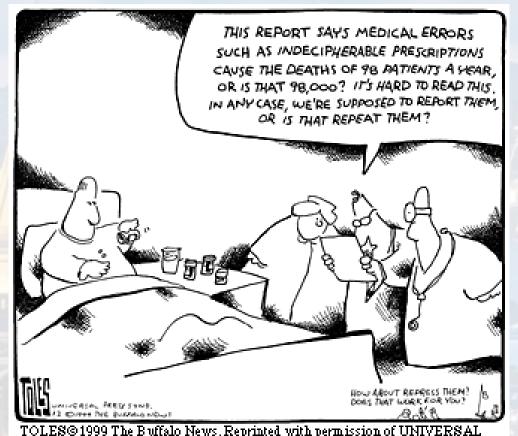


M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics



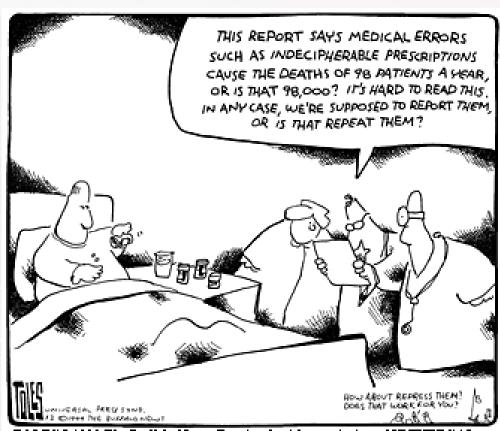
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| syllabus: | - Introduction to Unix & Python | (week 1 - 2) |
|-----------|---|--------------|
| | - Functions, Loops, Lists and Arrays | (week 3 - 4) |
| | - Visualization | (week 5) |
| | - Parsing, Data Processing and File I/O | (week 6) |
| | - 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) |
| | | |







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Outline:

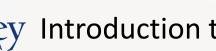
Basics

Most Common PDFs

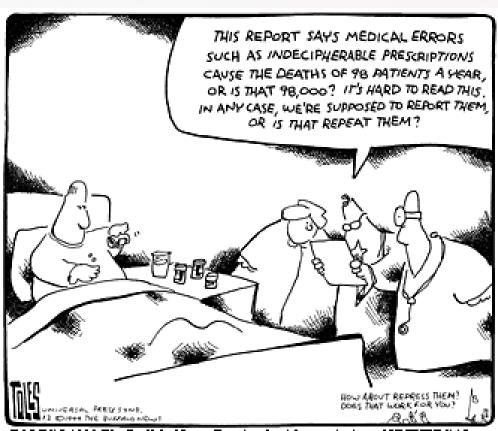
- uniform
- binomial
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics







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Outline:

Basics

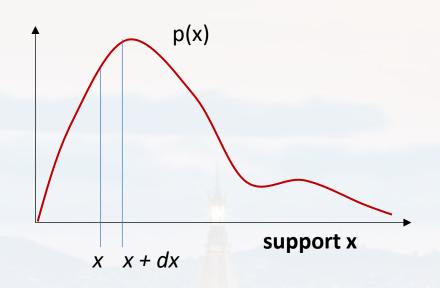
Most Common PDFs

 $[a \le x \le b]$



Berkeley Introduction to Computational Techniques in Physics:





probability **d**ensity **f**unction

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

Cumulative density function

$$P(x) = \int_{a}^{x} p(x) \ dx$$

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

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

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

$$\int_{a}^{m} p(x) \ dx = \frac{1}{2}$$





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

$$= E(x^2) - 2\mu E(x) + \mu^2 E(1) \qquad \int_a^b p(x) dx = 1$$

$$\int_{a}^{b} p(x) \ dx = 1$$

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

$$\mu = E(x)$$

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





mean

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

a, b = const

variance

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

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

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

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

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

$$a^2 var(x_1)$$

 $b^2 var(x_2)$

 $= a^{2}E(x_{1}^{2}) + 2ab E(x_{1}x_{2}) + b^{2} E(x_{2}^{2}) - a^{2}E(x_{1})^{2} - b^{2}E(x_{2})^{2} - 2abE(x_{1})E(x_{2})$





mean

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

a, b = const

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

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

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

$$= a^{2}E(x_{1}^{2}) + 2ab E(x_{1}x_{2}) + b^{2}E(x_{2}^{2}) - a^{2}E(x_{1})^{2} - b^{2}E(x_{2})^{2} - 2abE(x_{1})E(x_{2})$$

$$a^{2} var(x_{1})$$

$$b^{2} var(x_{2})$$

$$2ab cov(x_{1}, x_{2})$$

$$= a^2 var(x_1) + b^2 var(x_2) + 2ab cov(x_1, x_2)$$

$$cov(x_1, x_2) = cov(x_2, x_1) = E(x_1x_2) - 2E(x_1)E(x_2)$$

covariance

$$ab = c$$



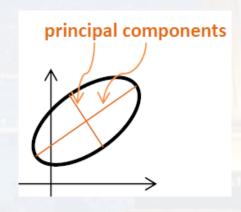


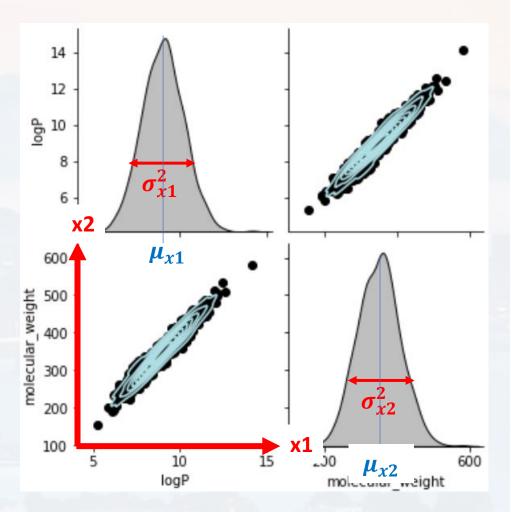
const =
$$a^2 var(x_1) + b^2 var(x_2) + 2c cov(x_1, x_2)$$

covariance matrix

$$const = \begin{pmatrix} x\mathbf{1} - \mu_{x1} \\ x\mathbf{2} - \mu_{x2} \end{pmatrix}^{T} \begin{pmatrix} a & c_{12} \\ c_{21} & b \end{pmatrix} \begin{pmatrix} x\mathbf{1} - \mu_{x1} \\ x\mathbf{2} - \mu_{x2} \end{pmatrix}$$

 $= v^T S v$... 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

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

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

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

note:

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

called nth *moment* of a pdf

covariance

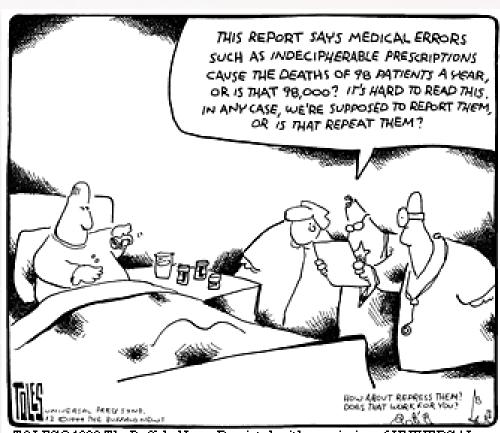
$$cov(x_1, x_1) = E(x_1x_2) - 2E(x_1)E(x_2)$$

correlation coefficient

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







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Outline:

Most Common PDFs

- uniform





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

$$S = -\int p(x) \ln(x) dx$$
 c: $\int p(x) dx = 1$

$$\int p(x) \ dx = 1$$

p(x) = const

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

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

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

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

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

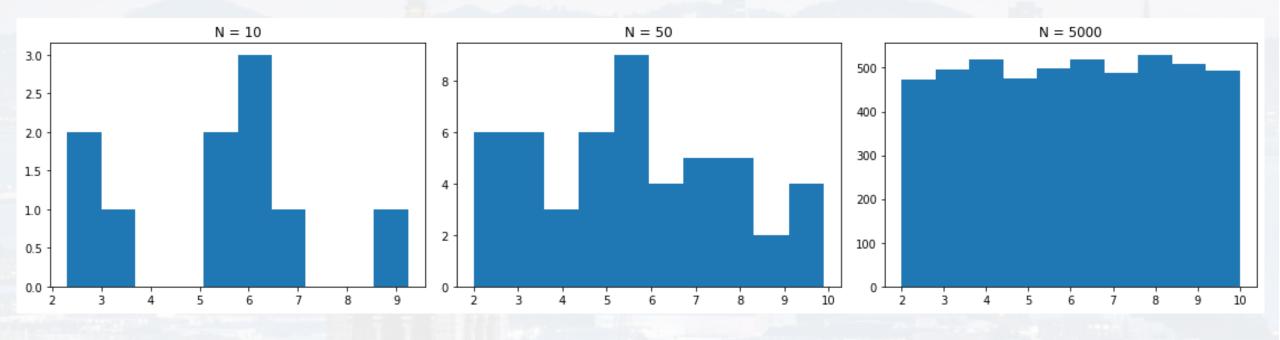




$$p(x) = const$$

plotting the pdf

continuous support





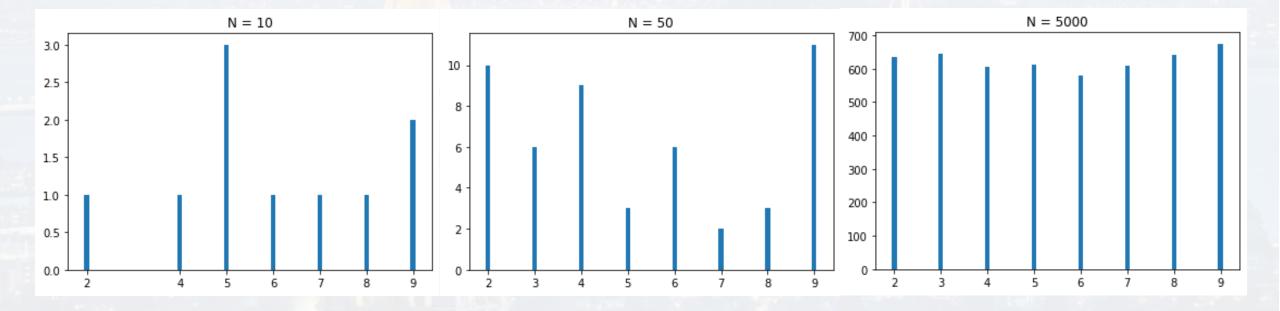
$$p(x) = const$$

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))
```



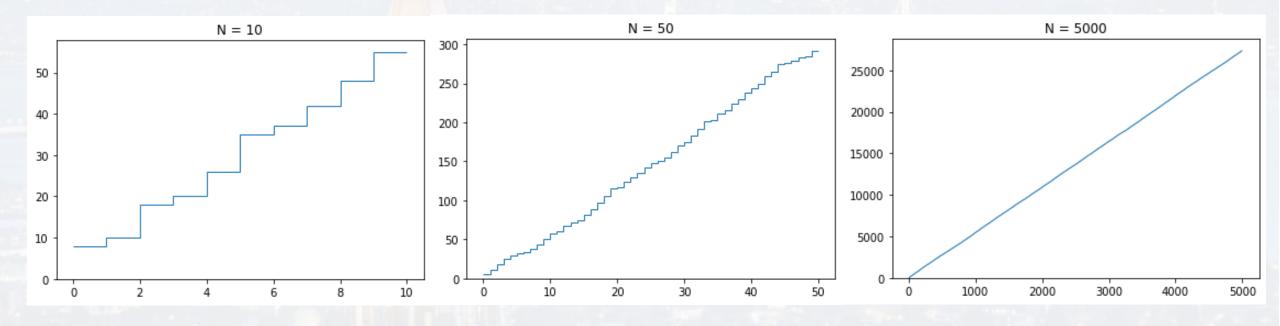


$$p(x) = const$$

plotting the cdf

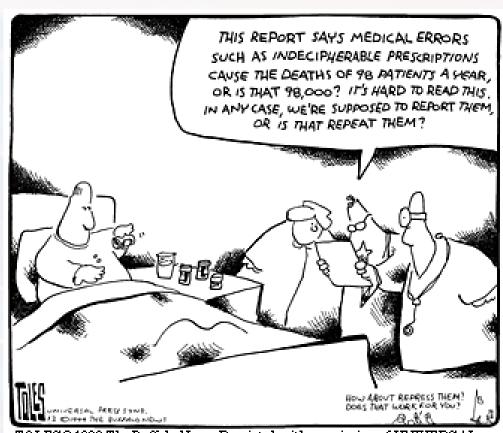
discrete support

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









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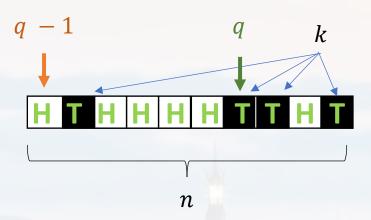
Outline:

Most Common PDFs

- binomial







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

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



fair coin? q = 0.5 ???

$$\frac{n!}{k!(n-k)!} =: \binom{n}{k}$$
 "in choose k"

Statistics – Binomial Dist



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

nial distribution
$$\mu = \sum_i x_i \ p(x_i)$$

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

$$P(k|q = 0.3, n = 36)$$

$$0.12$$

$$0.1$$

$$0.08$$

$$0.06$$

$$0.04$$

$$0.02$$

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$$0.04$$

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

$$var(k) = \sum_{k=0}^{n} (k - qn)^{2} {n \choose k} q^{k} (1 - q)^{n-k} = qn(1 - q)$$

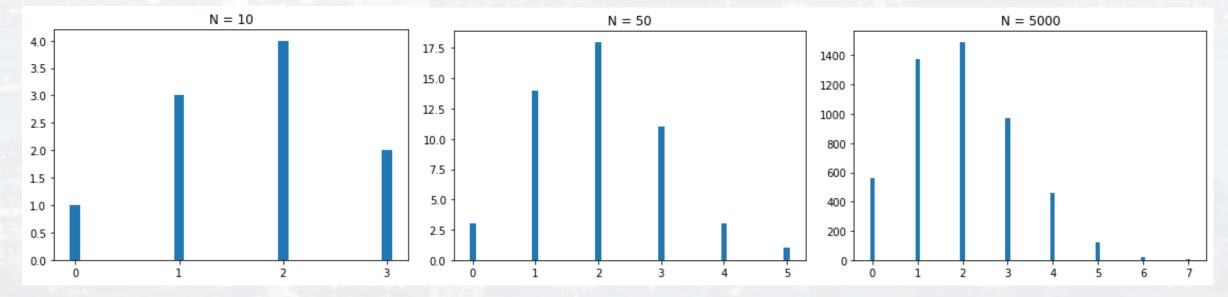




$$P(k|q,n) = \binom{n}{k} q^k (1-q)^{n-k}$$

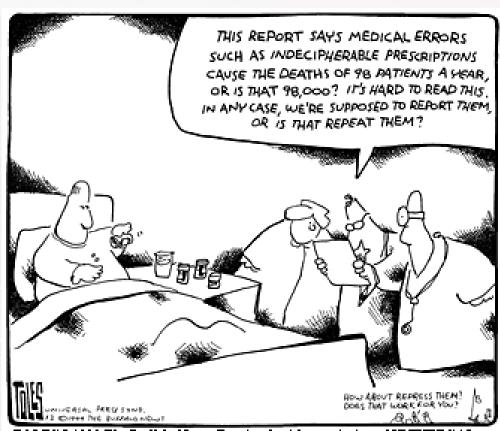
```
q = 0.2
n = 10
K = np.random.binomial(n, q, N)
```

```
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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Outline:

Most Common PDFs

- Poissonian





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

binomial distribution

rare events

$$\rightarrow$$
 q << 1

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

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

$$\rightarrow$$
 n $\rightarrow \infty$

Stirling's approximation for n!

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

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

Statistics – Poisson Dist



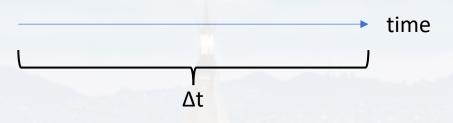
$$\binom{n}{k} q^k (1-q)^{n-k} \approx \frac{(nq)^k e^{-nq}}{k!}$$

often: $nq := \lambda$

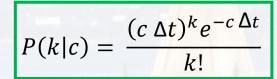
events per time interval: $\lambda = c \Delta t$







rate c = 4 tails per Δt



Poisson distribution

$$\mu = qn \rightarrow qn = \lambda$$

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

Statistics – Poisson Dist



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

Poisson distribution

$$\mu = \lambda$$

$$var(k) = \lambda$$

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

examples:

- 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))
```





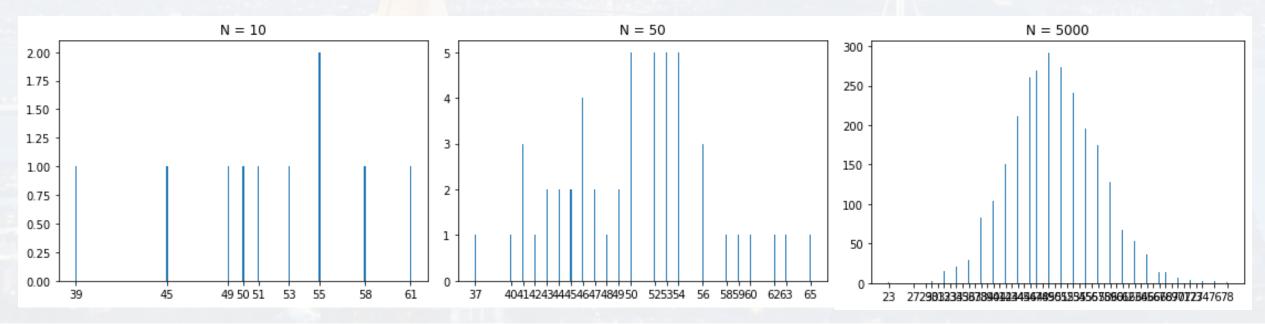
Poisson distribution

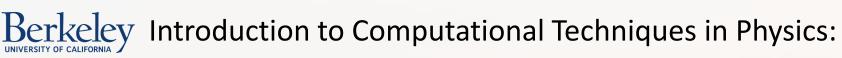
$$\mu = \lambda$$

$$var(k) = \lambda$$

```
delt = 10
lam = c * delt
     = 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))
```

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









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Outline:

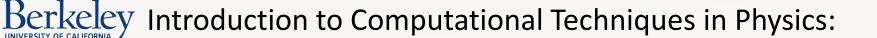
Basics

Most Common PDFs

- uniform
- binomia
- Poissoniar
- Normal/Gaussian

Error Estimation

Bayesian Statistics



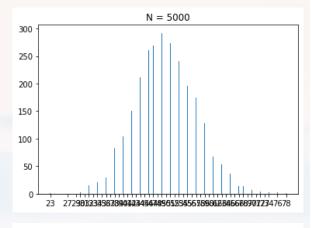
Statistics – Normal Dist

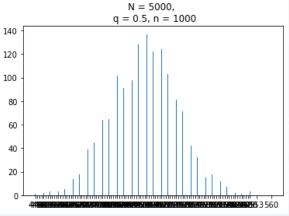


$$P(k|c) = \frac{(c \Delta t)^k e^{-c \Delta t}}{k!}$$

Poisson distribution

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





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





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
$$k := x$$

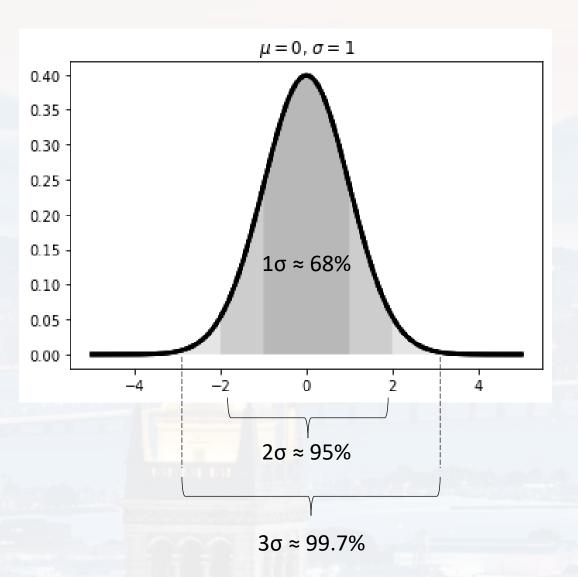
$$P(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi \sigma^2}} exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$
 Normal/Gauss distribution



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



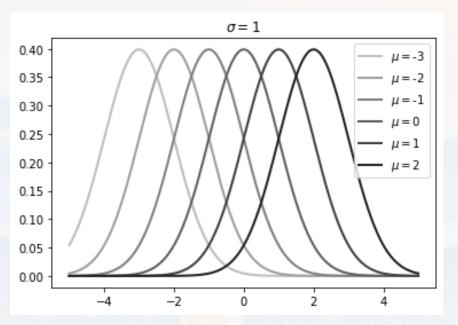


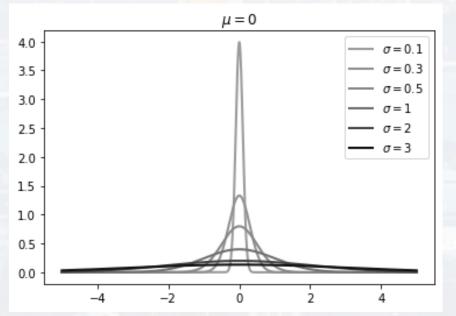


$$P(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi \sigma^2}} exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$





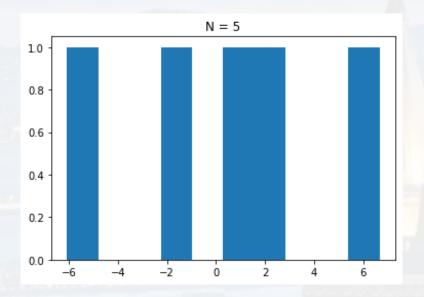


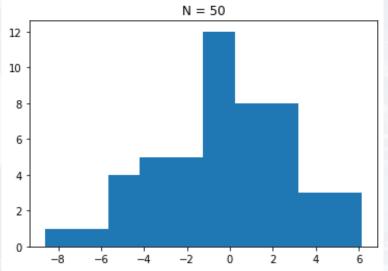


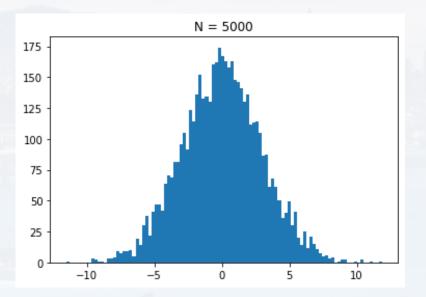
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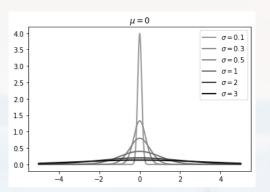






Statistics – Normal Dist





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

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
- $-\chi^2$ 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 | $\{a,a+1,\ldots,b-1,b\}$ |
| 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\]=rac{1}{p}$ | $\mathbb{N} \smallsetminus \{0\} = \{1,2,3,\dots\}$ |
| Exponential | $f(x) = \lambda \exp(-\lambda x)$ | $\mathbb{E}[\ X\]=rac{1}{\lambda}$ | $[0,\infty)$ |
| Laplace | $f(x) = rac{1}{2b} \expigg(-rac{ x-\mu }{b}igg)$ | $\mathbb{E}[\ X-\mu \]=b$ | $(-\infty,\infty)$ |
| Asymmetric Laplace | $f(x) = rac{\lambda \; \expig(-\left(x-m ight) \lambda s \kappa^sig)}{\left(\kappa + rac{1}{\kappa} ight)}$ where $s \equiv \mathrm{sgn}(x-m)$ | $\mathbb{E}[\;(X-m)\;s\;\kappa^s\;]=rac{1}{\lambda}$ | $(-\infty,\infty)$ |
| Pareto | $f(x)=rac{lpha\ x_m^lpha}{x^{lpha+1}}$ | $\mathbb{E}[\ln X] = rac{1}{lpha} + \ln(x_m)$ | $[x_m,\infty)$ |
| Normal | $f(x) = rac{1}{\sqrt{2\pi\sigma^2}} \exp\Biggl(-rac{(x-\mu)^2}{2\sigma^2}\Biggr)$ | $egin{array}{l} \mathbb{E}[\:X\:] &= \mu\:, \ \mathbb{E}[\:X^2\:] &= \sigma^2 + \mu^2 \end{array}$ | $(-\infty,\infty)$ |



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

examples:

- approx. stat. error of data points

- approx. distribution of body height/shoe sizes/ weight, IQ

- approx. blood pressure, blood values

- approx. retirement age

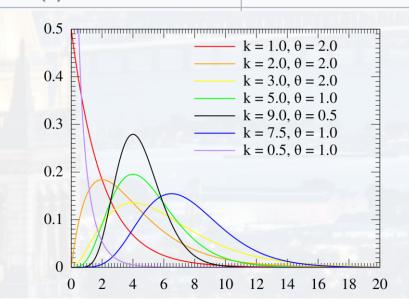
....

Gamma

$$f(x) = rac{x^{k-1} \exp\left(-rac{x}{ heta}
ight)}{ heta^k \Gamma(k)}$$

$$\begin{split} \mathbb{E}[\; X \;] &= k \; \theta \; , \\ \mathbb{E}[\; \ln X \;] &= \psi(k) + \ln \theta \end{split}$$

 $[0,\infty)$









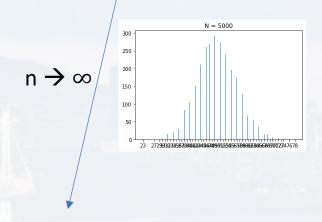
$$P(k|c) = \frac{(c \Delta t)^k e^{-c \Delta t}}{k!}$$

binomial distribution

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

N = 5000, q = 0.5, n = 1000

0 < p



The fact that that many datasets can be well approximated by a Normal distribution for n → ∞ is called

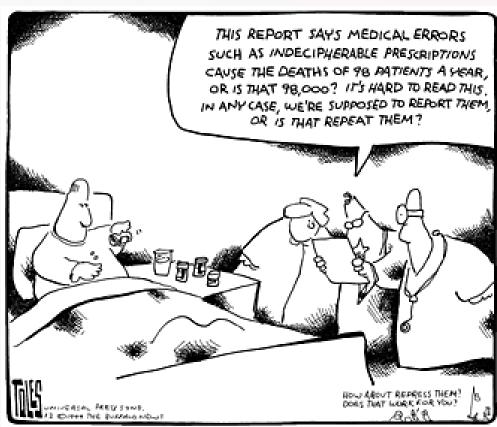
Central Limit Theorem

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









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Outline:

Basics

Most Common PDFs

- uniform
- binomia
- Poissonian
- Normal/Gaussian

Error Estimation

Bayesian Statistics