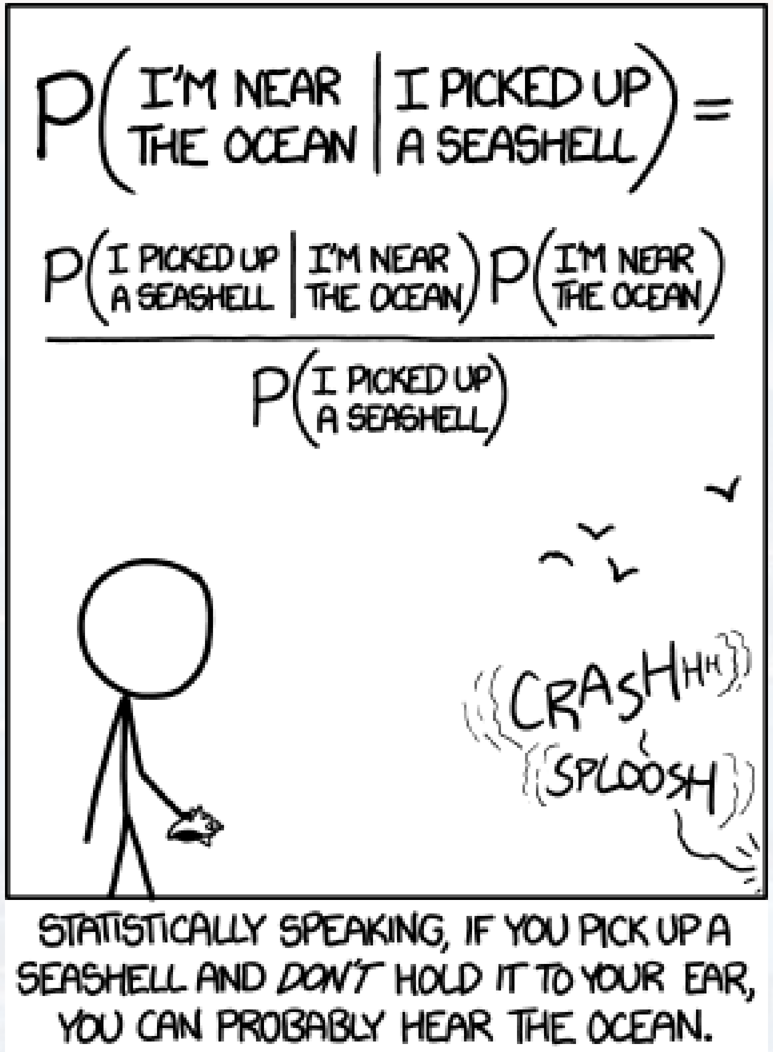
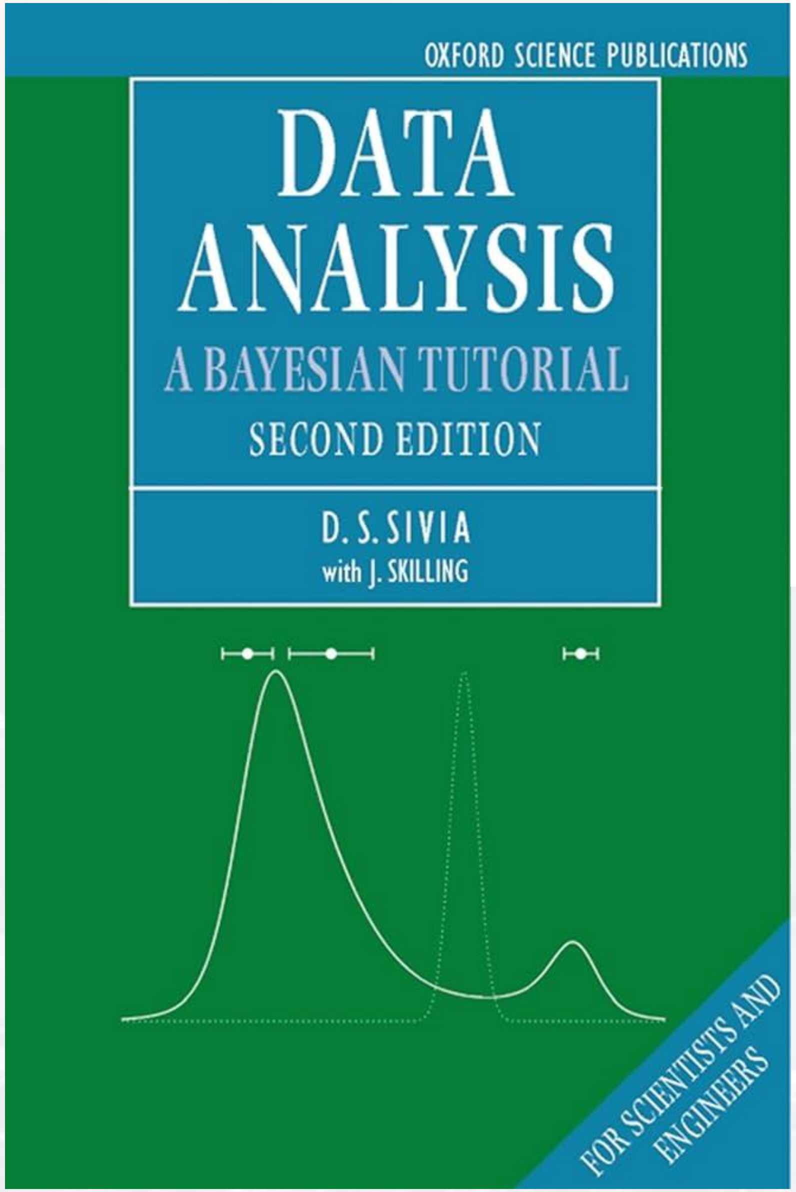

P(I'M NEAR THE OCEAN | I PICKED UP A SEASHELL) =
P(I PICKED UP A SEASHELL | I'M NEAR THE OCEAN) P(I'M NEAR THE OCEAN)
P(I PICKED UP A SEASHELL)
CRASHHH
SPLOOSH
STATISTICALLY SPEAKING, IF YOU PICK UP A SEASHELL AND DON'T HOLD IT TO YOUR EAR, YOU CAN PROBABLY HEAR THE OCEAN.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DATA ANALYSIS
A BAYESIAN TUTORIAL
SECOND EDITION
D. S. SIVIA
with J. SKILLING
FOR SCIENTISTS AND ENGINEERS

Thomas Bayes
(1701 - 1761)

$P(A \cap B)$ probability ***P*** that the events ***A*** **and** ***B*** occur

so far: A and B were independent $P(A \cap B) = P(A)P(B) = P(B)P(A)$

now: **conditional probabilities** | "given" or "under the condition"

$$P(A \cap B) = P(A|B)P(B) = P(B|A)P(A)$$

$$\boxed{P(A|B)P(B) = P(B|A)P(A)}$$

Bayes Theorem

$$\text{posterior} \quad P(A|B) = \frac{P(B|A)P(A)}{P(B)} \quad \text{prior}$$

$$\boxed{P(A|B)P(B) = P(B|A)\mathrm{P(A)}}$$ **Bayes Theorem**

Thomas Bayes
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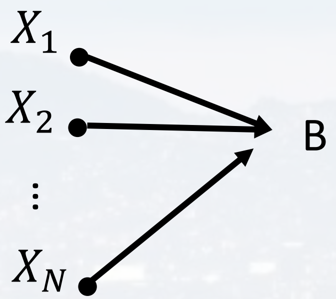
posterior $$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$ **prior**



$$P(B) = \sum_{n=1}^{N} P(B|X_n)P(X_n)$$

$$P(B) = \int P(B|X)P(X)\,dX$$

marginalization

Probability $P(B)$ that I am going to be too late for a meeting:

$$\begin{aligned} P(B) = {} & P(B|I\ forgot\ that\ I\ have\ a\ meeting)\ P(I\ forgot\ that\ I\ have\ a\ meeting) + \\ & P(B|I\ got\ sick)\ P(I\ got\ sick) + \\ & P(B|BART\ was\ too\ late)\ P(BART\ was\ too\ late) + \ \ldots \end{aligned}$$

example: cancer diagnosis from blood test

Bayes Theorem $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

Marginalization $P(B) = \sum_{n=1}^{N} P(B|X_n)P(X_n)$

+ : positive test result
D : diseased
H : health

statement 1: If a person is **diseased**, there is a **95% probability** that the test is **positive.**

statement 2: The **prevalence** for the disease in the average **population** is **0.001%** .

statement 3: **5% of healthy** patients have **a positive result** (aka p-value).

A person takes the test and gets a positive test result. **What is the probability that the person is sick**?

$$P(D|+) = \frac{P(+|D)P(D)}{P(+)} \underset{\text{statement 1}}{=} \frac{0.95\, P(D)}{P(+)} \underset{\text{statement 2}}{=} \frac{0.95 \cdot 0.00001}{P(+)} \underset{\text{marginalization}}{=} \frac{0.95 \cdot 0.00001}{P(+|D)P(D) + P(+|H)P(H)}$$

example: cancer diagnosis from blood test

Bayes Theorem $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

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$$P(D|+) = \frac{P(+|D)P(D)}{P(+)} = \frac{\mathbf{0.95}\, P(D)}{P(+)} = \frac{\mathbf{0.95 \cdot 0.00001}}{P(+)} = \frac{\mathbf{0.95 \cdot 0.00001}}{P(+|D)P(D) + P(+|H)P(H)}$$

statement 1 statement 2 marginalization

$$= \frac{\mathbf{0.95 \cdot 0.00001}}{P(+|D)P(D) + P(+|H)[\mathbf{1 - P(D)}]}$$

complement probability

example: cancer diagnosis from blood test

Bayes Theorem $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

+ : **positive test result**
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$$P(D|+) = \frac{P(+|D)P(D)}{P(+|D)P(D) + P(+|H)[1 - P(D)]}$$

$$\boxed{= \frac{1}{1 + \frac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}} = \frac{1}{1 + \frac{\mathbf{0.05}\,[1 - \mathbf{0.00001}]}{\mathbf{0.95} \cdot \mathbf{0.00001}}} = \mathbf{1/5000}$$

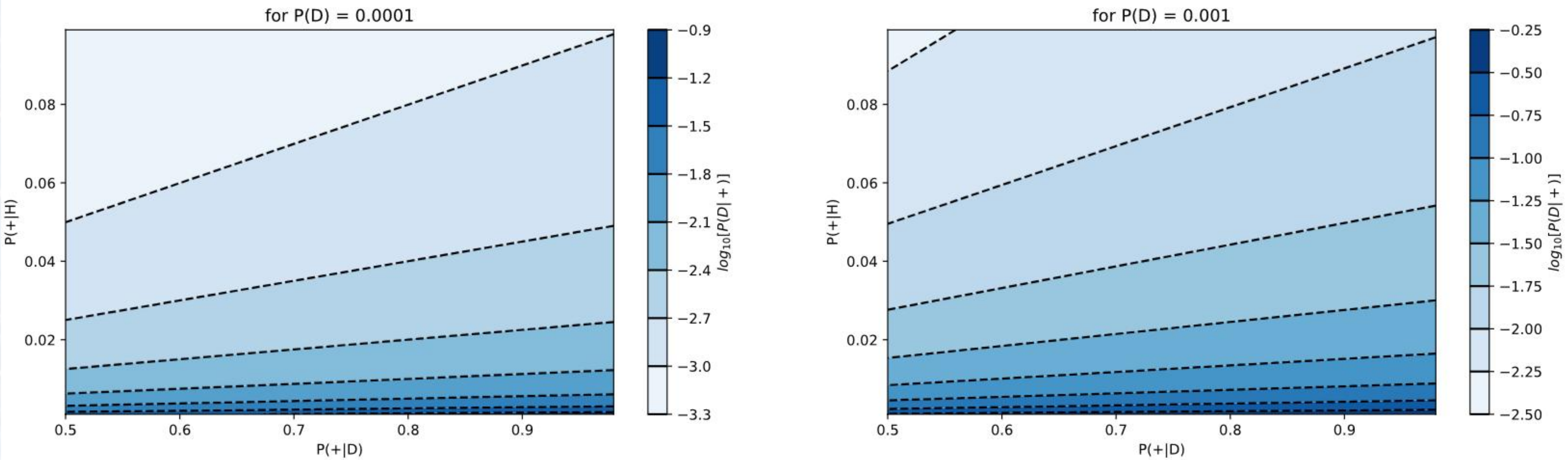
example: cancer diagnosis from blood test

+ : **positive test result**
D : **diseased**
H : **health**

statement 1:	sensitivity	P(D|+) = 95%
statement 2:	prior	P(D) = 0.001%
statement 3:	p-value or false positive rate	P(+|H) = 5%

$$P(D|+) = \frac{1}{1 + \frac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

check: `PlotPD_Plus.py`



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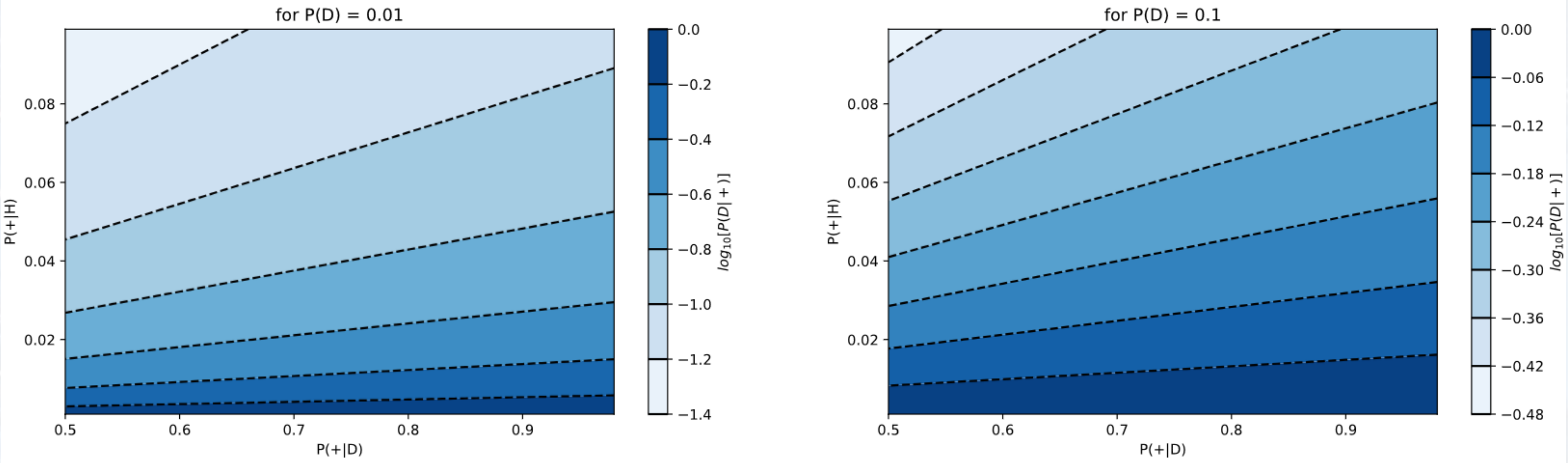

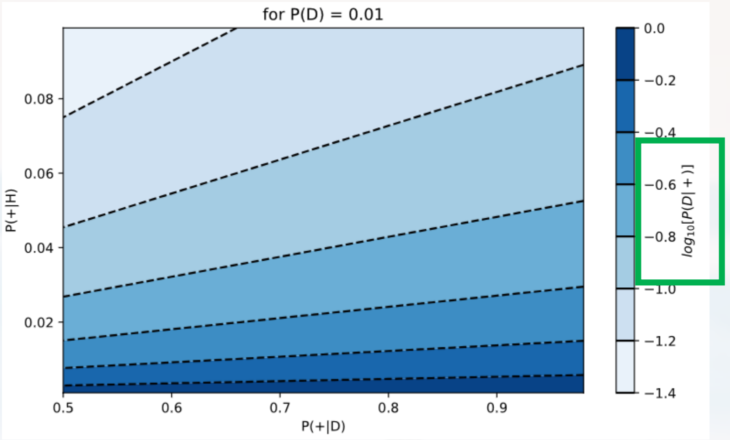

statement 1:	sensitivity	**P(D|+) = 95%**
statement 2:	prior	**P(D) = 0.001%**
statement 3:	p-value or false positive rate	**P(+|H) = 5%**

odds ratios:

$$\rho_1 = \frac{P(+|H)}{P(+|D)}$$

$$\rho_2 = \frac{1 - P(D)}{P(D)}$$

$$P(D|+) = \frac{1}{1 + \frac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

log odds ratios:

$$r_1 = \log\left[\frac{P(+|H)}{P(+|D)}\right]$$

$$r_2 = \log\left[\frac{1 - P(D)}{P(D)}\right]$$

$$P(D|+) = \frac{1}{1 + e^{r_1} e^{r_2}}$$

log odds ratios: $$r_1 = \log\left[\frac{P(+|H)}{P(+|D)}\right]$$

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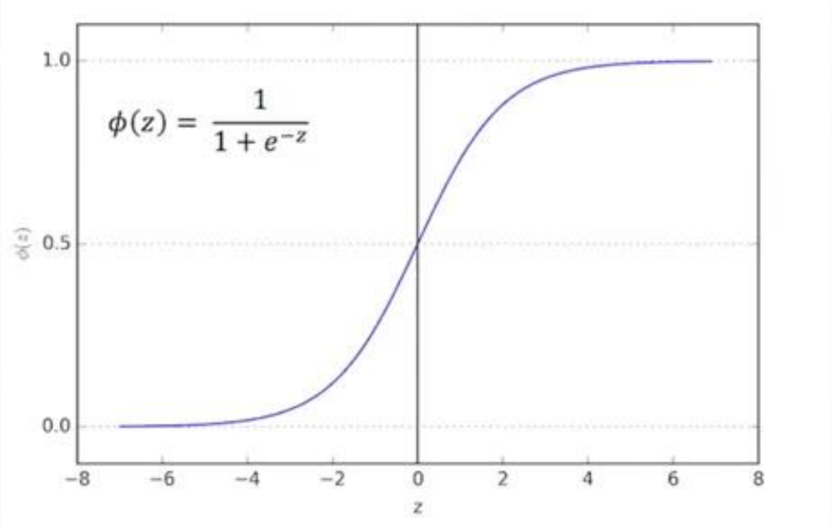
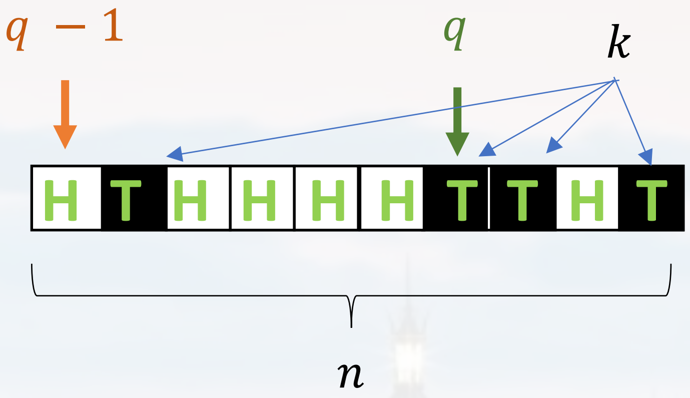
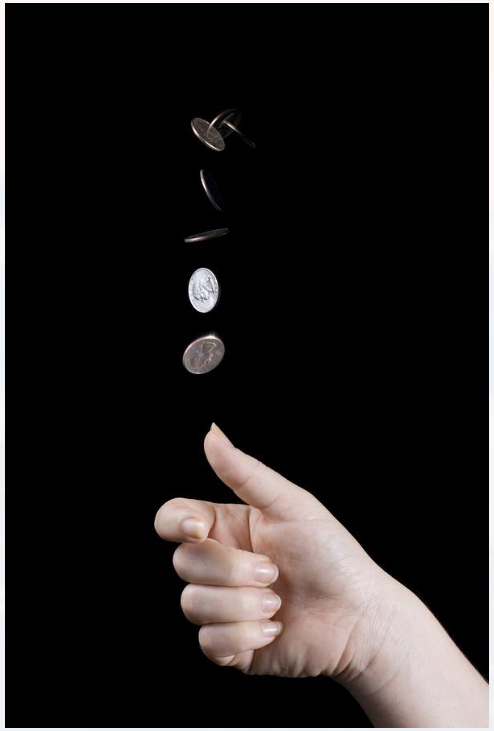
$$\boxed{P(D|+) = \frac{1}{1+e^{r_1}e^{r_2}}}$$

logistic (or logit or sigmoid) function

- logistic regression
- transfer function ANN
- bound growth (Verhulst equation)
- binding affinity ligand/receptor







fair coin? q = 0.5 ???

probability of having **a** sequence of **k tails** and **n-k heads**

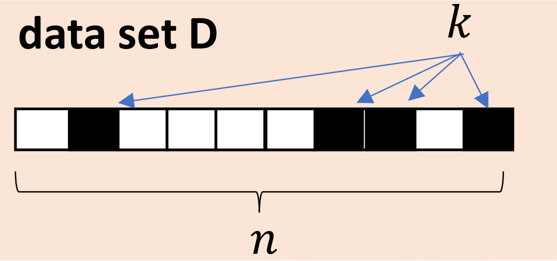
$$p_{tot} = \prod_i q_i^{\,n_i} = \; q^k \;(1-q)^{n-k}$$

probability of having **any** sequence of **k tails** and **n-k heads**

$$\boxed{P(k|q,n) = \binom{n}{k} \; q^k \;(1-q)^{n-k}}$$

binomial distribution

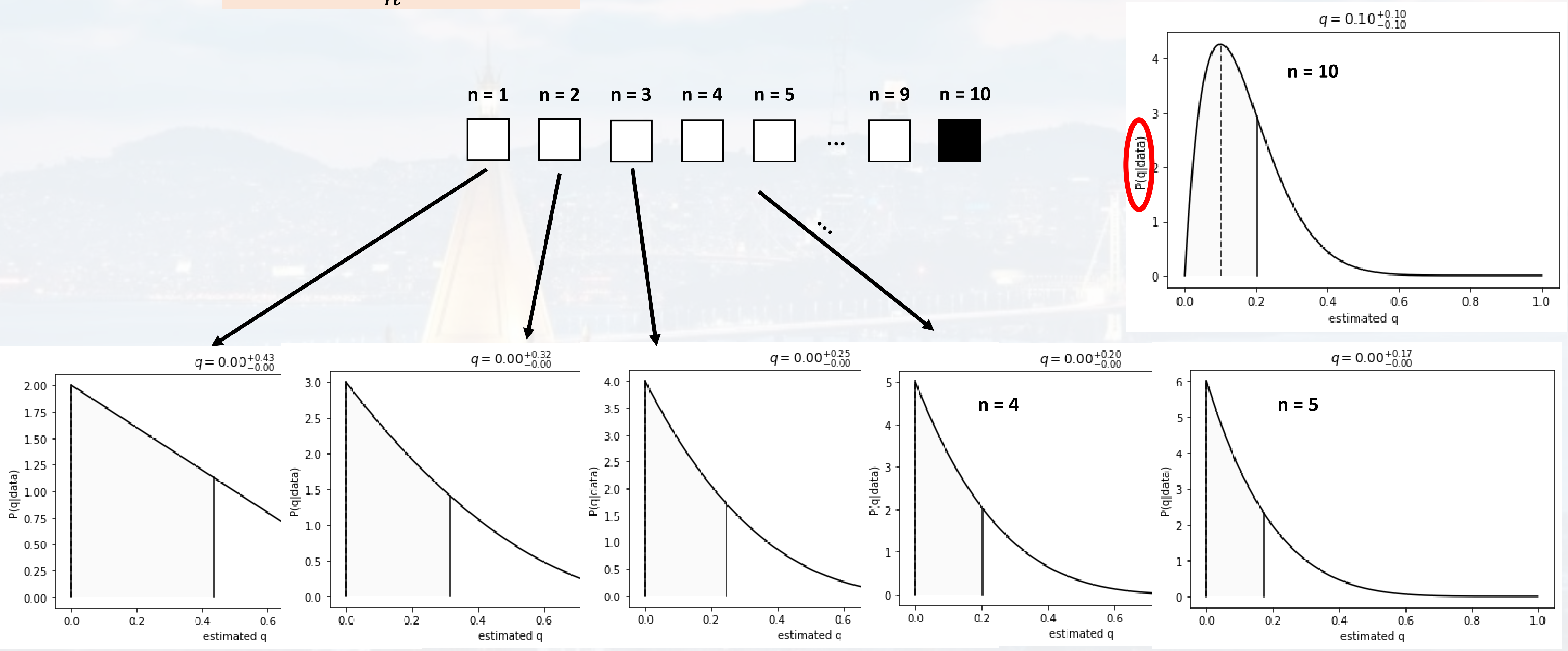
$$\frac{\boldsymbol{n!}}{\boldsymbol{k!(n-k)!}} =: \binom{\boldsymbol{n}}{\boldsymbol{k}}$$ **``n choose k''**



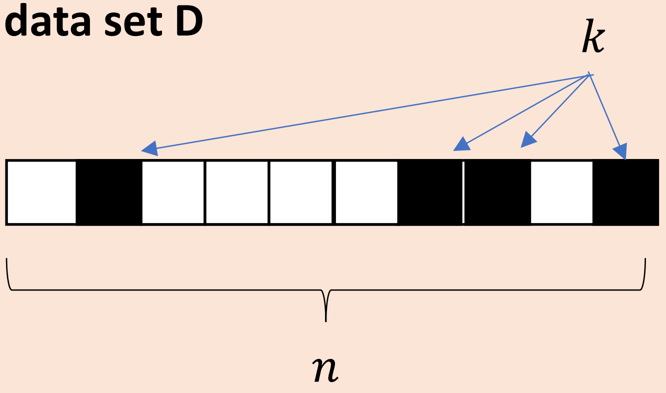
$\boldsymbol{q} = ?$

goal:

- **P(q|D)** **Parameter Estimation**
- the larger ***D***, the more certain ***q***
  → learning



data set D



$\boldsymbol{q} = ?$

goal:
- **P(q|D)**
- the larger ***D***, the more certain ***q***
  → learning

$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$$

Bayes' theorem:

likelihood function **(here: binomial)**

$$P(q|data\ set) = \frac{\boxed{P(data\ set|q)}\boxed{P(q)}}{\boxed{P(data\ set)}}$$

prior

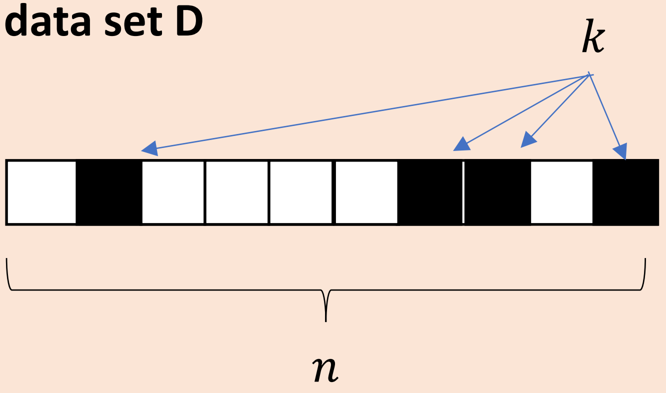
evidence **(const wrt q)**

$$= \frac{\binom{n}{k} q^k (1-q)^{n-k}}{P(D)} P(q)$$

$$\sim q^k (1-q)^{n-k}\, P(q)$$

$P(D)$ and $\binom{n}{k}$ are no functions of q

data set D



$\boldsymbol{q} = ?$

goal:
- **P(q|D)**
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$$P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$$

$$P(q|data\ set) = \frac{P(data\ set|q)P(q)}{P(data\ set)}$$

$$= \frac{\binom{n}{k} q^k (1-q)^{n-k}}{P(D)} P(q)$$

$$\sim q^k (1-q)^{n-k}\ P(q)$$

max. entropy: $\mathrm{P}(q) = const$
if no prior information about q

$$\sim q^k (1-q)^{n-k}$$

$$\boxed{P(q|data\ set) = \frac{q^k (1-q)^{n-k}}{\int_0^1 q^k (1-q)^{n-k}\ dq}}$$

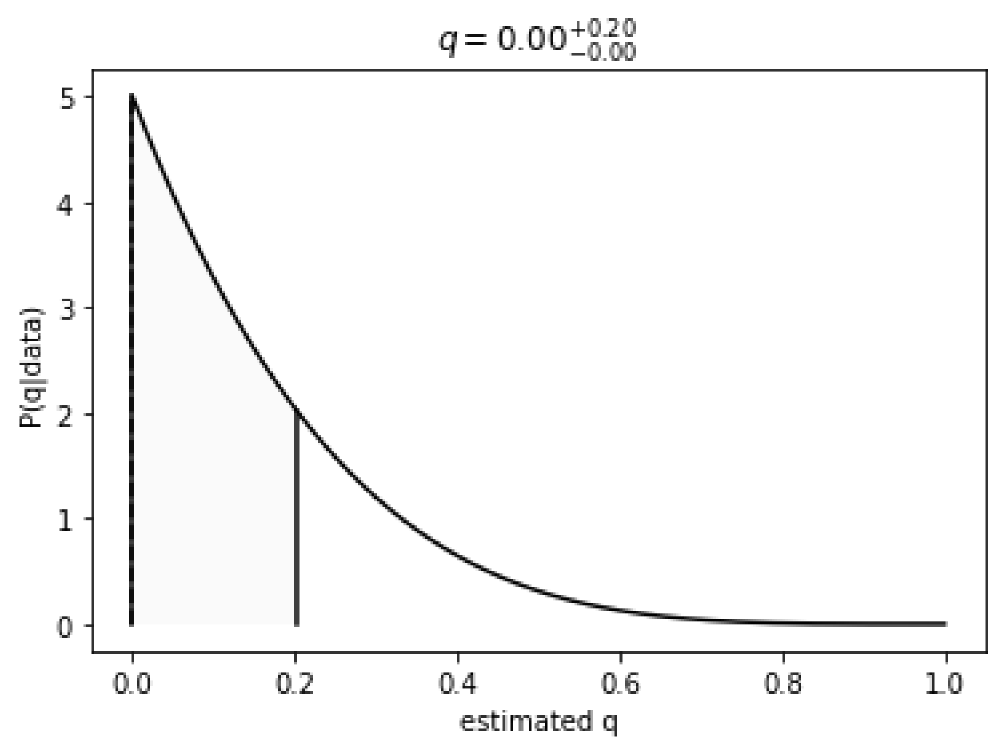
check out bayesian_bino.py

$$P(q|data\ set) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}$$

```
n1 = 4
k1 = np.random.binomial(n1, 0.25)
```

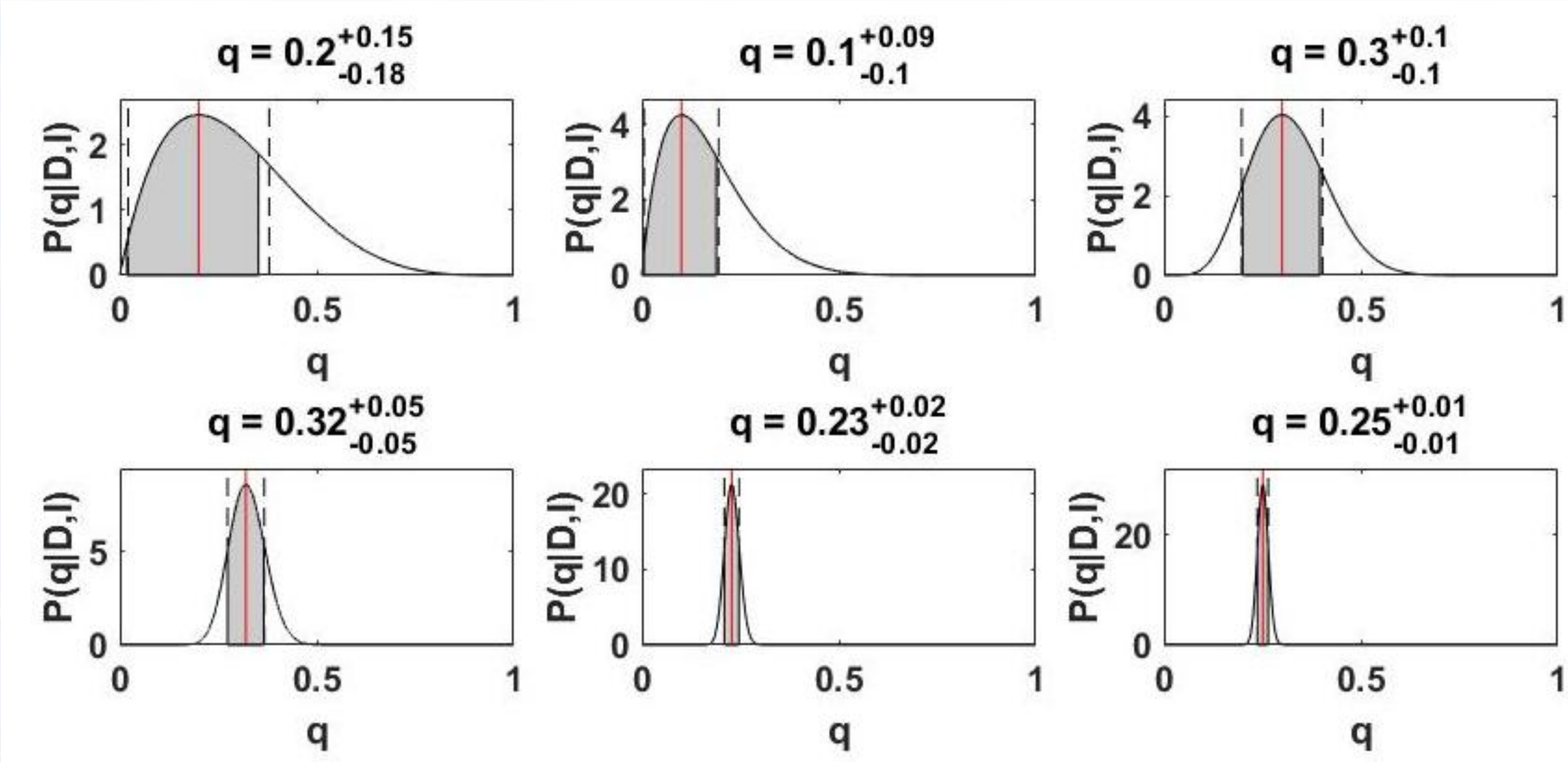
creating artificial data set
note: in reality ***q*** is unknown!

```
[q1, b, _] = bayesian_bino(n1, k1)
```



check out `bayesian_bino.py`

$$P(q|data\ set) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}$$



n	estimated q
5	$0.2^{+0.15}_{-0.18}$
10	$0.1^{+0.09}_{-0.1}$
20	$0.3^{+0.1}_{-0.1}$
50	$0.2^{+0.05}_{-0.06}$
100	$0.32^{+0.05}_{-0.05}$
500	$0.23^{+0.02}_{-0.02}$
1,000	$0.25^{+0.01}_{-0.01}$
infinity	0.25

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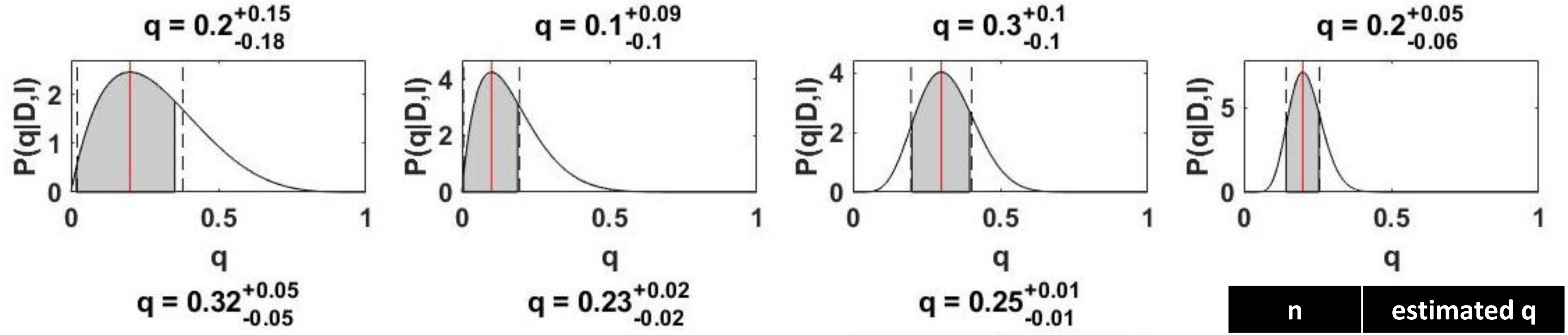

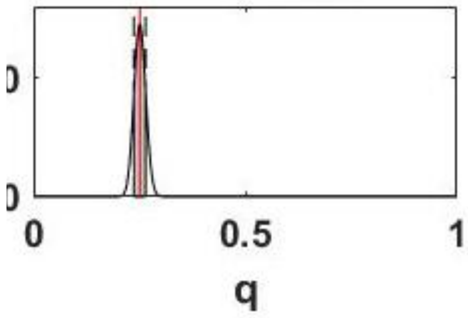

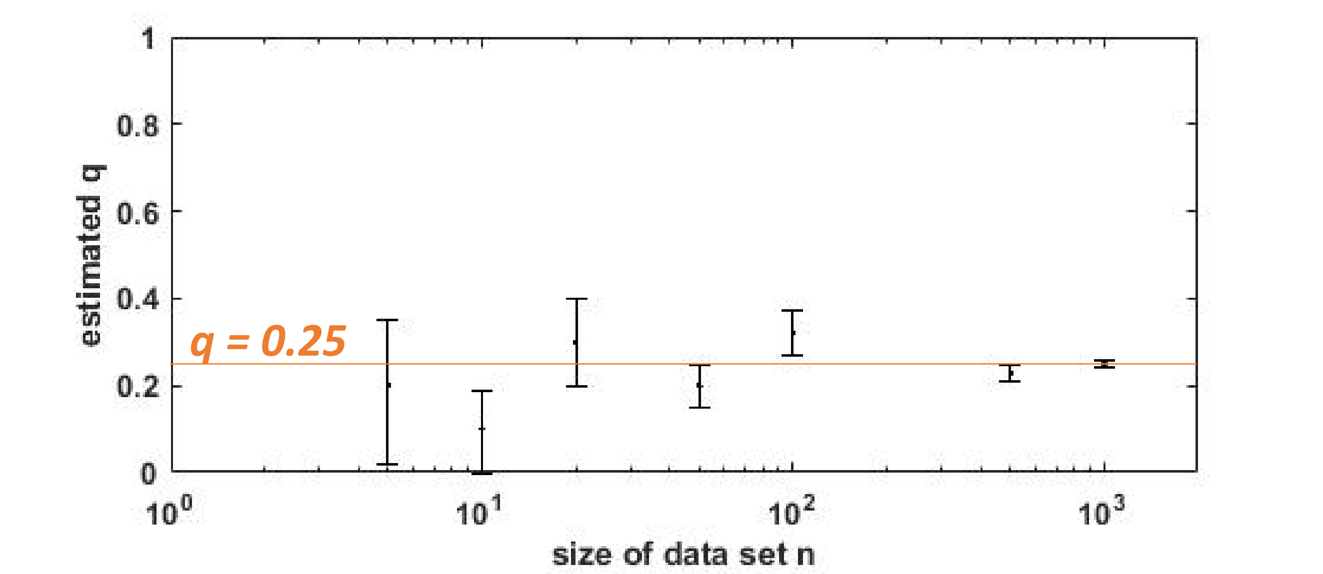

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Of course, Bayesian Parameter Estimation works with **any other pdf**

goal: - **P(q|D)**
- the larger ***D***, the more certain ***q***
→ learning

likelihood function

$$P(q|data\ set) = \frac{\boxed{P(data\ set|q)}\boxed{P(q)}}{\boxed{P(data\ set)}}$$

prior

evidence **(const wrt q)**

<u>What is the average number of WhatsUp messages I get every day?</u>

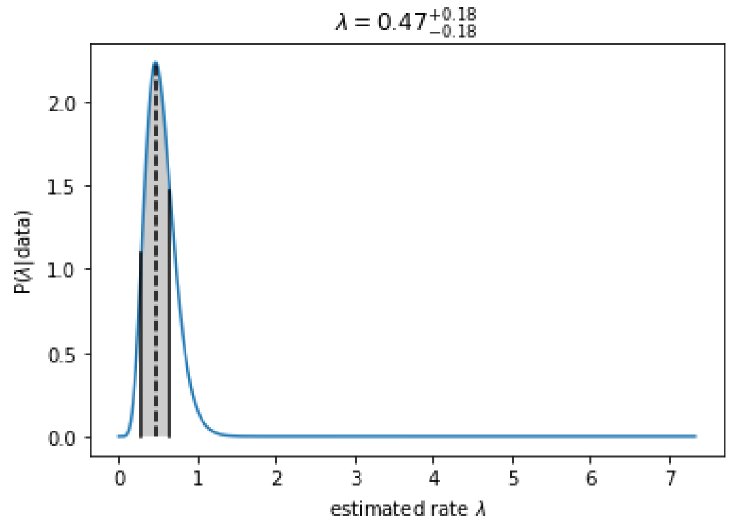
Mon:	5
Tue:	7
Wed:	1
Thu:	3
Fri:	9
Sat:	2
Sun:	5

event - has no duration
- is rare

→ Poissonian

$$P(k|\lambda) = \frac{\lambda^k}{k!}\, e^{-\lambda}$$

```
data = np.random.poisson(lam = 0.4, 15)
poissfit(data)
```



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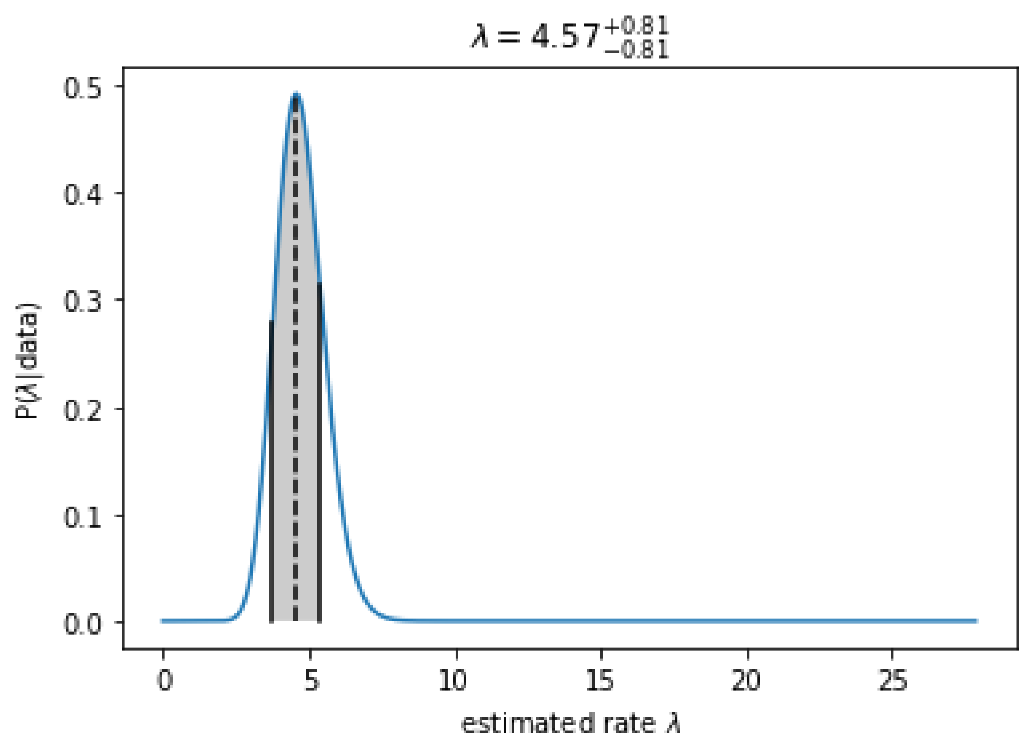
event
- has no duration
- is rare

→ Poissonian

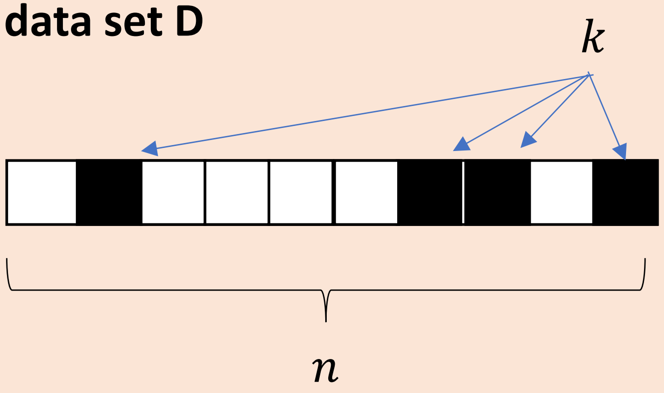
$$P(k|\lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$$

```
poissfit([5, 7, 1, 3, 9, 2, 5])
```



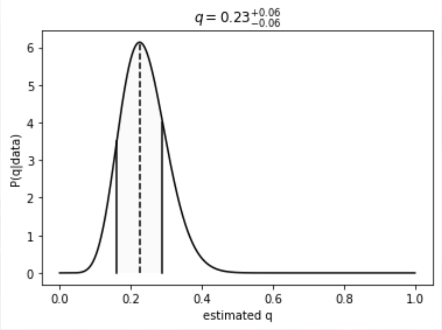
What if there is new data?

data set D

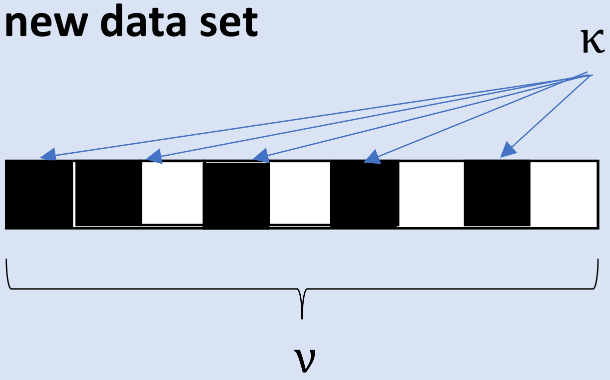


$\cancel{q = ?}$

$$\boxed{P(q|data\ set) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}}$$



new data set



if there **is** prior information ***I*** about *q*:

$$P(q|new\ data\ set, I) = \frac{P(new\ data\ set|q, I)\ \boldsymbol{P(q, I)}}{P(new\ data\ set)}$$

What if there is new data?

$$P(q|data\ set) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}$$

$$P(q|new\ data\ set, I) = \frac{P(new\ data\ set|q, I)\ \boldsymbol{P(q, I)}}{P(new\ data\ set)}$$

$$= \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ q^k(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ q^k(1-q)^{n-k}\ dq}$$

$$= \frac{q^{k+\kappa}(1-q)^{\nu-\kappa+n-k}}{\int_0^1 q^{k+\kappa}(1-q)^{\nu-\kappa+n-k}\ dq}$$

often: $\kappa = \alpha - 1$

$\beta = \nu - \kappa - 1$

$$= \frac{q^{k+\alpha-1}(1-q)^{n-k+\beta-1}}{\boxed{\int_0^1 q^{k+\alpha-1}(1-q)^{n-k+\beta-1}\ dq}}$$

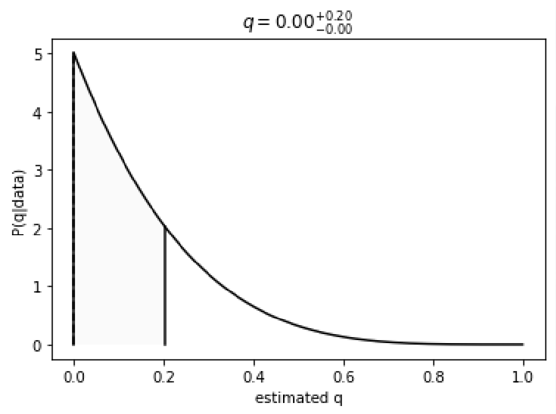
Beta function

What if there is new data?

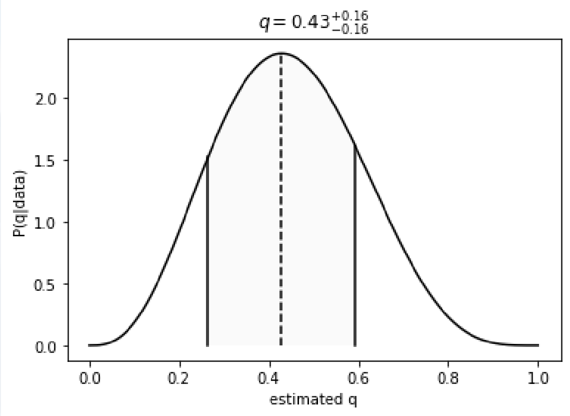
$$P(q|new\ data\ set, I) = \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}\ dq}$$

```python
n1 = 4
k1 = np.random.binomial(n1, q = 0.2)
[_, _, Prior] = bayesian_bino(n1, k1)
```

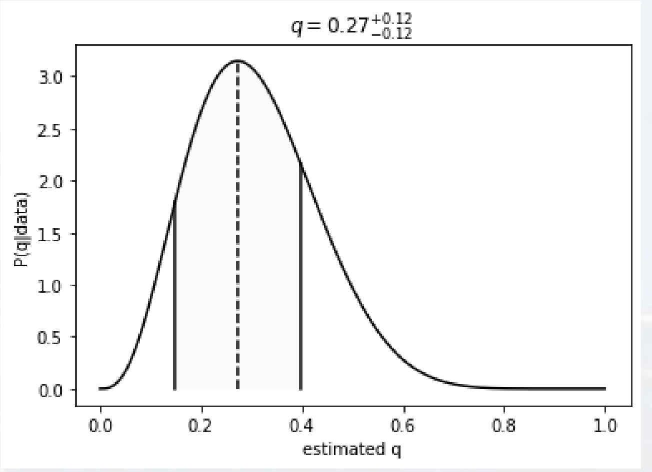
```python
n2 = 7
k2 = np.random.binomial(n2, q = 0.2)
[_, _, _] = bayesian_bino(n2, k2)
```



$$P(q, I) = \frac{q^{k}(1-q)^{n-k}}{\int_0^1 q^{k}(1-q)^{n-k}\ dq}$$




```python
[_ , _, _] = bayesian_bino(n2, k2, Prior = Prior)
```



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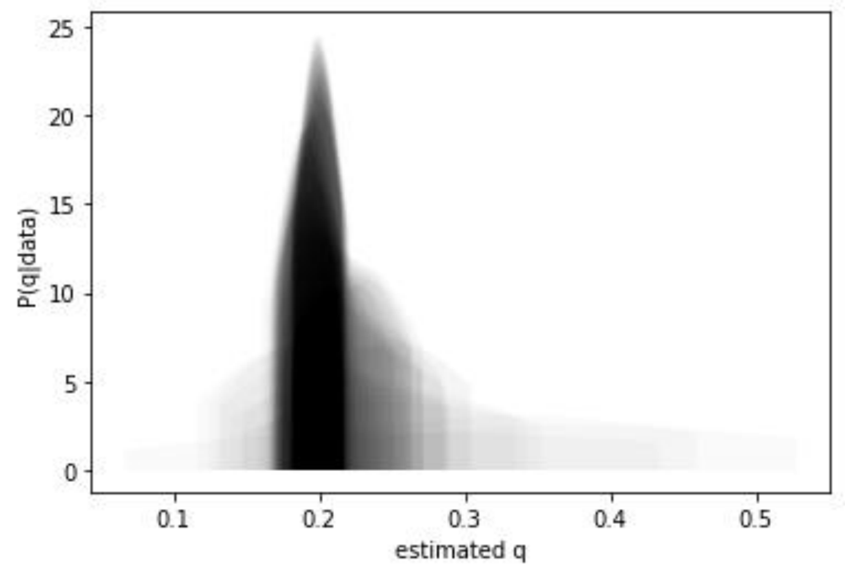
The **posterior** from the **previous** experiment is the **prior** of the **next** experiment



→ we become more certain about the model parameters
→ learning!

→ see e.g. **V**ariational **A**uto **E**ncoders

2D images → 3D objects

credit: StableAI

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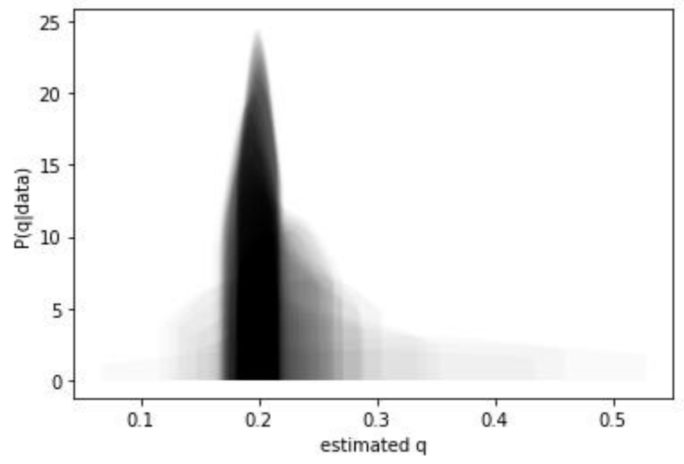

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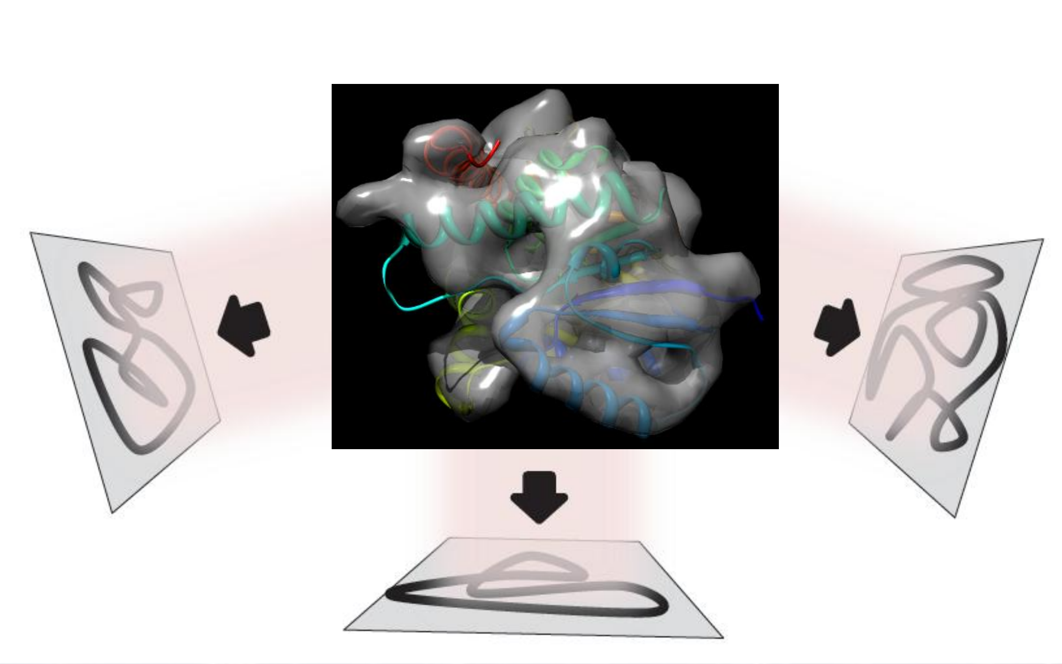
Cryo – EM: 3D structure from 2D images/projections



(image courtesy: Thomas Becker, GC LMU Munich)

Thank you very much for your attention!