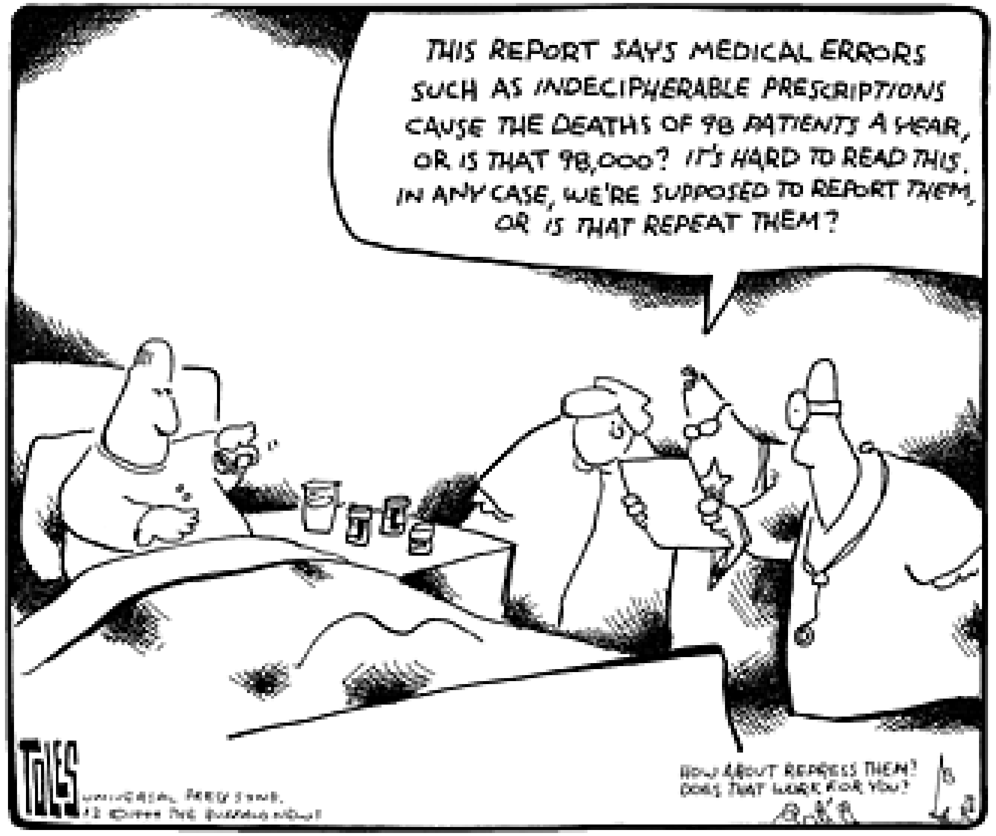
Berkeley
UNIVERSITY OF CALIFORNIA

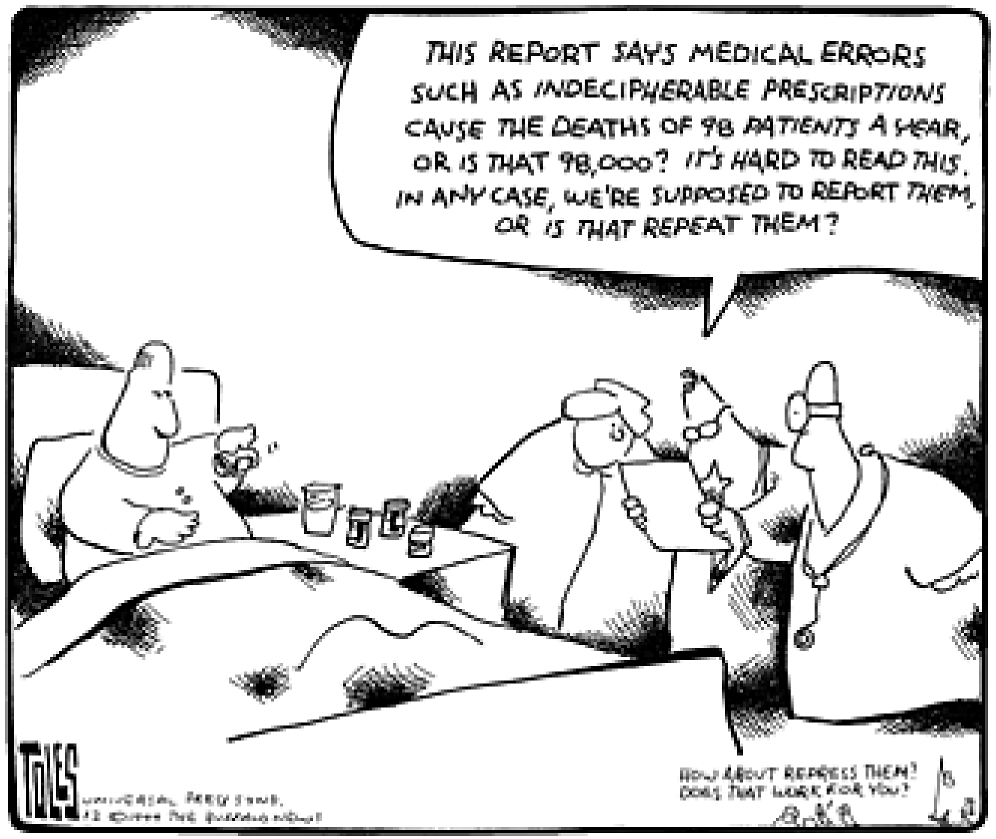
M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



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)



Outline:

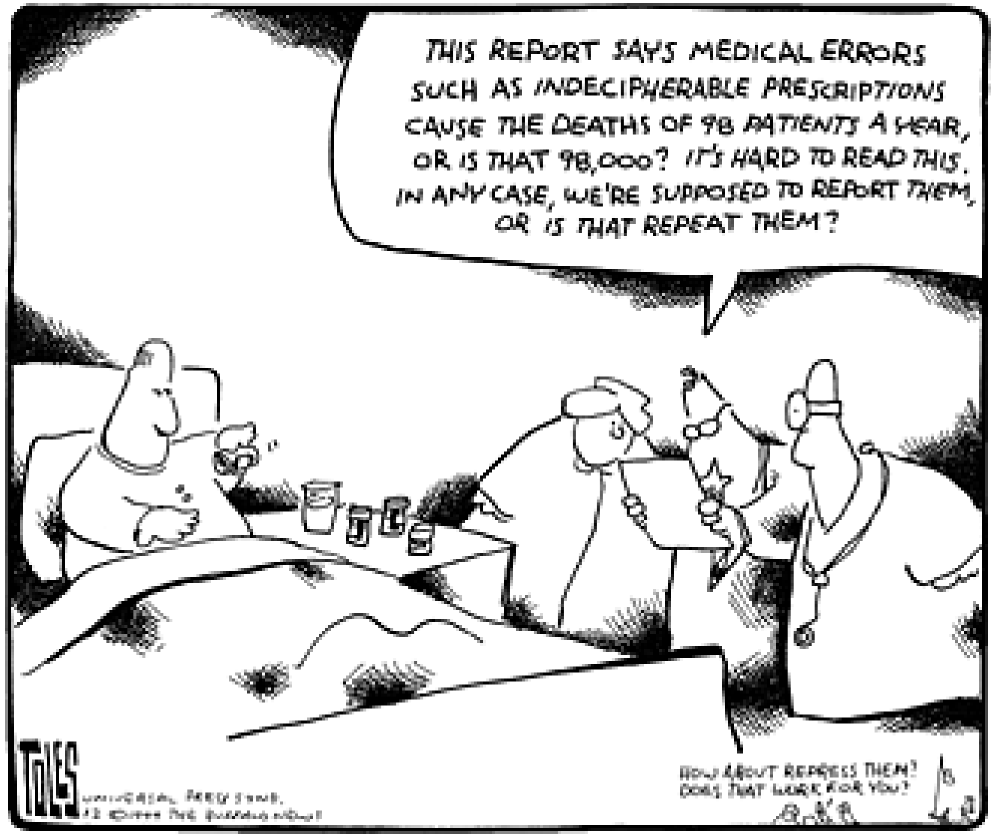
Basics

Most Common PDFs

- uniform
- binomial
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics



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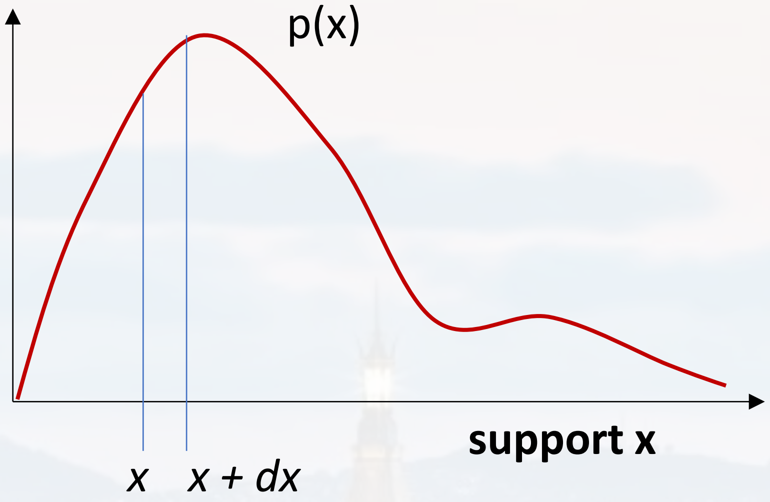


probability **d**ensity **f**unction [a ≤ x ≤ b]

p(x) dx $\int_a^b p(x)\,dx = 1$

Cumulative **d**ensity **f**unction

$$P(x) = \int_a^x p(x)\,dx$$

mean $\mu = E(x) = \int x\,p(x)\,dx$

What is the mean of a fair, six sided die?

variance $\sigma^2 = var(x) = \int (x-\mu)^2\,p(x)\,dx$

median *m* $\int_a^m p(x)\,dx = \frac{1}{2}$

mean $\mu = E(x) = \int x\, p(x)\, dx$

variance $\sigma^2 = var(x) = \int (x-\mu)^2\, p(x)\, dx$

$$var(x) = \int (x-\mu)^2\, p(x)\, dx = E([x-\mu]^2)$$

$$= E(x^2 - 2x\mu + \mu^2)$$

the mean is a linear operator

$$= E(x^2) - 2\mu\, E(x) + \mu^2 \boxed{E(1)}$$

$$\int_a^b p(x)\, dx = 1$$

$$= E(x^2) - 2\mu\, E(x) + \mu^2$$

$$\mu = E(x)$$

$$\boldsymbol{\sigma^2 = E(x^2) - E(x)^2}$$

mean $\mu = E(x) = \int x\, p(x)\, dx$

a, b = const

variance $\sigma^2 = var(x) = \int (x-\mu)^2\, p(x)\, dx$

$$var([a\,x_1 + b\,x_2]) = E([a\,x_1 + b\,x_2]^2) - E(a\,x_1 + b\,x_2)^2$$

$$\sigma^2 = E(x^2) - E(x)^2$$

$$= E(a^2\,x_1^2 + 2ab\,x_1 x_2 + b^2\,x_2^2) - E(a\,x_1 + b\,x_2)^2$$

$$= a^2 E(x_1^2) + 2ab\,E(x_1 x_2) + b^2\,E(x_2^2) - E(a\,x_1 + b\,x_2)^2$$

$$= a^2 E(x_1^2) + 2ab\,E(x_1 x_2) + b^2\,E(x_2^2) - [aE(x_1) + b\,E(x_2)]^2$$

$$= \boxed{a^2 E(x_1^2)} + 2ab\,E(x_1 x_2) + \boxed{b^2\,E(x_2^2)} \boxed{- a^2 E(x_1)^2} - \boxed{b^2 E(x_2)^2} - 2abE(x_1)E(x_2)$$

$\boldsymbol{a^2\, var(x_1)}$ $\boldsymbol{b^2\, var(x_2)}$

mean $\mu = E(x) = \int x\, p(x)\, dx$

a, b = const

variance $\sigma^2 = var(x) = \int (x-\mu)^2\, p(x)\, dx$

$$var([a\,x_1 + b\,x_2]) = E([a\,x_1 + b\,x_2]^2) - E(a\,x_1 + b\,x_2)^2$$

$$\sigma^2 = E(x^2) - E(x)^2$$

$$= \boxed{a^2 E(x_1^2)} + \boxed{2ab\, E(x_1 x_2)} + \boxed{b^2\, E(x_2^2)} \boxed{- a^2 E(x_1)^2} \boxed{- b^2 E(x_2)^2} - \boxed{2abE(x_1)E(x_2)}$$

$\boldsymbol{a^2\, var(x_1)}$ $\boldsymbol{b^2\, var(x_2)}$ $\boldsymbol{2ab\, cov(x_1, x_2)}$

$$= \boldsymbol{a^2\, var(x_1)} + \boldsymbol{b^2\, var(x_2)} + \boldsymbol{2ab\, cov(x_1, x_2)}$$

$$\boldsymbol{cov(x_1, x_2)} = \boldsymbol{cov(x_2, x_1)} = E(x_1 x_2) - E(x_1)E(x_2)$$ **covariance**

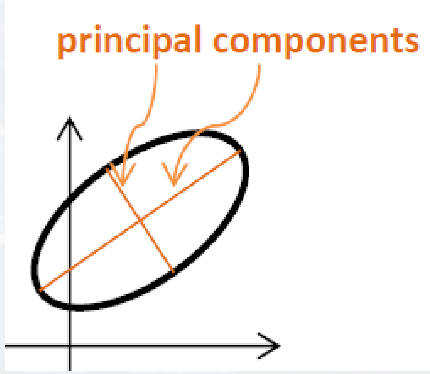
$$ab = c$$

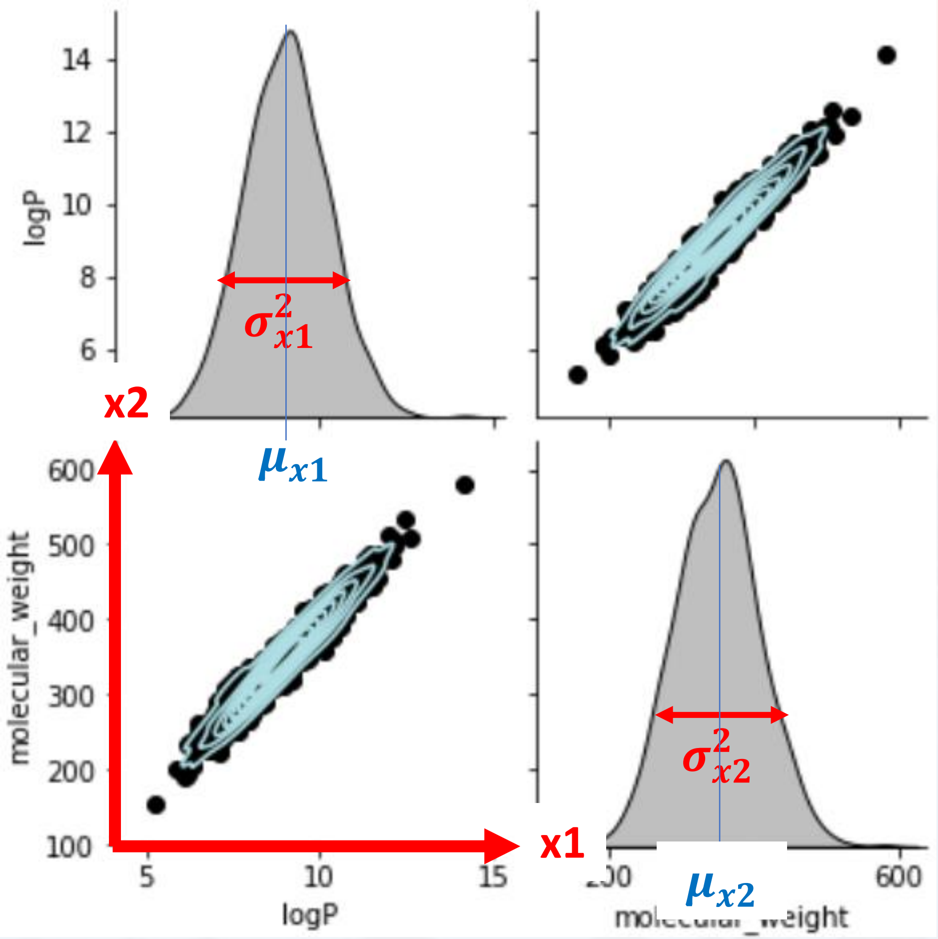
const $= a^2\, var(x_1) + b^2\, var(x_2) + 2c\, cov(x_1, x_2)$

covariance matrix

$$const = \begin{pmatrix} x1-\mu_{x1} \\ x2-\mu_{x2} \end{pmatrix}^T \boxed{\begin{pmatrix} a & c_{12} \\ c_{21} & b \end{pmatrix}} \begin{pmatrix} x1-\mu_{x1} \\ x2-\mu_{x2} \end{pmatrix}$$

$= v^T S v$ ... called **quadric** (also in N-D)





PCA: data in eigen coordinates → variances are the eigenvalues

mean $\mu = E(x) = \int x\, p(x)\, dx$

median *m* $\int_a^m p(x)\, dx = \frac{1}{2}$

variance $\sigma^2 = var(x) = \int (x-\mu)^2\, p(x)\, dx$

$$\sigma^2 = E(x^2) - E(x)^2$$

$$\sigma_{tot}^2 = \sigma_1^2 + \sigma_2^2 + 2\, cov(x_1, x_2)$$

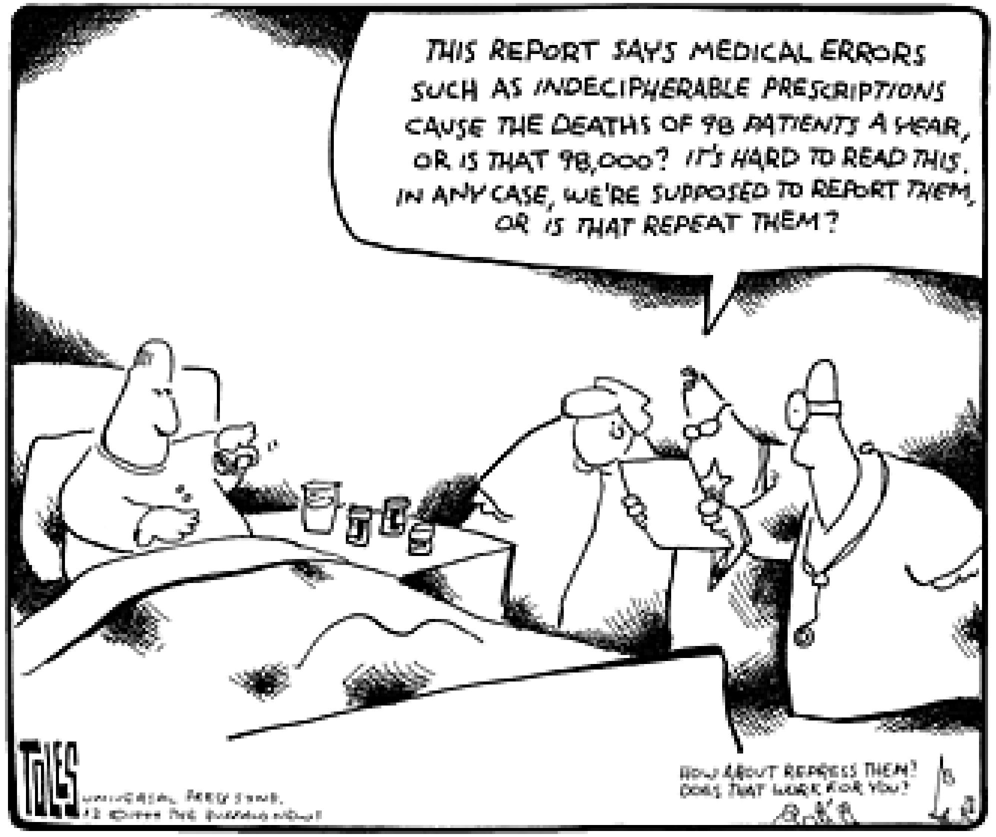
note:

$\int (x-\mu)^n\, p(x)\, dx$

called nth *moment* of a pdf

covariance $cov(x_1, x_2) = E(x_1 x_2) - E(x_1)E(x_2)$

correlation coefficient $\rho(x_1, x_2) = \frac{cov(x_1, x_2)}{\sqrt{\sigma_1^2 \sigma_2^2}}$



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finding those $p(x)$ that maximize the **entropy S**, given constrains **C**

$$S = -\int p(x) \ln[p(x)]\, dx$$

C: $\int p(x)\, dx = 1 \longrightarrow p(x) = const$

$$\mu = \int_a^b x\, p(x)\, dx = const \int_a^b x\, dx = const\, \frac{1}{2}(b^2 - a^2)$$

$$\int_a^b p(x)\, dx = 1 \qquad const \int_a^b dx = 1 \qquad \rightarrow const = \frac{1}{b-a}$$

$$\boxed{\mu = \frac{1}{2}\frac{b^2 - a^2}{b - a}}$$

$$\boxed{\sigma^2 = \frac{1}{12}(b-a)^2}$$

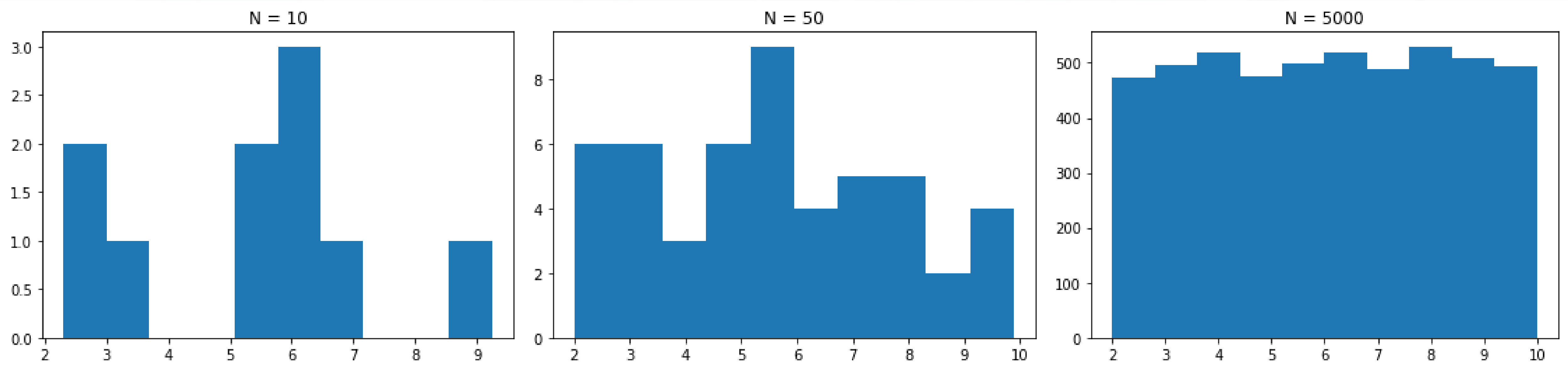
Note: the uniform distribution has the largest entropy
→ maximum ignorance = no prior information = unbiased

$p(x) = const$

plotting the pdf

```
U = np.random.uniform(low, high, shape)
plt.hist(U)
```

continuous support



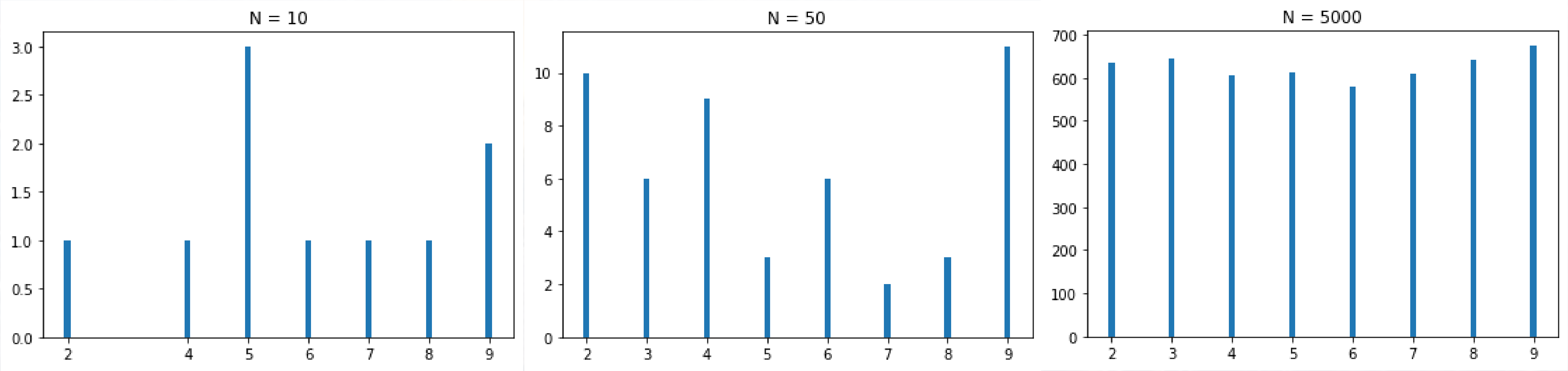
$p(x) = const$

plotting the pdf

```
U = np.random.randint(low, high, shape)
```

discrete support

```
labels, counts = np.unique(U, return_counts = True)
plt.bar(labels, counts, align = 'center', width = 0.1)
plt.gca().set_xticks(labels)
plt.title('N = ' + str(N))
```



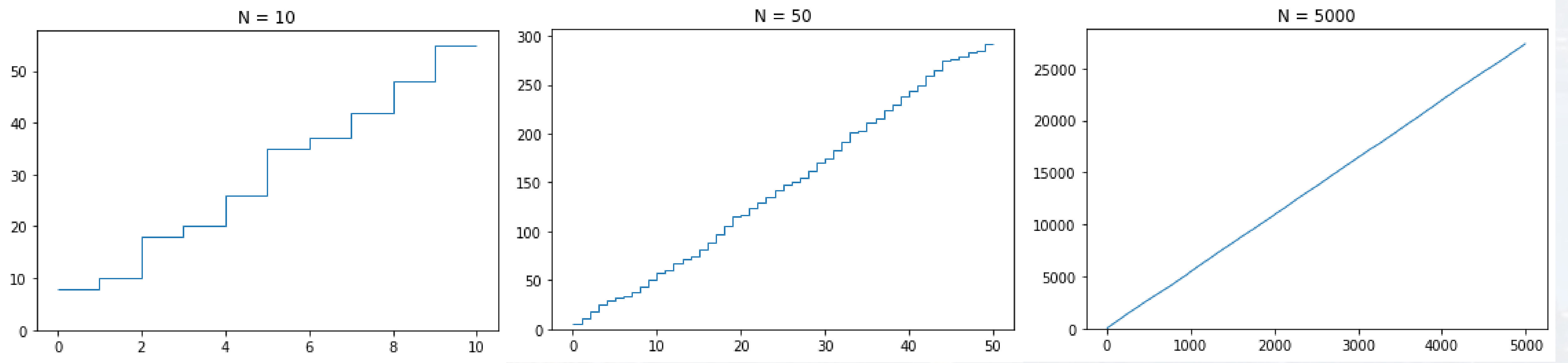
$p(x) = const$

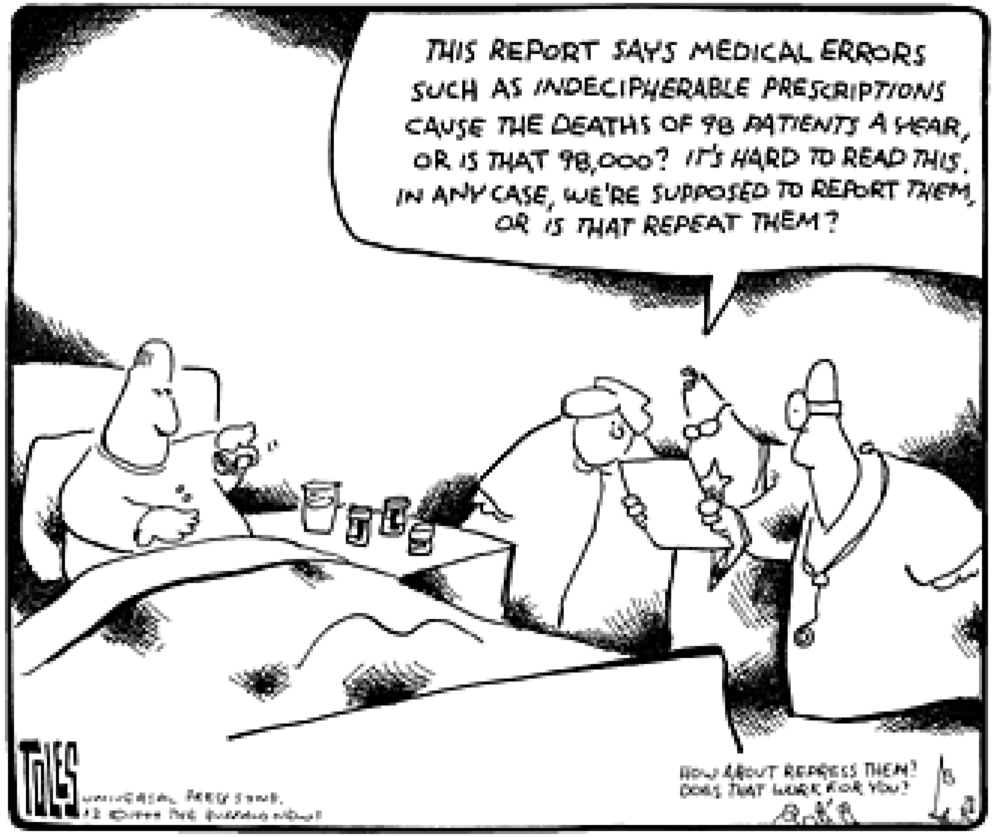
plotting the cdf

```
U = np.random.randint(low, high, shape)

C = np.cumsum(U)
plt.stairs(C, baseline = None)
plt.title('N = ' + str(N))
```

discrete support





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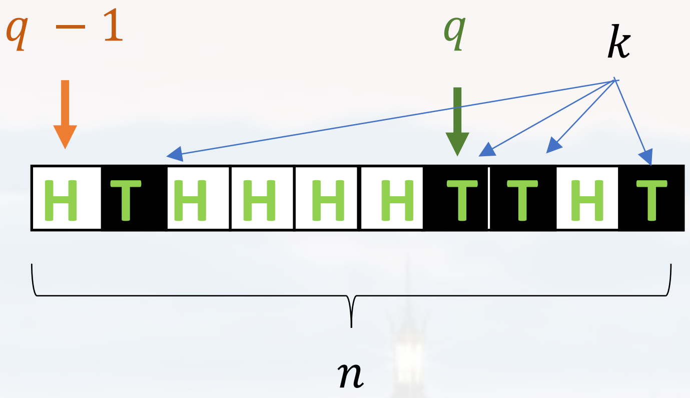
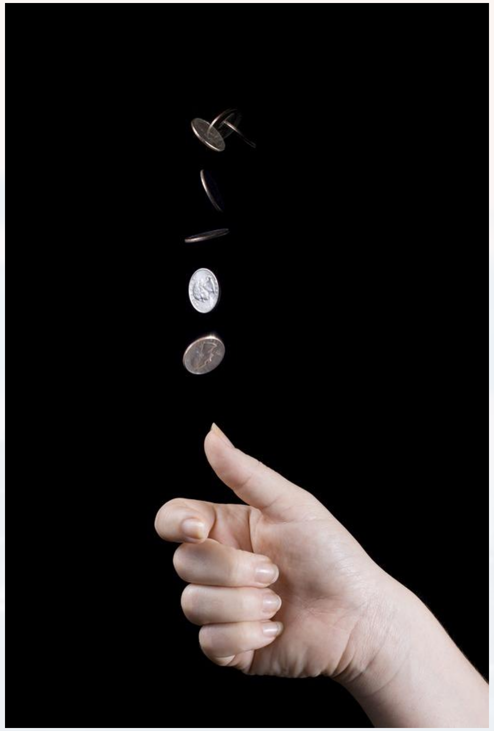




fair coin? q = 0.5 ???

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

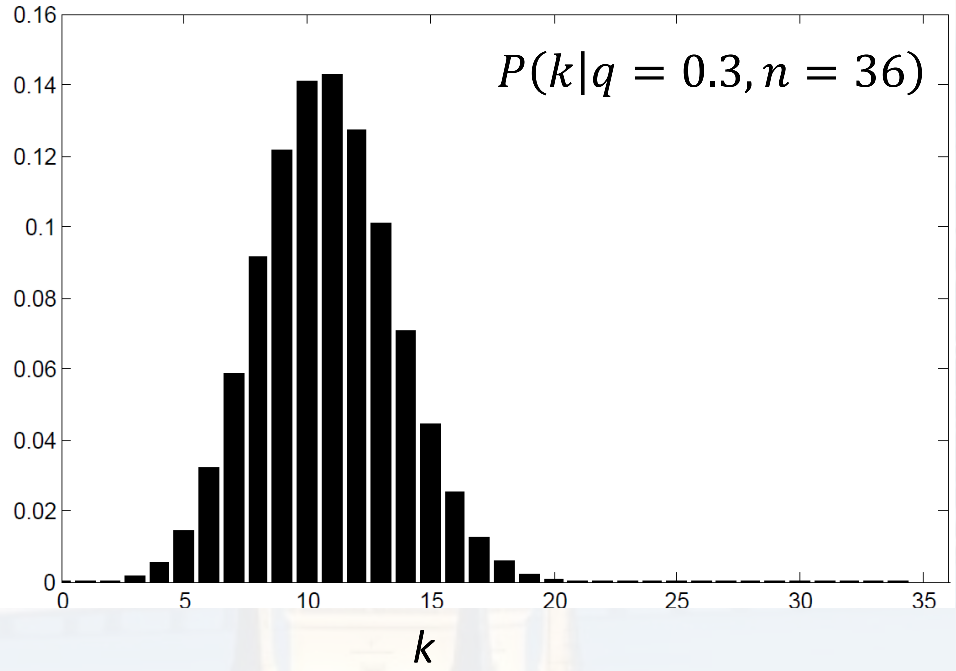
$$\frac{\boldsymbol{n!}}{\boldsymbol{k!(n-k)!}} =: \binom{\boldsymbol{n}}{\boldsymbol{k}}$$ **``n choose k''**

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

binomial distribution

$$\mu = \sum_i x_i\, p(x_i)$$

$$\mu = \int x\, p(x)\, dx$$



$$\mu = \sum_{k=0}^{n} k \binom{n}{k} q^k\,(1-q)^{n-k} = \boldsymbol{qn}$$

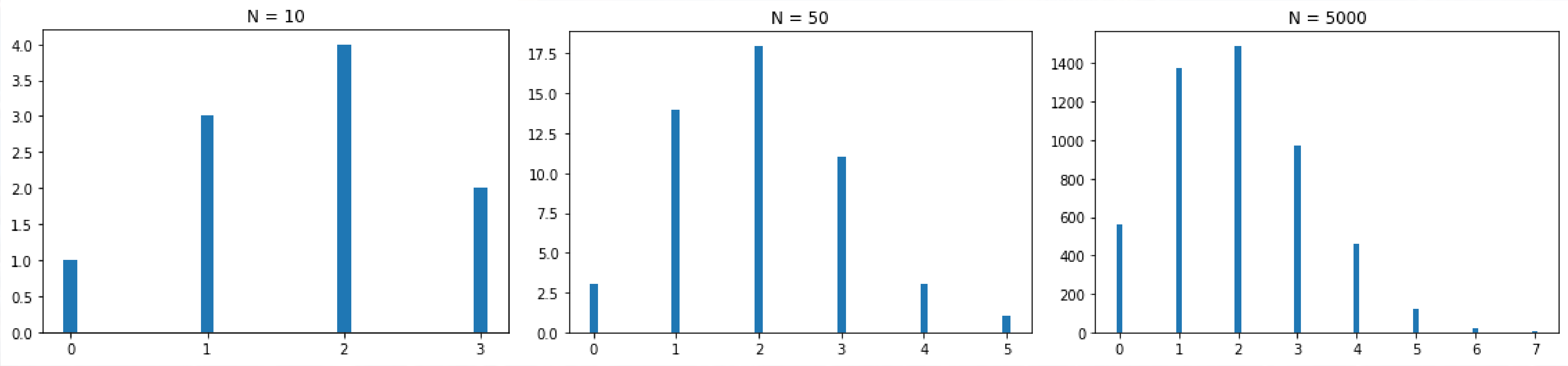
$$var(k) = \sum_{k=0}^{n} (\,k - qn\,)^2 \binom{n}{k}\; q^k\,(1-q)^{n-k} = \boldsymbol{qn(1-q)}$$

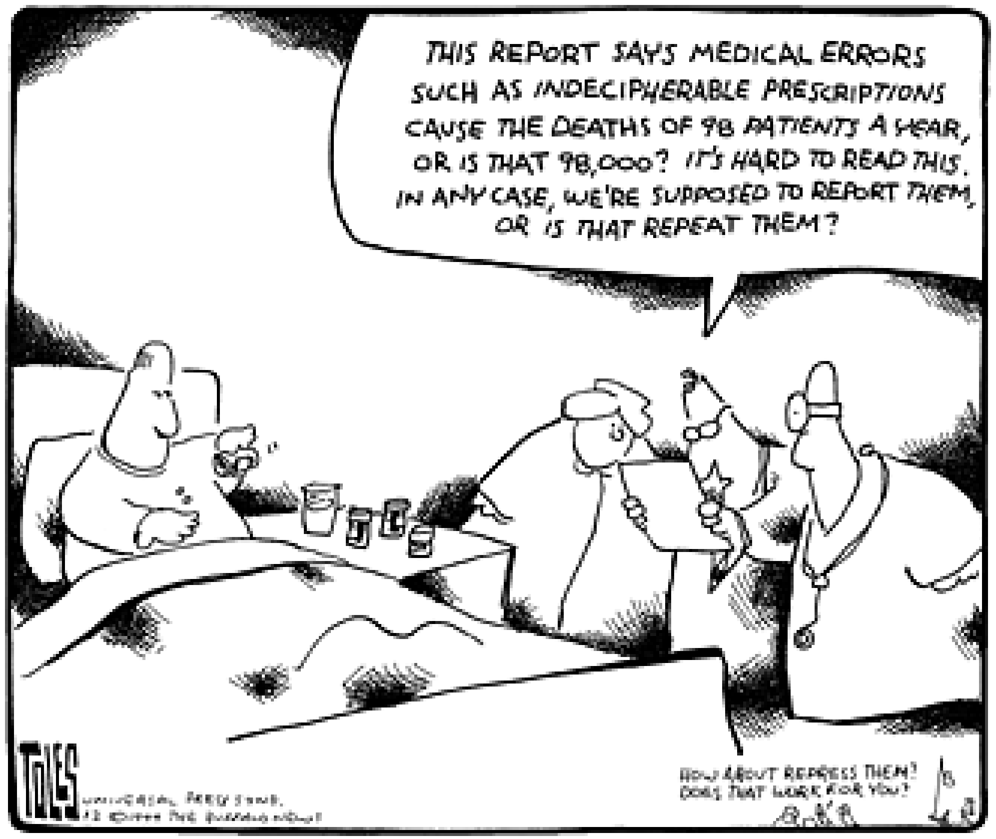
$$P(k|q,n) = \binom{n}{k}\, q^k\, (1-q)^{n-k}$$

binomial distribution

```
q = 0.2
n = 10
K = np.random.binomial(n, q, N)

labels, counts = np.unique(K, return_counts = True)
plt.bar(labels, counts, align = 'center', width = 0.1)
plt.gca().set_xticks(labels)
plt.title('N = ' + str(N))
```





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

binomial distribution

rare events → q << 1

Taylor expansion for $(1-q)^{n-k}$ around q = 0

$$(1-q)^{n-k} = 1 - nq + \frac{(nq)^2}{2} - \frac{(nq)^3}{6} + \ldots = e^{-nq}$$

→ n → ∞

Stirling's approximation for n!

$$\frac{n!}{(n-k)!} \approx \sqrt{\frac{n}{n-k}} \frac{n^n e^{n-k}}{e^n (n-k)^{n-k}} \approx n^k$$

$$\binom{n}{k} q^k (1-q)^{n-k} \approx \frac{(nq)^k e^{-nq}}{k!}$$

Introduction to Computational Techniques in Physics:

$$\binom{n}{k} q^k (1-q)^{n-k} \approx \frac{(nq)^k e^{-nq}}{k!}$$

often: nq : = λ

events per time interval: λ = c Δt

H	T	H	H	H	H	T	T	H	T

time

$\underbrace{\hspace{6cm}}_{\Delta t}$

rate c = 4 tails per Δt

$$\boxed{P(k|c) = \frac{(c\,\Delta t)^k e^{-c\,\Delta t}}{k!}}$$

Poisson distribution

$$\mu = qn \rightarrow \mathbf{qn = \lambda}$$

$$var(k) = qn(1-q) \rightarrow \mathbf{qn = \lambda}$$

$$\boxed{P(k|c) = \frac{(c\,\Delta t)^k e^{-c\,\Delta t}}{k!}}$$

Poisson distribution

$$\mu = \lambda$$

$$var(k) = \lambda$$

- **rare** events
- events are mutually **independent**
- events have **no duration**

<u>examples:</u>

- radioactive decay
- single photon detection
- lightning
- mutation of a gene
- receiving WhatsApp messages/SMS

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

Poisson distribution

$$\mu = \lambda$$
$$var(k) = \lambda$$

```
c    = 5
delt = 10
lam  = c * delt

K    = np.random.poisson(lam, N)

labels, counts = np.unique(K, return_counts = True)
plt.bar(labels, counts, align = 'center', width = 0.1)
plt.gca().set_xticks(labels)
plt.title('N = ' + str(N))
```

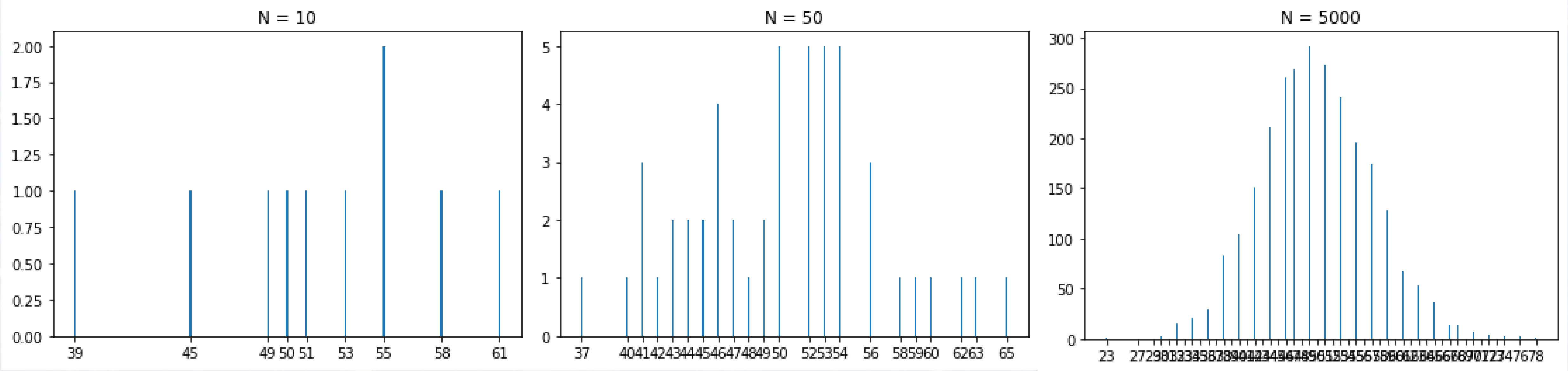
$$P(k|c) = \frac{(c\,\Delta t)^k e^{-c\,\Delta t}}{k!}$$

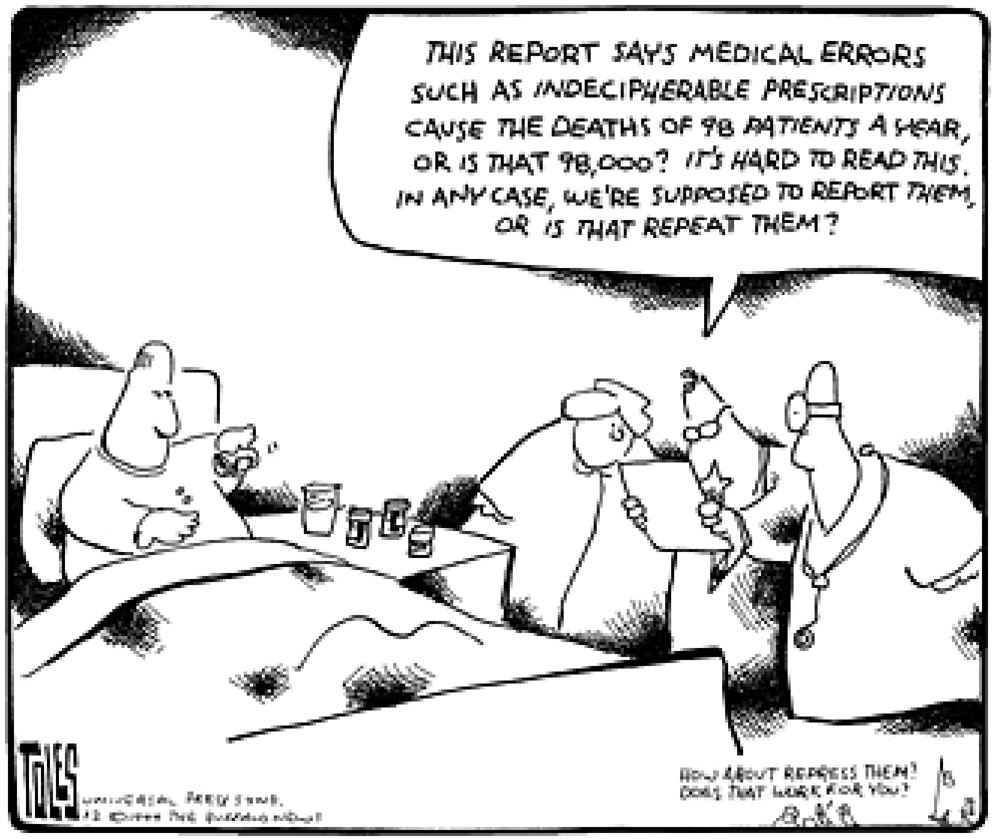
Poisson distribution

$$\mu = \lambda$$

$$var(k) = \lambda$$

```python
c    = 5
delt = 10
lam  = c * delt
K    = np.random.poisson(lam, N)
labels, counts = np.unique(K, return_counts = True)
plt.bar(labels, counts, align = 'center', width = 0.1)
plt.gca().set_xticks(labels)
plt.title('N = ' + str(N))
```





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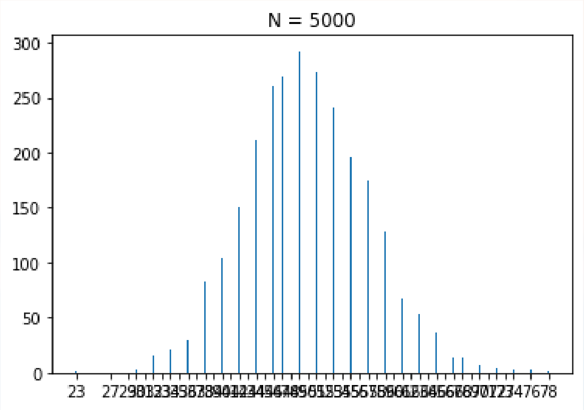
Introduction to Computational Techniques in Physics: Statistics – Normal Dist

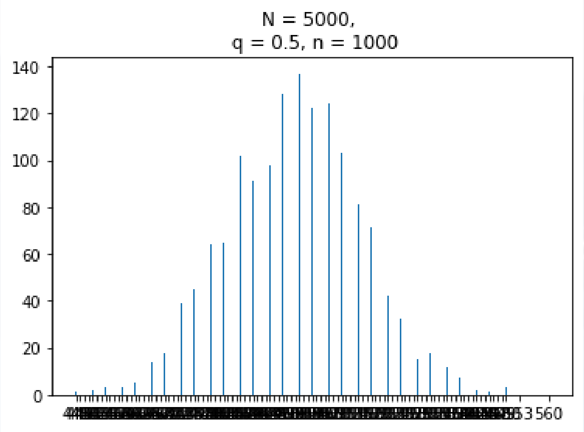
$$\boxed{P(k|c) = \frac{(c\,\Delta t)^k e^{-c\,\Delta t}}{k!}}$$

Poisson distribution



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

binomial distribution



Stirling's approximation for even larger n

$$P(k|n,p) \approx \frac{1}{\sqrt{2\pi\, nq(1-q)}} \exp\left[-\frac{(k-nq)^2}{2nq(1-q)}\right]$$

Stirling's approximation for even larger n

$$P(k|n,p) \approx \frac{1}{\sqrt{2\pi\, nq(1-q)}} \exp\left[-\frac{(k-nq)^2}{2nq(1-q)}\right]$$

using $\sigma^2 = var(k) = qn(1-q)$

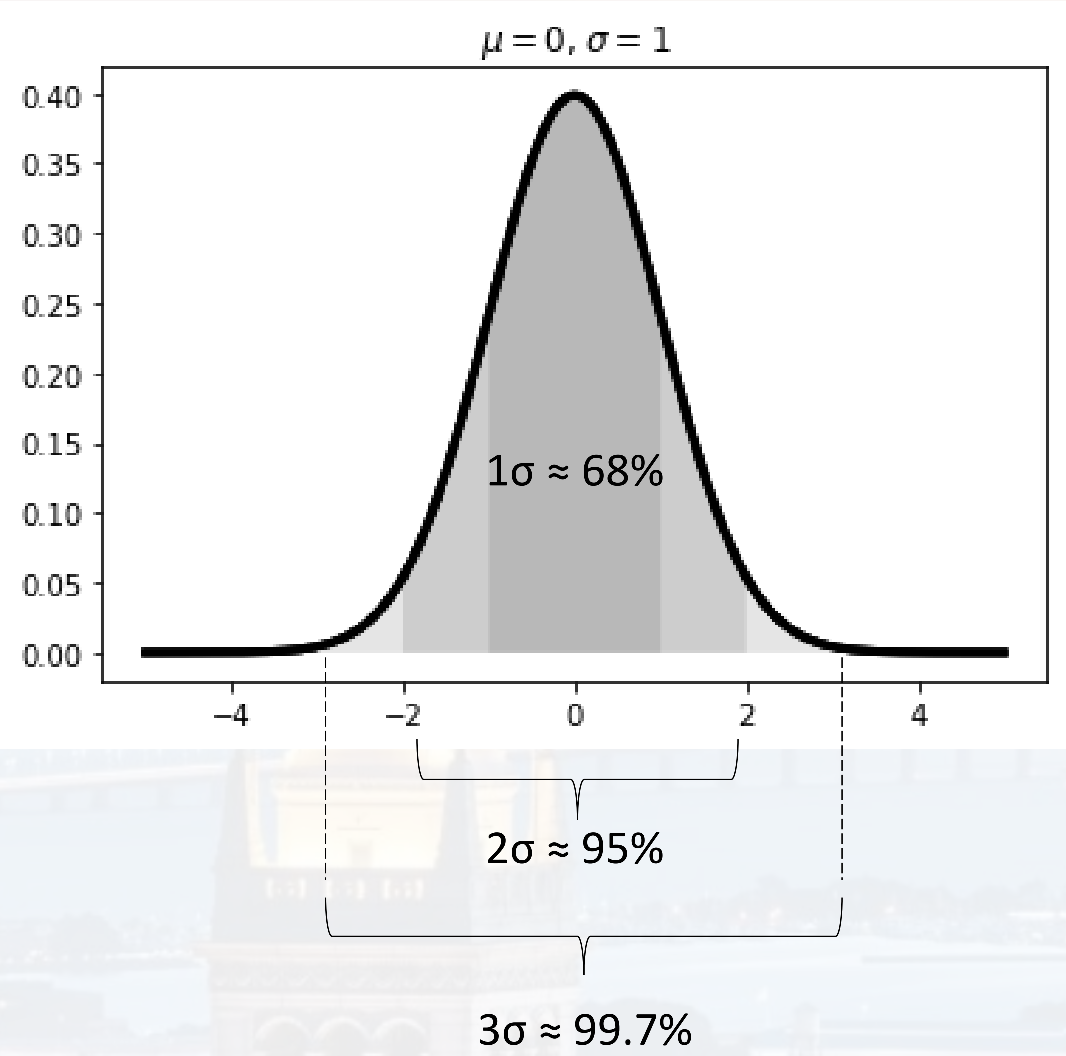
$\mu \;= qn$

and $k := x$

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

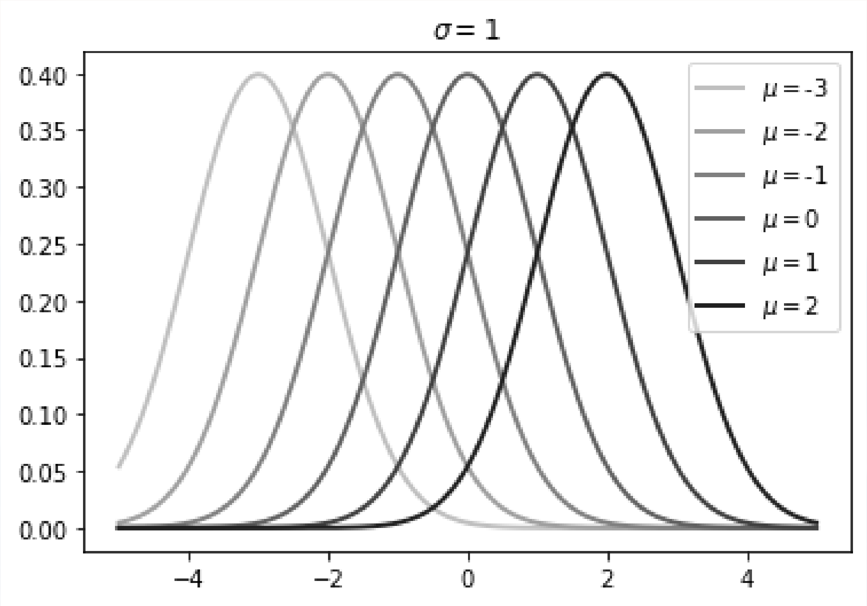
Normal/Gauss distribution

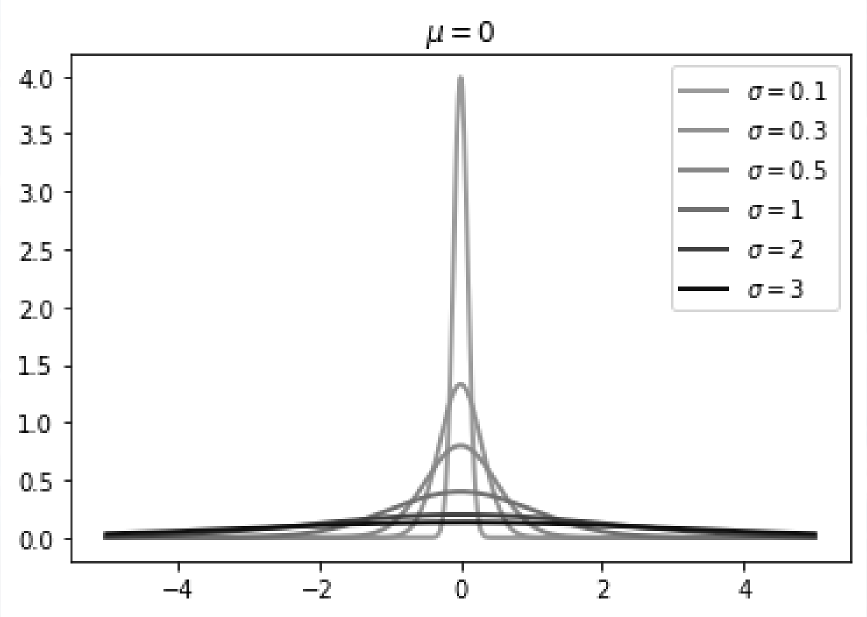
Note, that the **Poisson** and the **Binomial distribution** are *discrete*, whereas the **Normal distribution** is *continuous*!



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

Normal/Gauss distribution





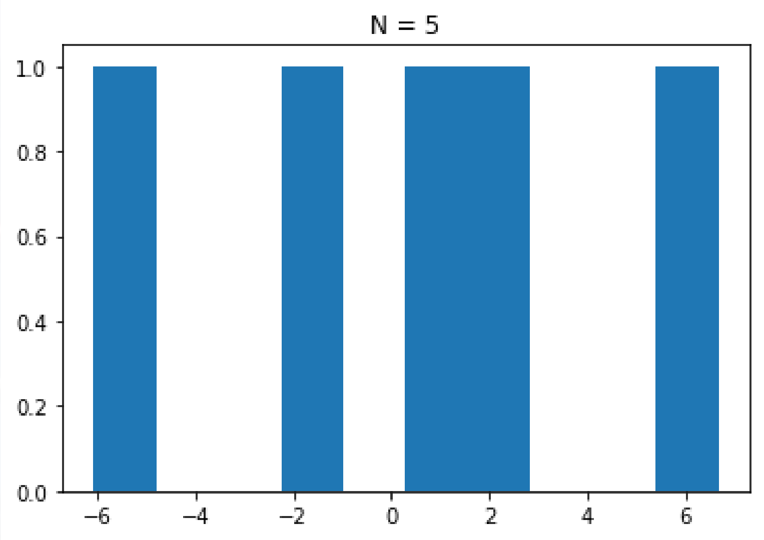
$$\boxed{P(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\,\sigma^2}}\,exp\left[-\frac{(x-\mu)^2}{2\,\sigma^2}\right]}$$

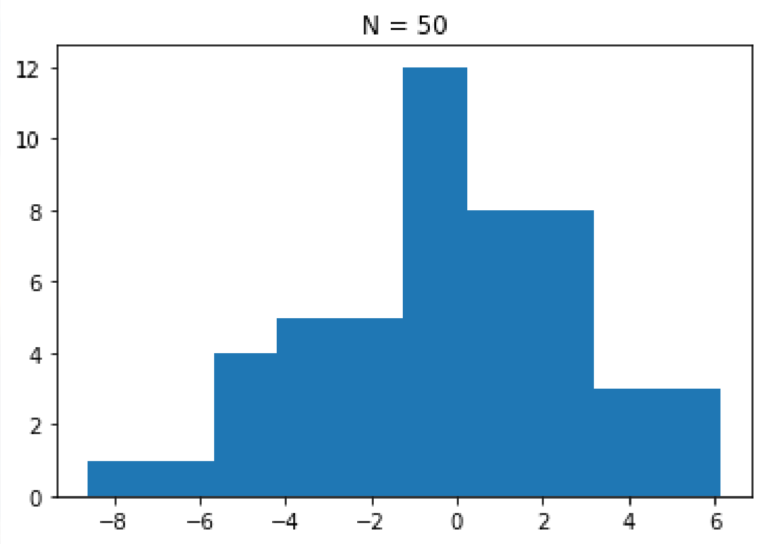
Normal/Gauss distribution

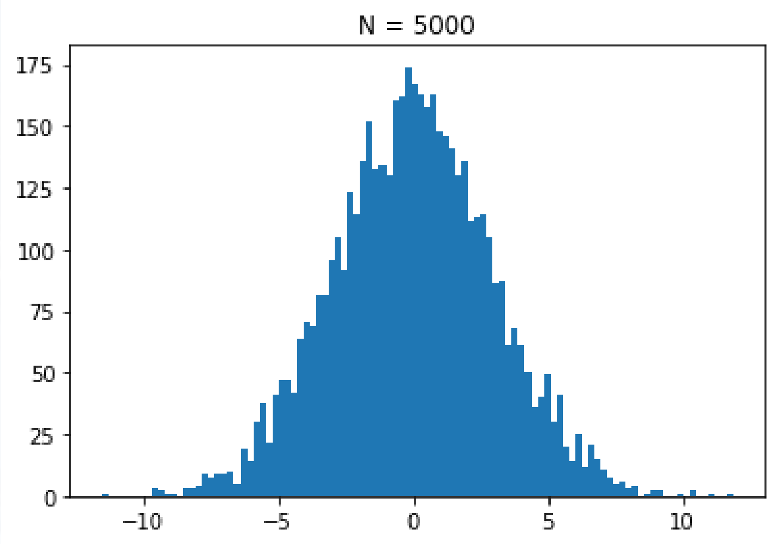
```
mu = 0
s  = 1
P  = np.random.normal(mu, s, N)
plt.hist(P)
plt.title('N = ' + str(N))
```

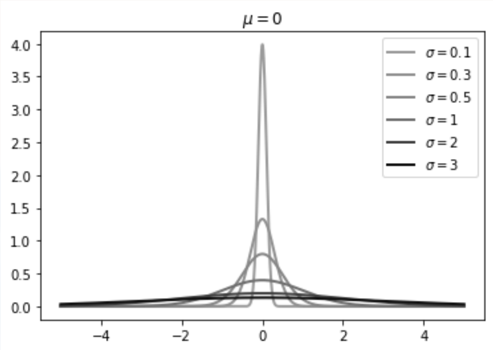
$$P(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\,\sigma^2}}\, exp\left[-\frac{(x-\mu)^2}{2\,\sigma^2}\right]$$

Normal/Gauss distribution









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

Normal/Gauss distribution

examples:
- diffusion processes
- approx. stat. error of data points
- approx. distribution of body height/shoe sizes/ weight, IQ
- approx. blood pressure, blood values
- approx. retirement age

….

applications:
- significance tests
- t-test
- ANOVA/MANOVA
- χ^2 - test
- χ^2 itself and students-t distribution

…

Why do so many quantities follow a normal distribution?

Why do so many quantities follow a normal distribution?

At the end… all probability distributions are **Maximum Entropy** Distributions, subject to a **set of constrains**

Distribution name	Probability density / mass function	Maximum Entropy constraint	Support
Uniform (discrete)	$f(k)=\frac{1}{b-a+1}$	None	$\{a,a+1,\dots,b-1,b\}$
Uniform (continuous)	$f(x)=\frac{1}{b-a}$	None	$[a,b]$
Bernoulli	$f(k)=p^k(1-p)^{1-k}$	$\mathbb{E}[\,K\,]=p$	$\{0,1\}$
Geometric	$f(k)=(1-p)^{k-1}\,p$	$\mathbb{E}[\,K\,]=\frac{1}{p}$	$\mathbb{N}\smallsetminus\{0\}=\{1,2,3,\dots\}$
Exponential	$f(x)=\lambda\exp(-\lambda x)$	$\mathbb{E}[\,X\,]=\frac{1}{\lambda}$	$[0,\infty)$
Laplace	$f(x)=\frac{1}{2b}\exp\left(-\frac{\lvert x-\mu\rvert}{b}\right)$	$\mathbb{E}[\,\lvert X-\mu\rvert\,]=b$	$(-\infty,\infty)$
Asymmetric Laplace	$f(x)=\frac{\lambda\,\exp\left(-(x-m)\,\lambda\,s\,\kappa^s\right)}{(\kappa+\frac{1}{\kappa})}$ where $s\equiv\operatorname{sgn}(x-m)$	$\mathbb{E}[\,(X-m)\,s\,\kappa^s\,]=\frac{1}{\lambda}$	$(-\infty,\infty)$
Pareto	$f(x)=\frac{\alpha\,x_m^\alpha}{x^{\alpha+1}}$	$\mathbb{E}[\,\ln X\,]=\frac{1}{\alpha}+\ln(x_m)$	$[x_m,\infty)$
Normal	$f(x)=\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$	$\mathbb{E}[\,X\,]=\mu$, $\mathbb{E}[\,X^2\,]=\sigma^2+\mu^2$	$(-\infty,\infty)$

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<u>examples:</u>

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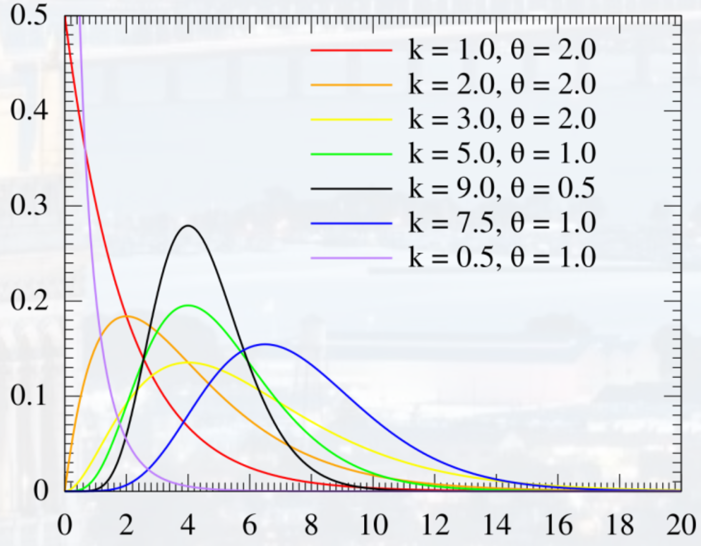
- approx. retirement age

….

Gamma	$f(x) = \dfrac{x^{k-1} \exp\left(-\frac{x}{\theta}\right)}{\theta^k \, \Gamma(k)}$	$\mathbb{E}[\,X\,] = k\,\theta\,,$ $\mathbb{E}[\,\ln X\,] = \psi(k) + \ln\theta$	$[0, \infty)$



Poisson distribution

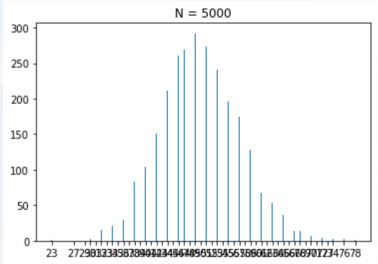
$$P(k|c) = \frac{(c\,\Delta t)^k e^{-c\,\Delta t}}{k!}$$

$q \rightarrow 0$

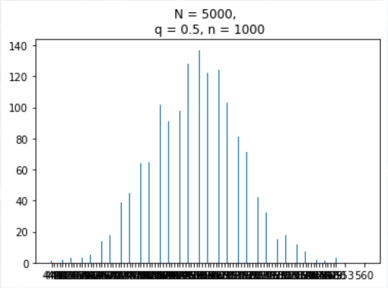
binomial distribution

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

$n \rightarrow \infty$



$n \rightarrow \infty$

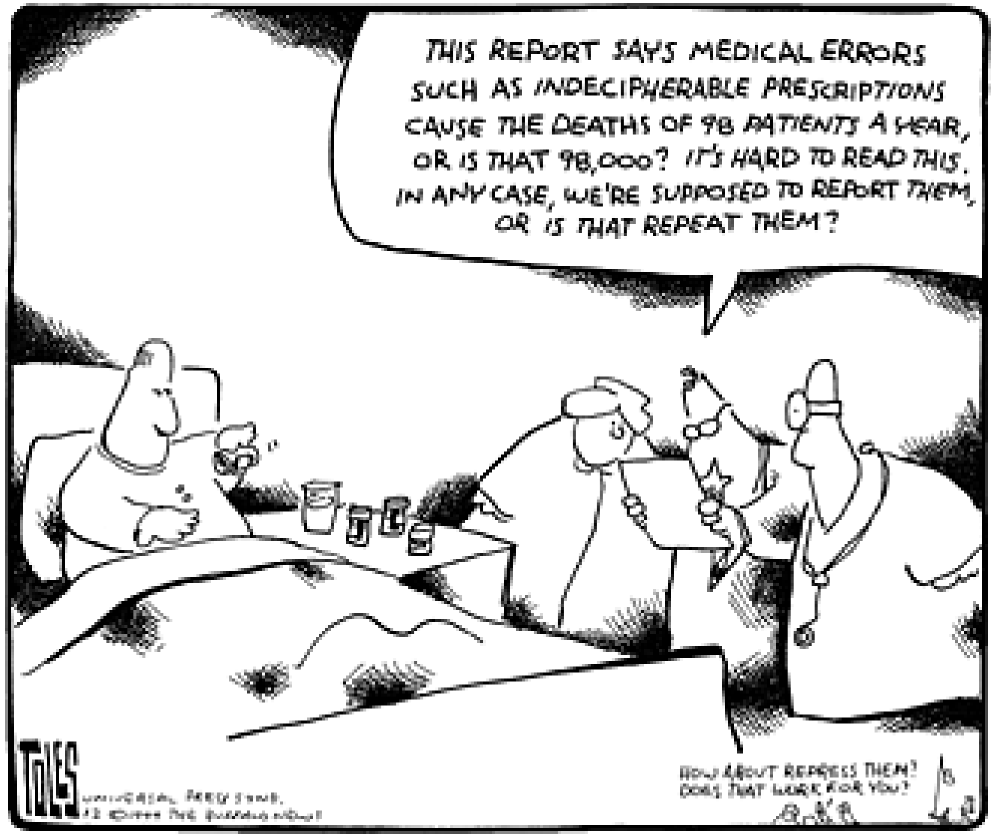


Normal/Gauss distribution

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

The fact that that many datasets can be well approximated by a Normal distribution for $n \rightarrow \infty$ is called

Central Limit Theorem



Outline:

Basics

Most Common PDFs

- uniform
- binomial
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics