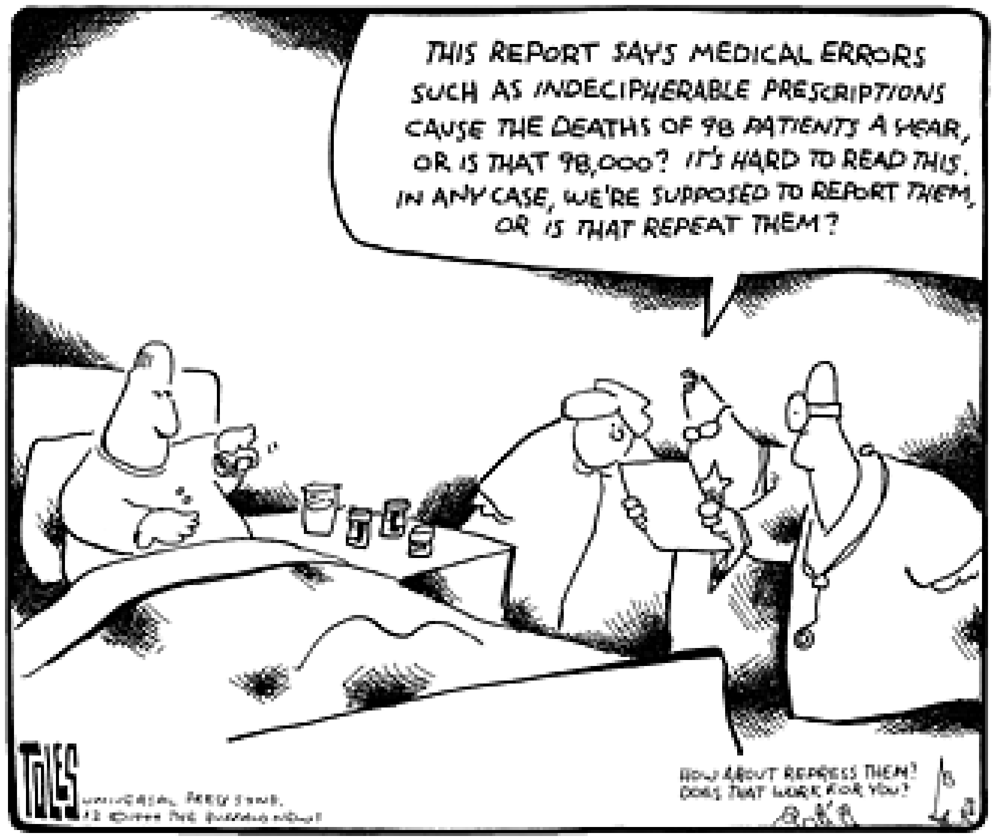


Outline:

Basics

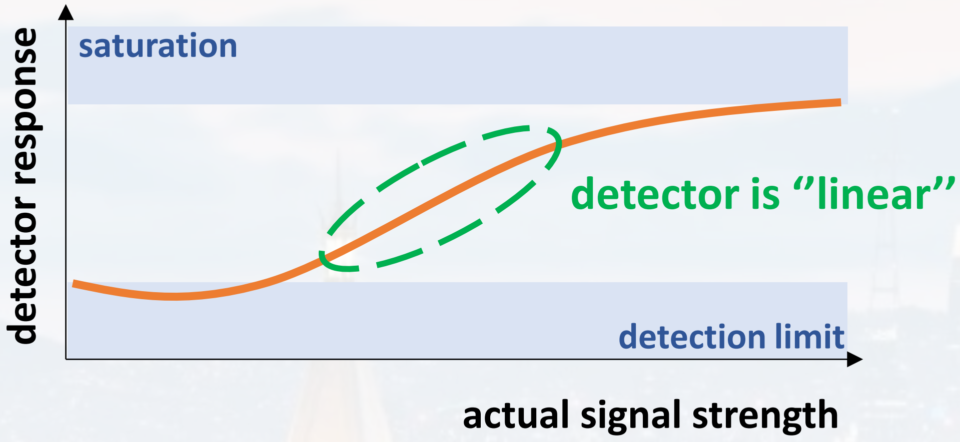
Most Common PDFs

- uniform
- binomial
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics

- **systematic errors:** calibration, non-linearity of the detector



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

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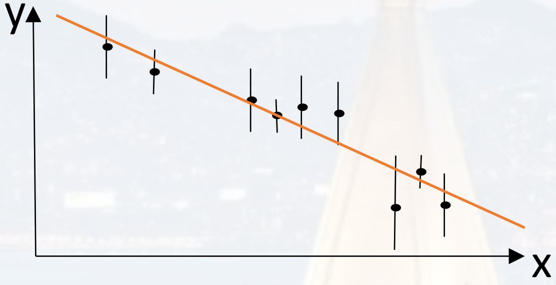
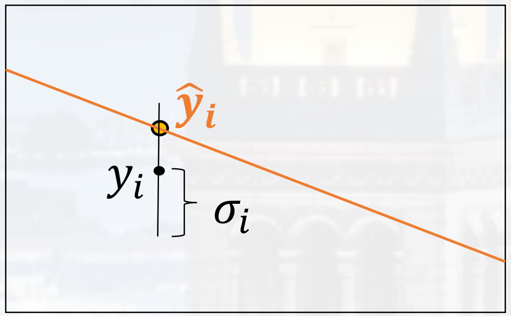
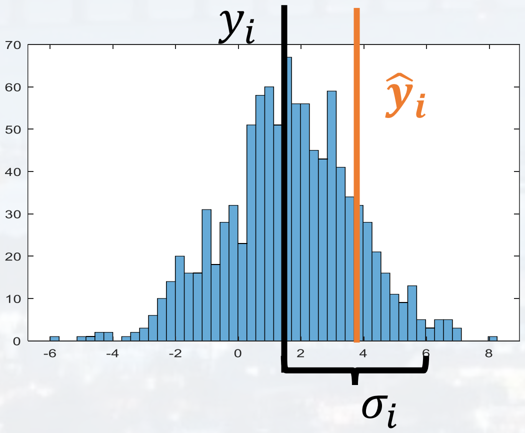
  → spread of the data around **an average value**

assumption: far from the detection limit and the saturation → the spread follows a normal distribution



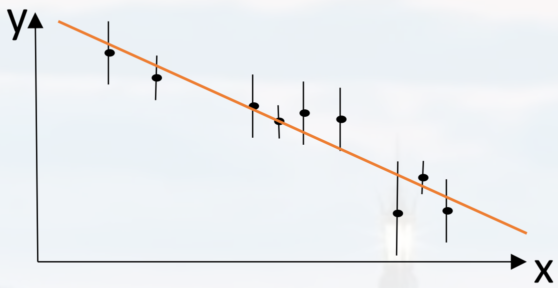
$$P(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\,\sigma^2}}\,exp\left[-\frac{(x-\mu)^2}{2\,\sigma^2}\right]$$

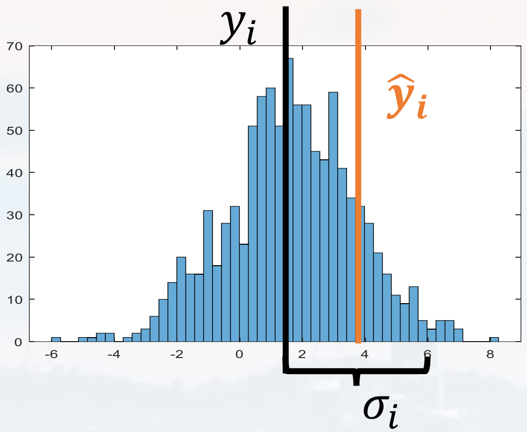




$$p_i(y_i|\hat{y}_i,\sigma_i) = \frac{1}{\sqrt{2\pi}\sigma_i}\,exp\left[-\frac{1}{2}\frac{(y_i-\hat{y}_i)^2}{{\sigma_i}^2}\right]$$

assumption: far from the detection limit and the saturation → the spread follows a **normal distribution**





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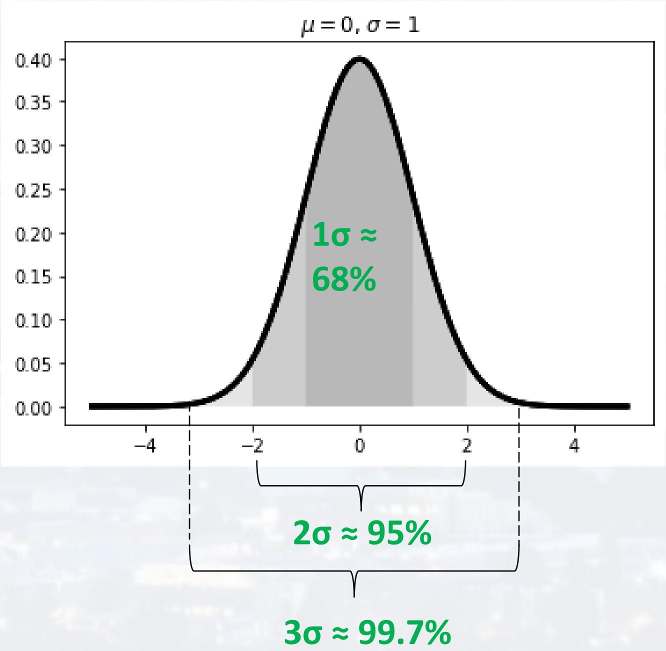
for large **(> 50…100)** N **(number of data points)**:

≈ **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



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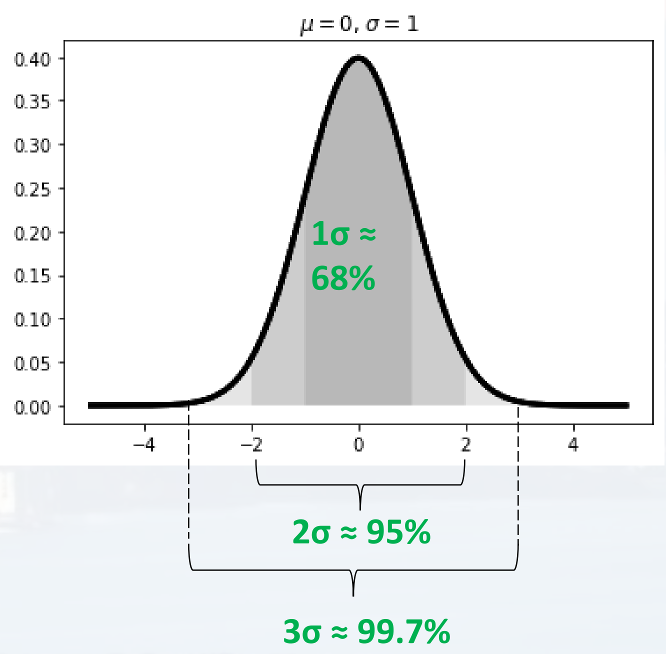


$$\chi^2_{red} = \frac{1}{df}\sum_{i=1}^{N}\left(\frac{y_i-\hat{y}_i}{\sigma_i}\right)^2 \qquad df = N - p - 1$$

rule of thumb:

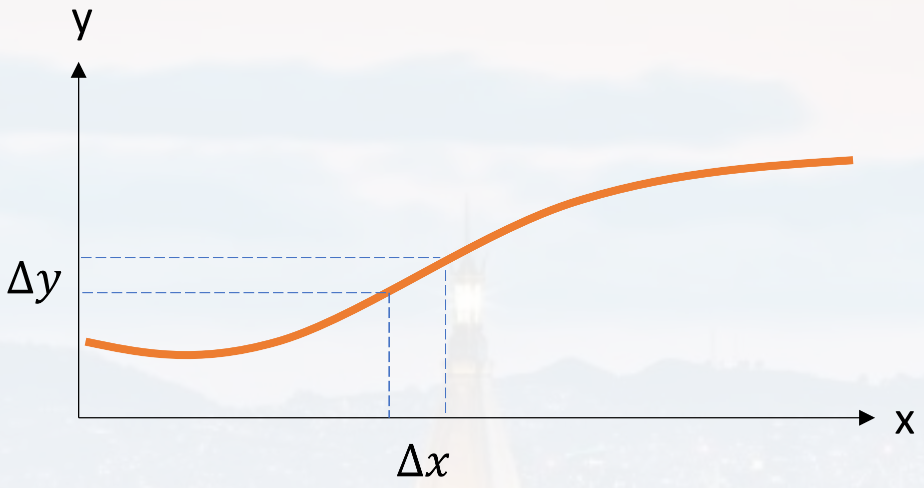
reduced χ^2 ≈

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!

y_i: measured value of data point
σ_i: statistical error of y_i (often aka ey_i)
$\hat{y}_i$: prediction by the model *after the fit*
N : number of data points
p: number of fit parameter

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:

$$V = \frac{4}{3}\pi r^3$$

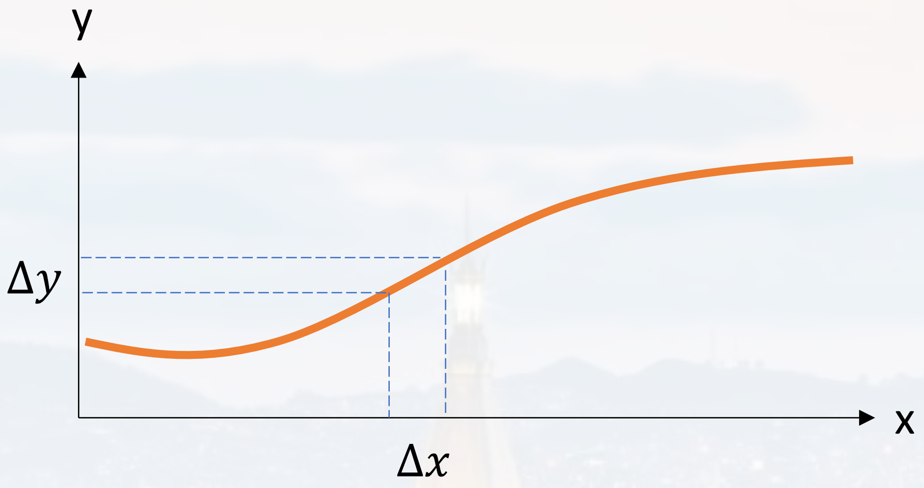
$\Delta V = ?$ given Δr

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

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

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

error propagation



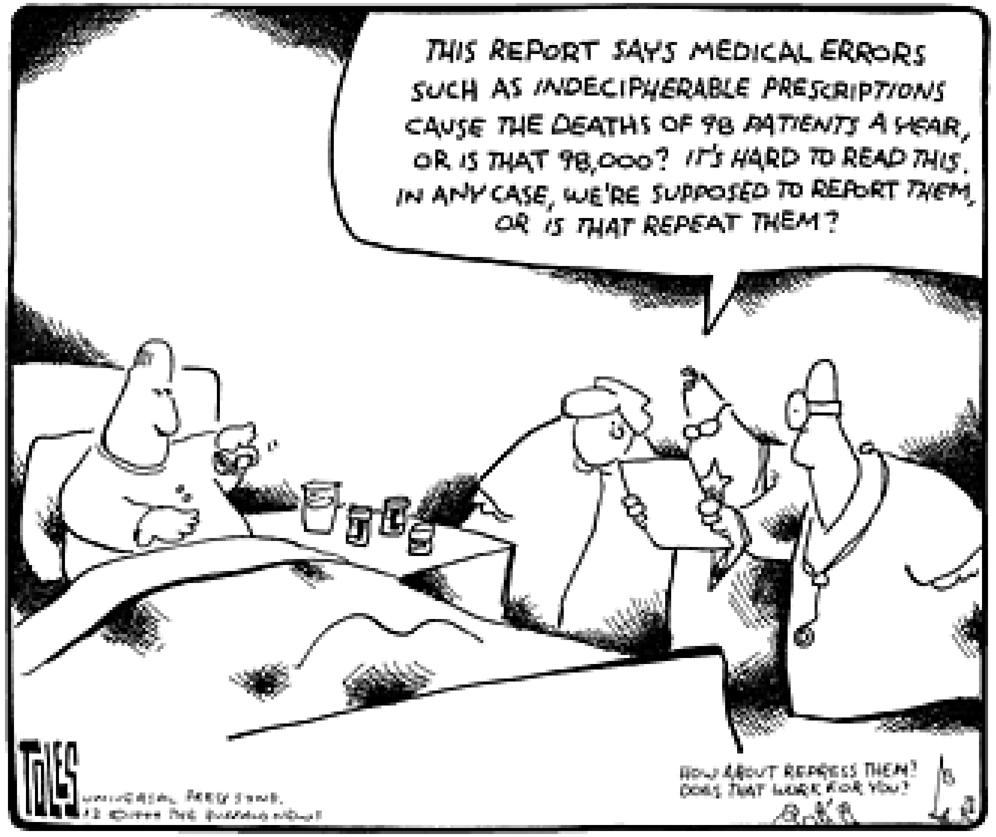
general:

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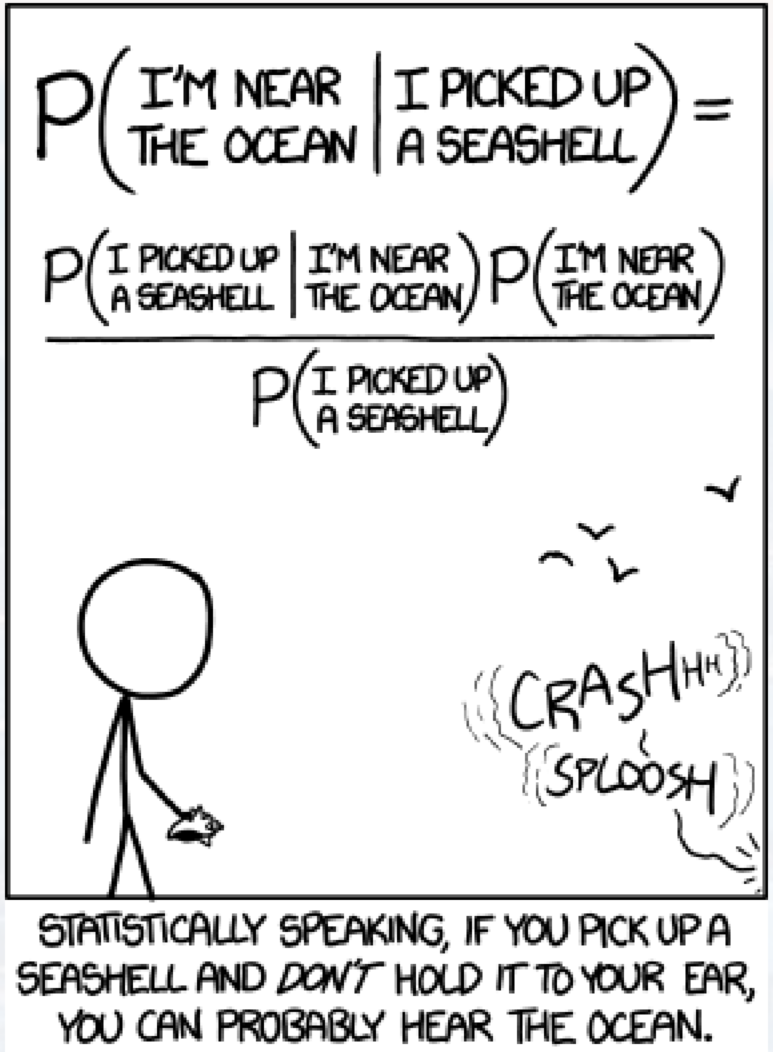
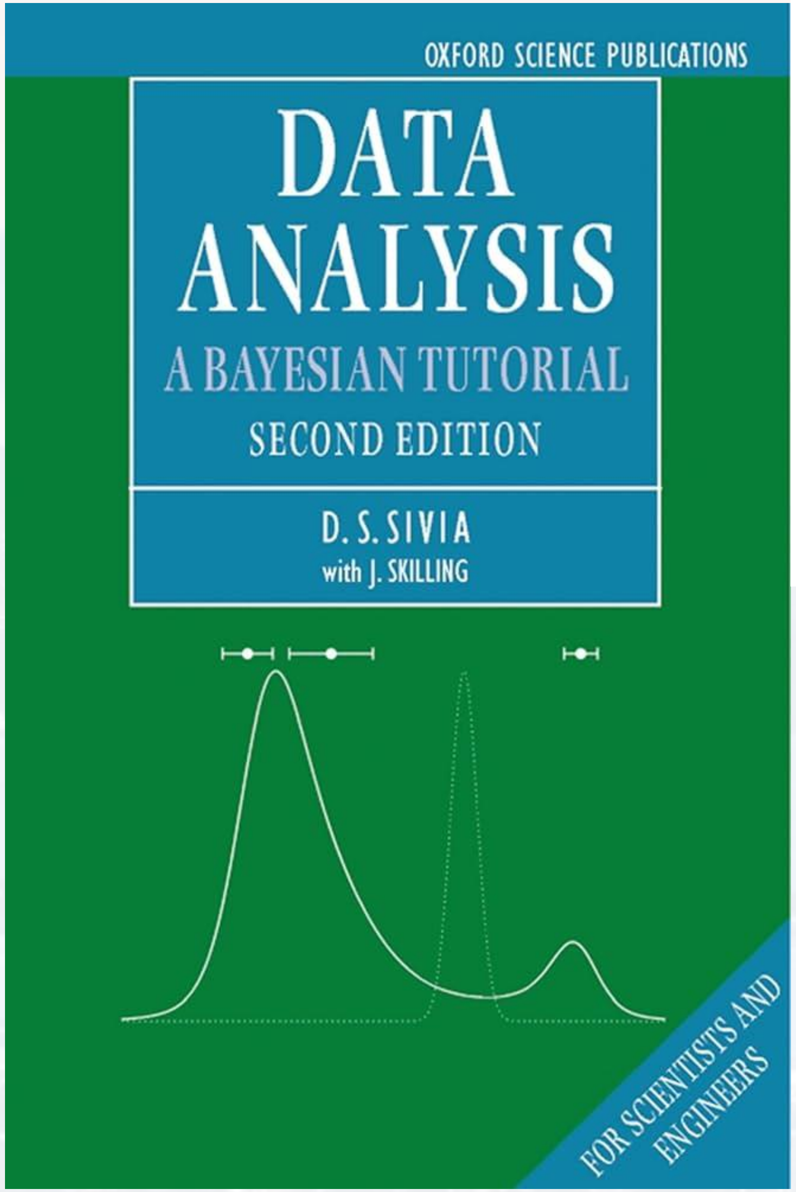

P(I'M NEAR THE OCEAN | I PICKED UP A SEASHELL) =
P(I PICKED UP A SEASHELL | I'M NEAR THE OCEAN) P(I'M NEAR THE OCEAN)
P(I PICKED UP A SEASHELL)
CRASHHH
SPLOOSH
STATISTICALLY SPEAKING, IF YOU PICK UP A SEASHELL AND *DON'T* HOLD IT TO YOUR EAR, YOU CAN PROBABLY HEAR THE OCEAN.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A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

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

Thomas Bayes (1701 - 1761)

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

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

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

Bayes Theorem

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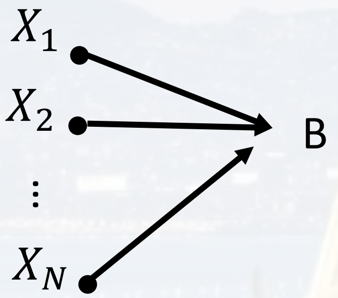
posterior $$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$ **prior**



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

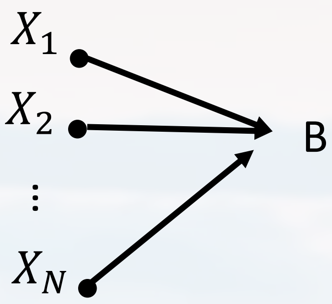
$$P(B) = \int P(B|X)P(X)\, dX$$

marginalization

example:

model: M
data: D

$$P(D|M) = \int P(D|all\ model\ param, M)\ P(all\ model\ param|M)\ \ d\ all\ model\ param$$



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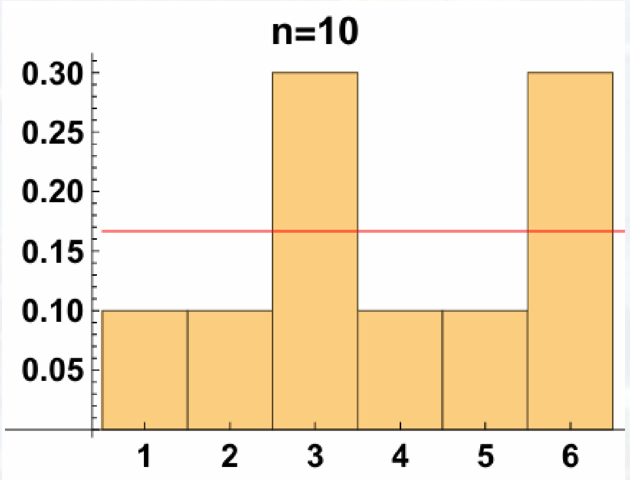
marginalization

Thomas Bayes
(1701 - 1761)

for a normal distribution $\mathcal{N}(\mu,\sigma)$ $\quad P(D|\mathcal{N}(\mu,\sigma)) = \int P(D|\mathcal{N}(\mu,\sigma))\,P(\mu,\sigma|\mathcal{N}(\mu,\sigma))\,d\,\Omega_{\mu,\sigma}$

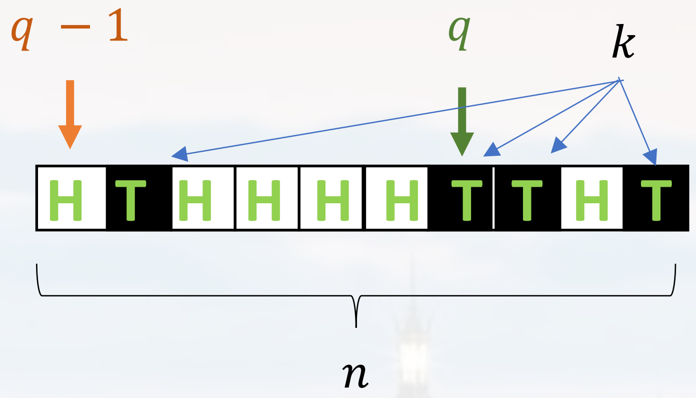


σ = 2, μ = 3.5

σ = 2, μ = 5.0

σ = 1.5, μ = 3.5

σ = 7.0, μ = 1.0



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

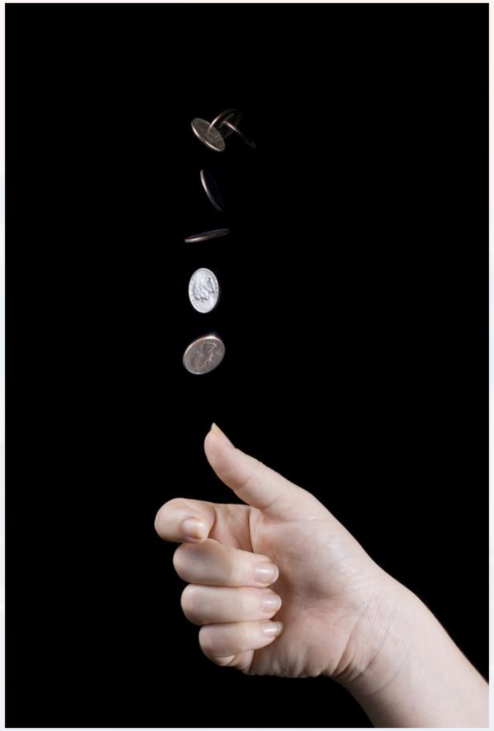
$$p_{tot} = \prod_i q_i{}^{n_i} = q^k \, (1-q)^{n-k}$$

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

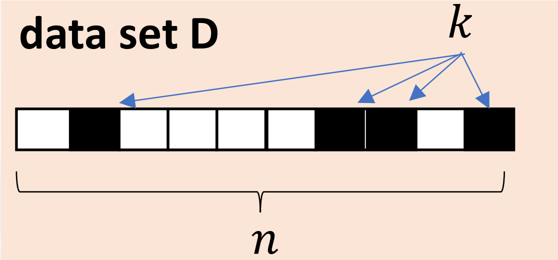
$$\boxed{P(k|q,n) = \binom{n}{k} \, q^k \, (1-q)^{n-k}}$$

binomial distribution

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



fair coin? q = 0.5 ???

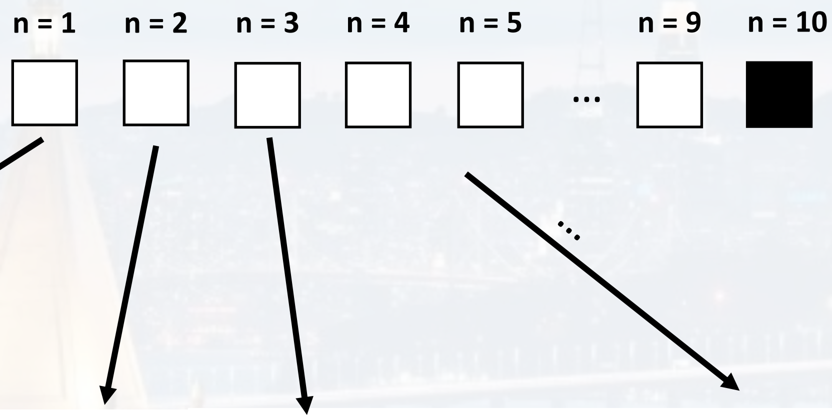


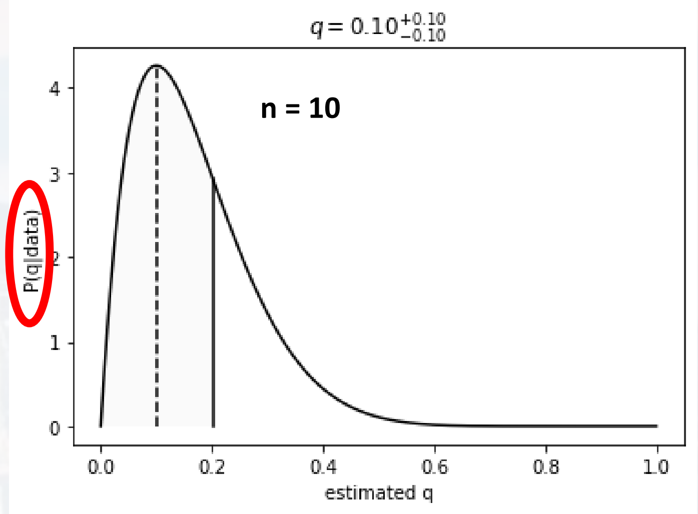
$\boldsymbol{q} = ?$

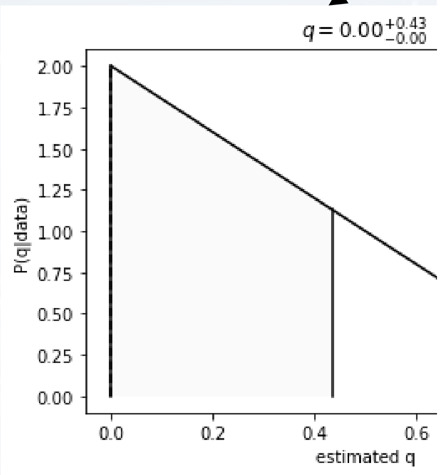
goal:

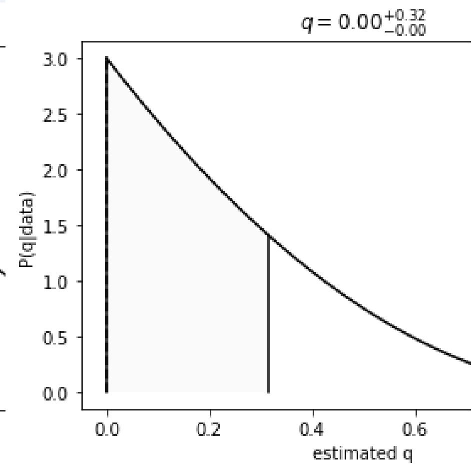
- **P(q|D)** **Parameter Estimation**
- the larger ***D***, the more certain ***q***

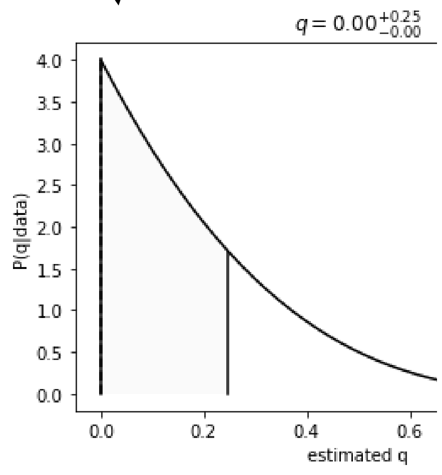
  → learning

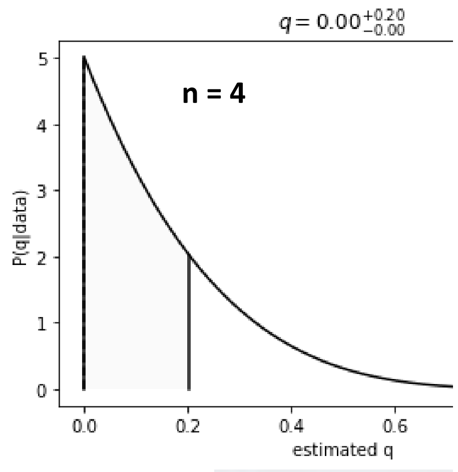


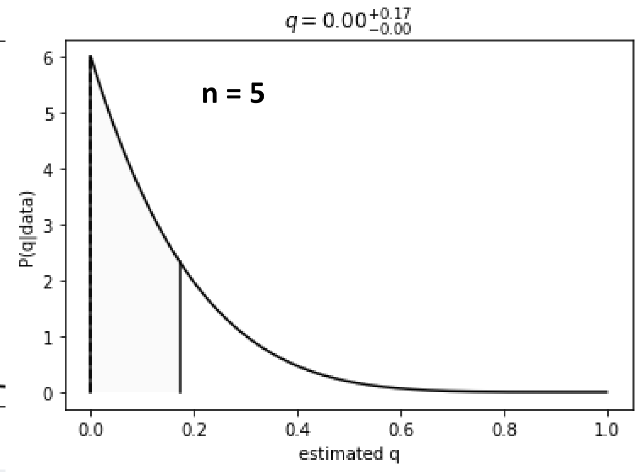


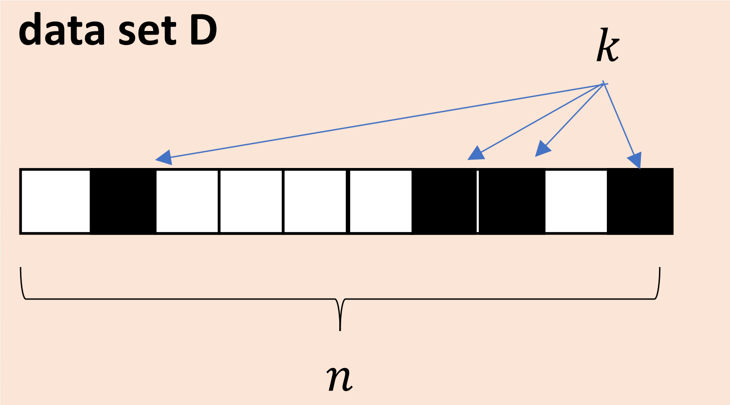












$\boldsymbol{q} = ?$

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)**

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

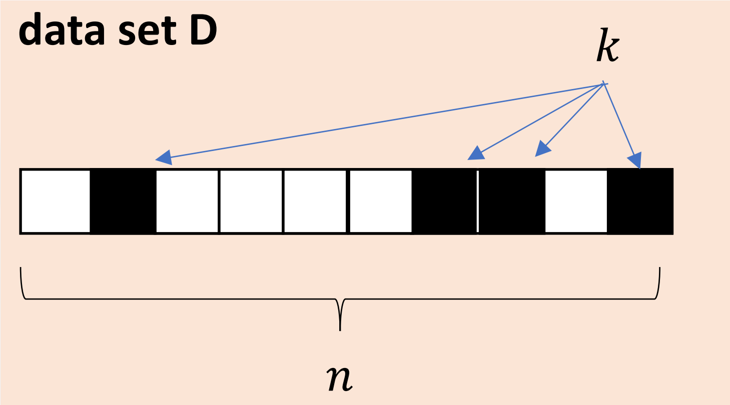
prior

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



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

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

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

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

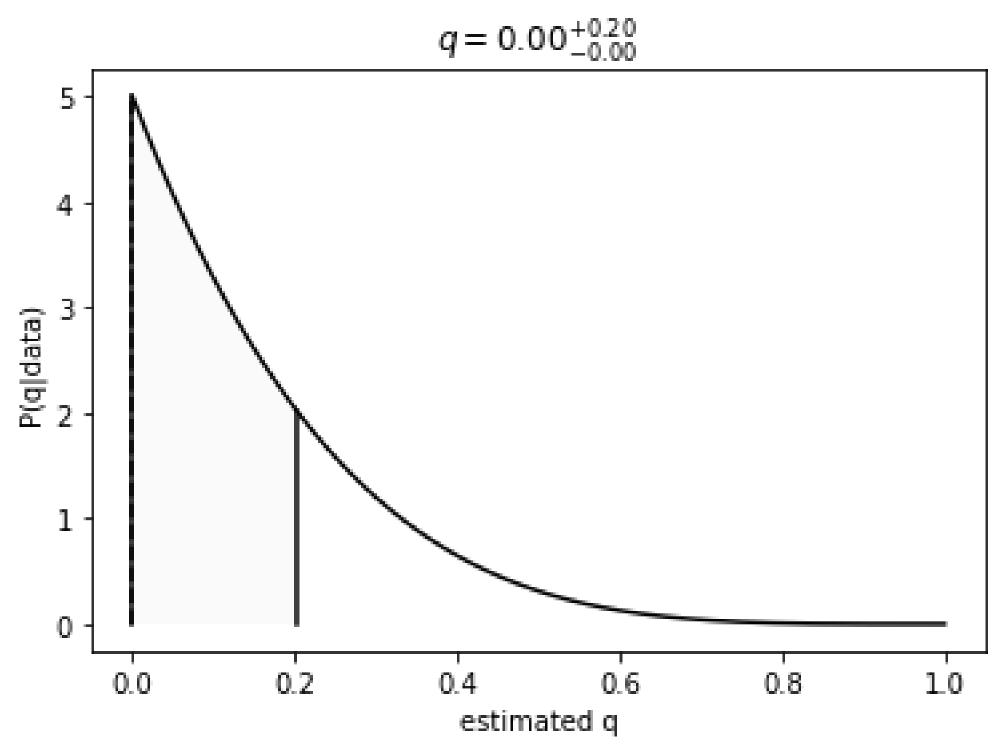
check out `bayesian_bino.py`

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

```
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)
```



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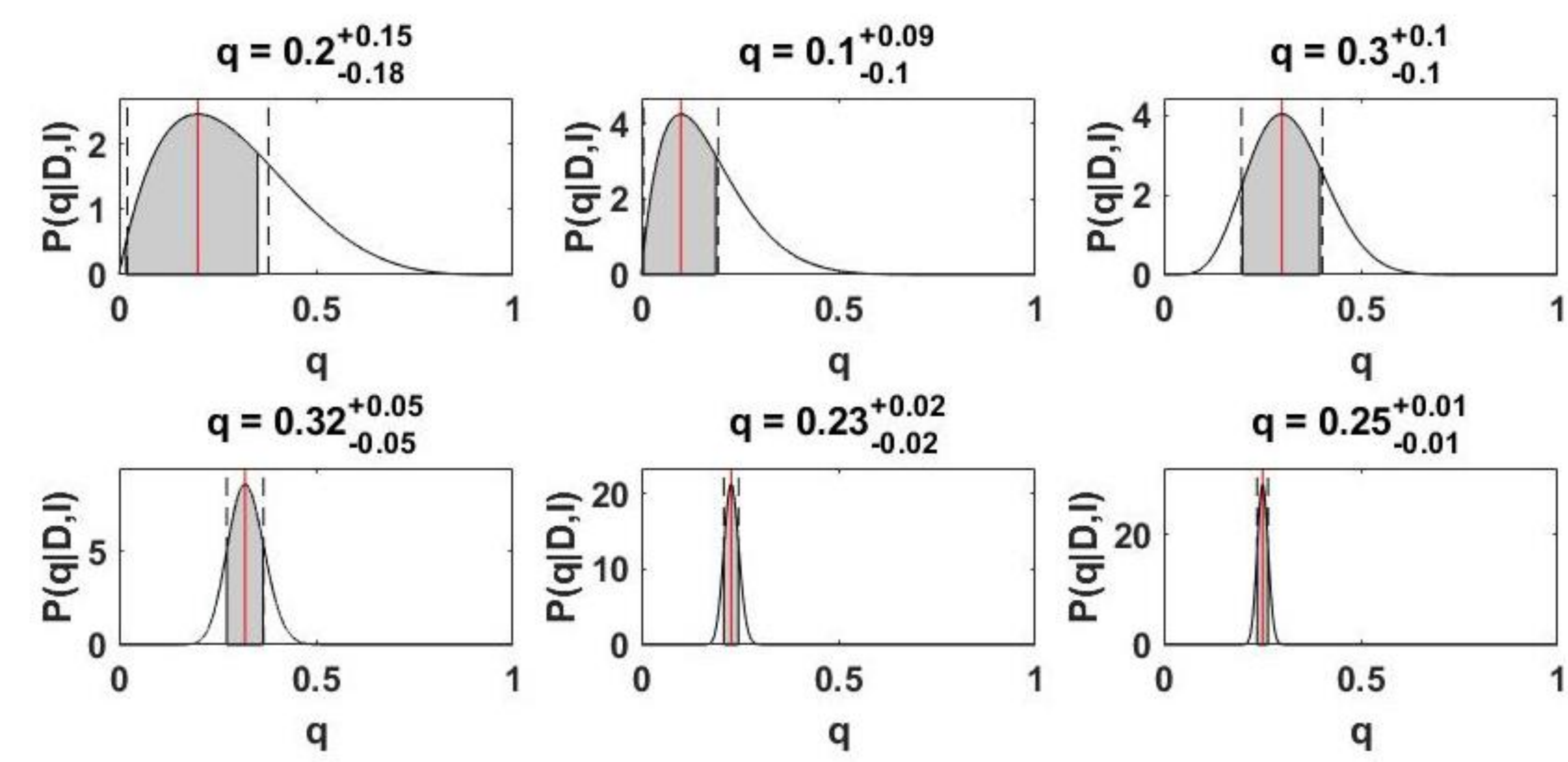

n	estimated q
5	$0.2^{+0.15}_{-0.18}$
10	$0.1^{+0.09}_{-0.1}$
20	$0.3^{+0.1}_{-0.1}$
50	$0.2^{+0.05}_{-0.06}$
100	$0.32^{+0.05}_{-0.05}$
500	$0.23^{+0.02}_{-0.02}$
1,000	$0.25^{+0.01}_{-0.01}$
infinity	0.25

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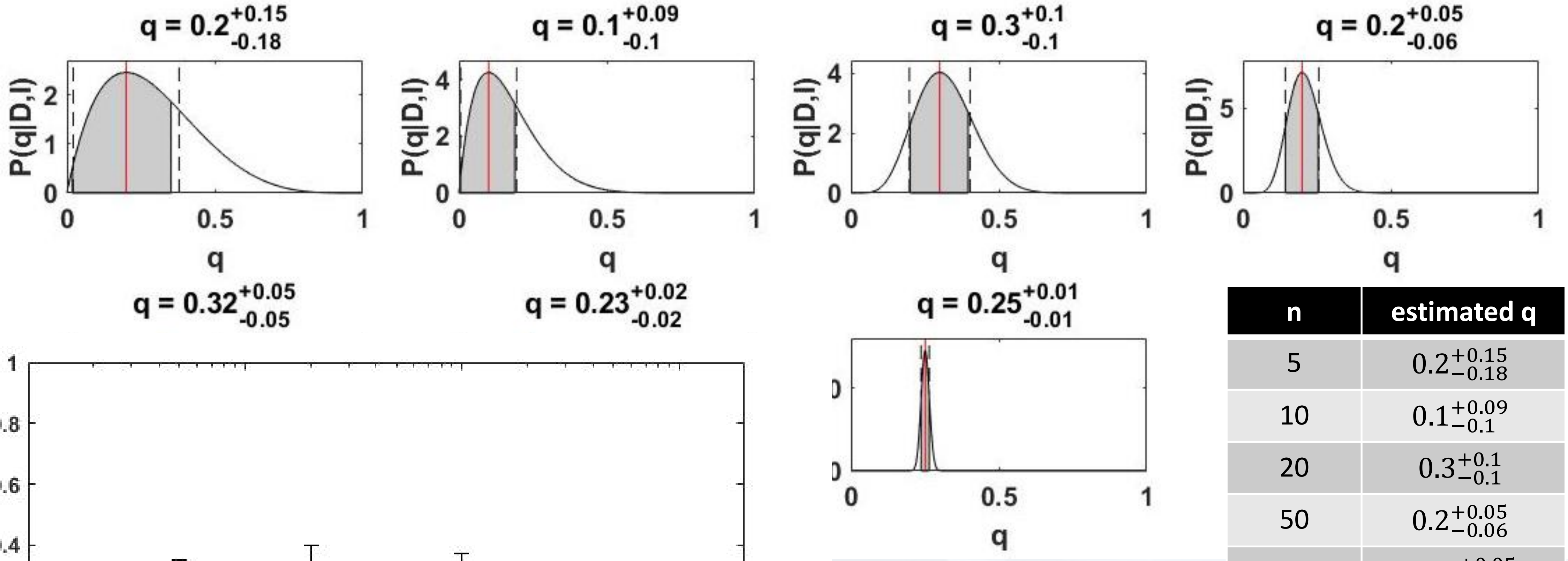

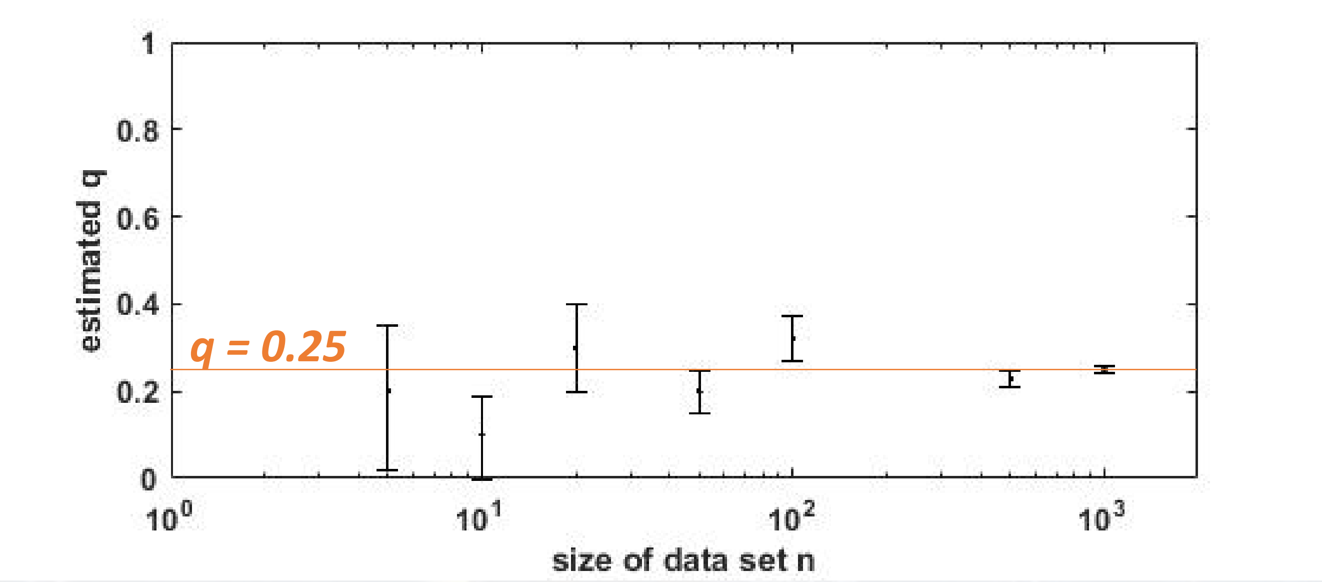

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infinity	0.25

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

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likelihood function

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

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evidence **(const wrt q)**

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

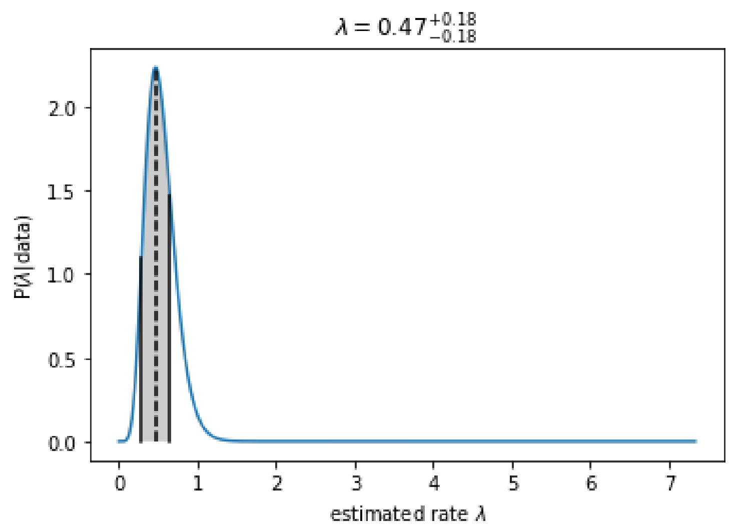
Mon:	5
Tue:	7
Wed:	1
Thu:	3
Fri:	9
Sat:	2
Sun:	5

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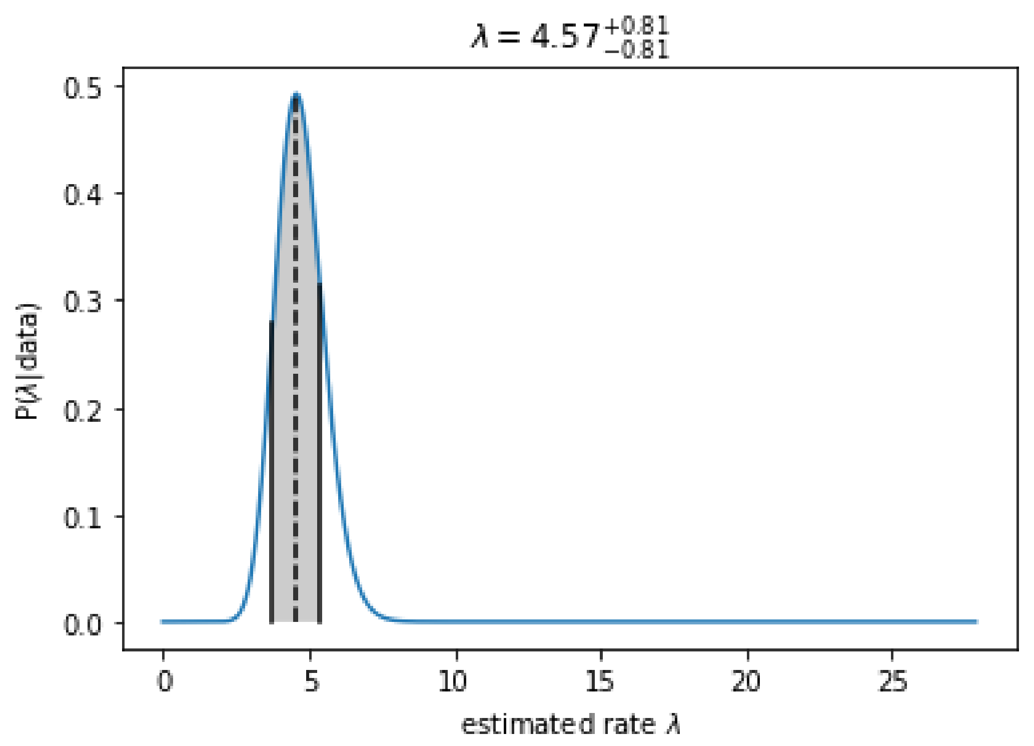
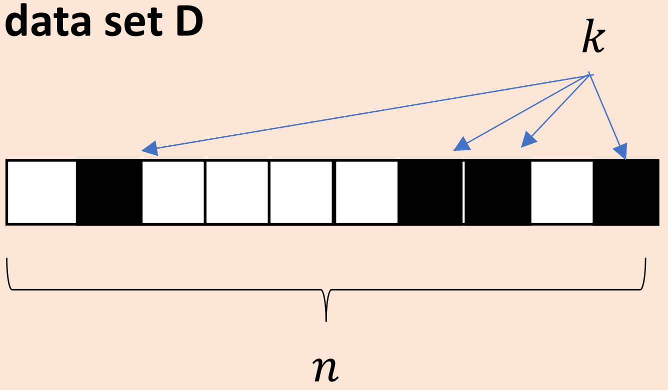
```
poissfit([5, 7, 1, 3, 9, 2, 5])
```



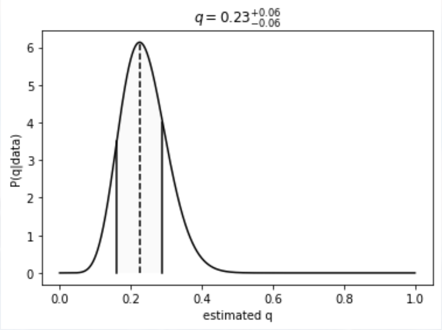
What if there is new data?

data set D

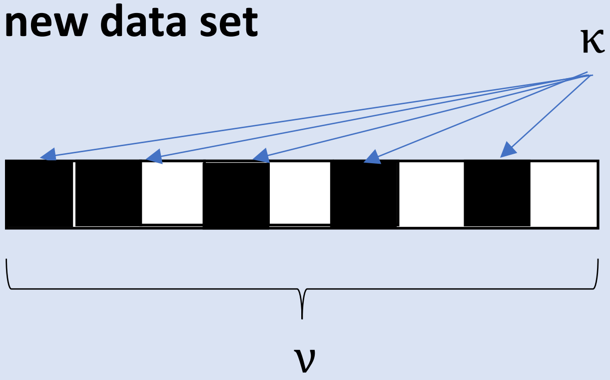


$\cancel{q = ?}$

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



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: $\kappa = \alpha - 1$

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

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

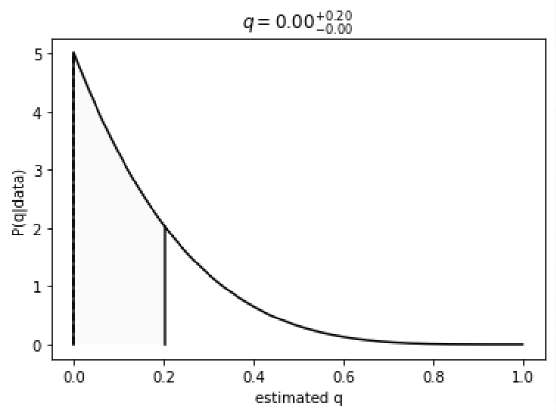
Beta function

What if there is new data?

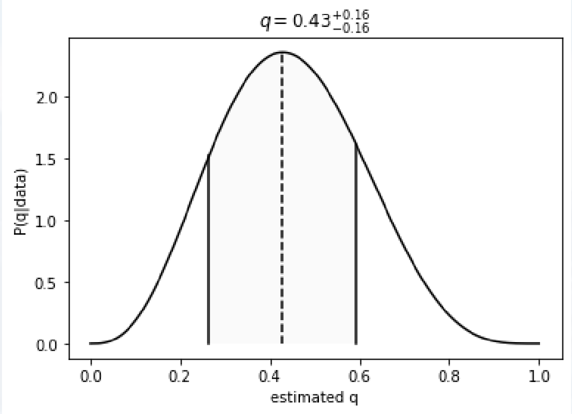
$$P(q|new\ data\ set, I) = \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}\ dq}$$

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

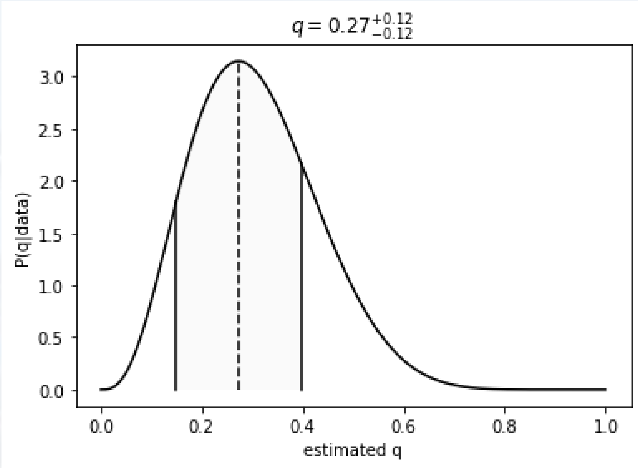
```
n2 = 7
k2 = np.random.binomial(n2, q = 0.2)
[_, _, _] = bayesian_bino(n2, k2)
```



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



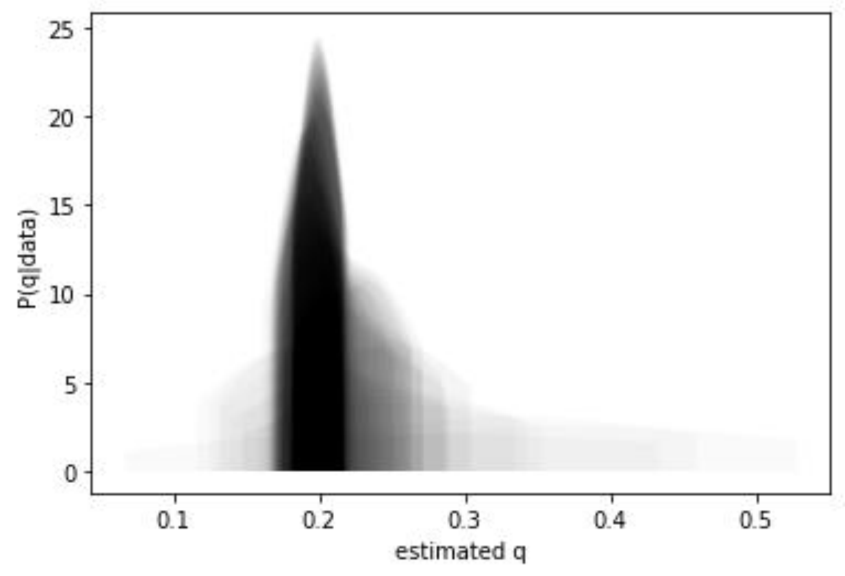

```
[_ , _, _] = bayesian_bino(n2, k2, Prior = Prior)
```



What if there is new data?

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

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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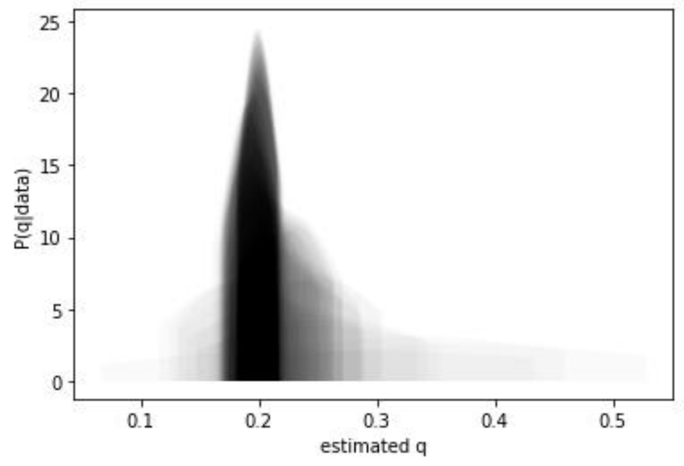
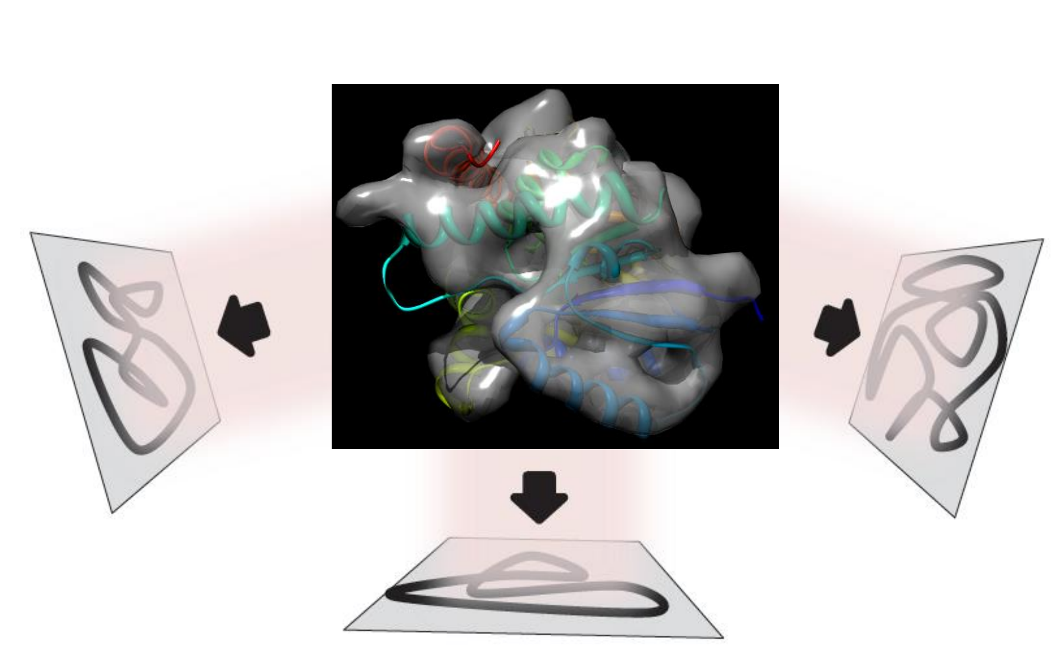


→ we become more certain about the model parameters
→ learning!

→ see e.g. **V**ariational **A**uto **E**ncoders   2D images → 3D objects

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



(image courtesy: Thomas Becker, GC LMU Munich)

Thank you very much for your attention!