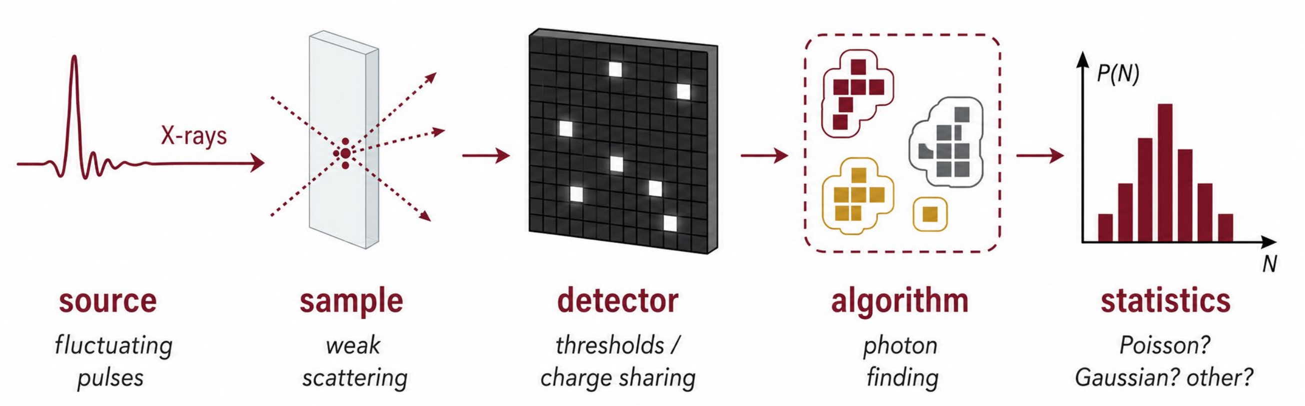
Counting statistics beyond the basics

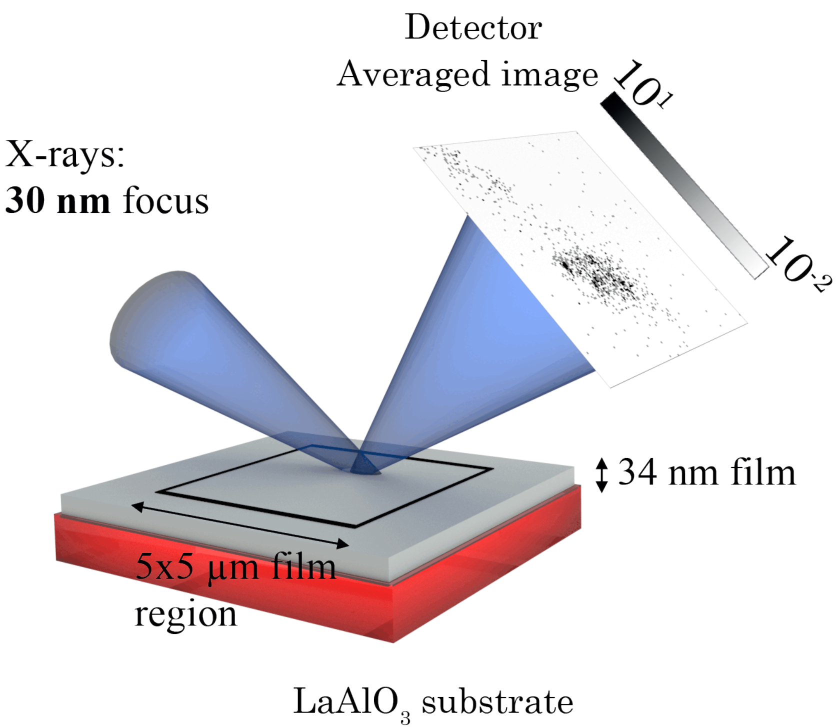
Oleg Gorobtsov

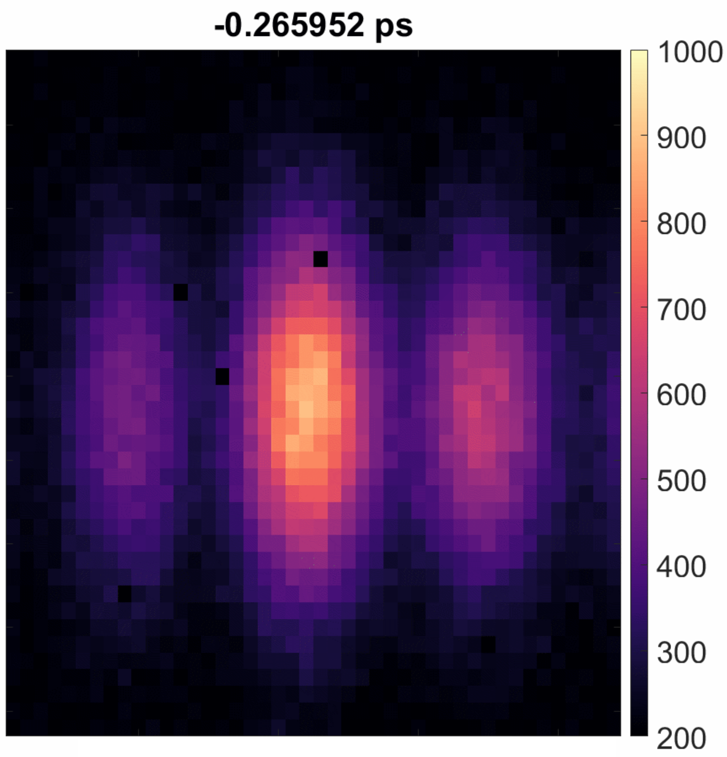
- Introduction
- Probability distributions
- Processes and examples



Note: chatbots were used to assist with non-scientic graphics

Why are counting statistics important?





Every measurement includes counting the signal; errors can be non-trivial!

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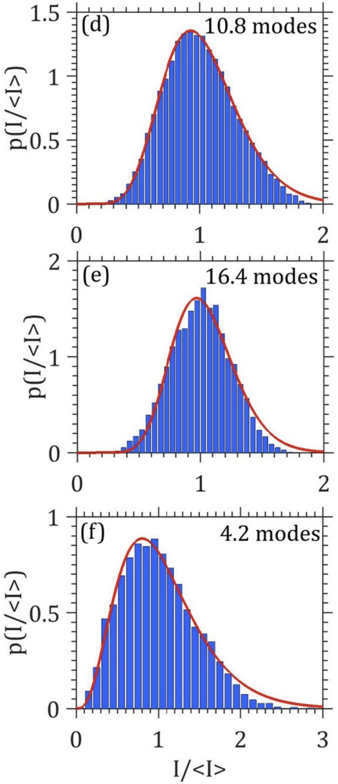
Are counting statistics always "normal"?

Common assumption:

continuous signal → Gaussian statistics and errors
discrete signal → Poisson statistics and errors

In fact, this assumption needs conditions:

- independent events
- fixed mean signal
- ideal detection
- no algorithm-induced correlations
- no "unknown unknowns"…



Counter-example: probability distribution intensity I measured at a free electron laser depends strongly on source properties

O. Yu. Gorobtsov et al. *PRA* 2017

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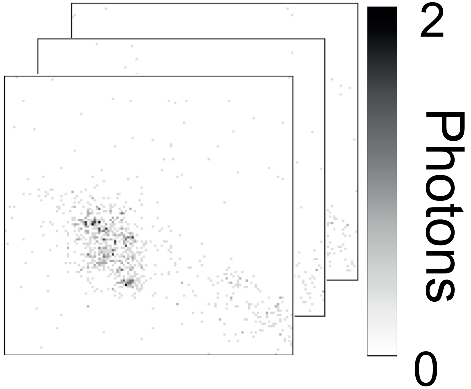
Low counts: more likely than you think

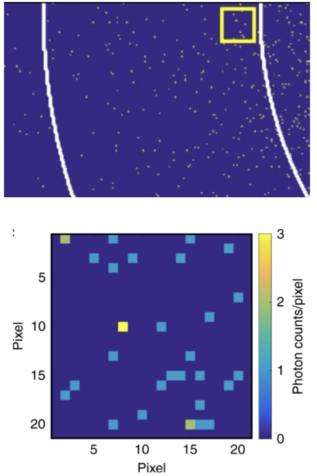
High signal at the source does not guarantee high signal when measuring

Science is done at the limits of detection:

- small scattering volumes: thin films, nanoparticles, dilute samples
- fast dynamics → exposure time
- regions far from strong diffraction peaks



Syncrotron, thin Ca_2RuO_4 film



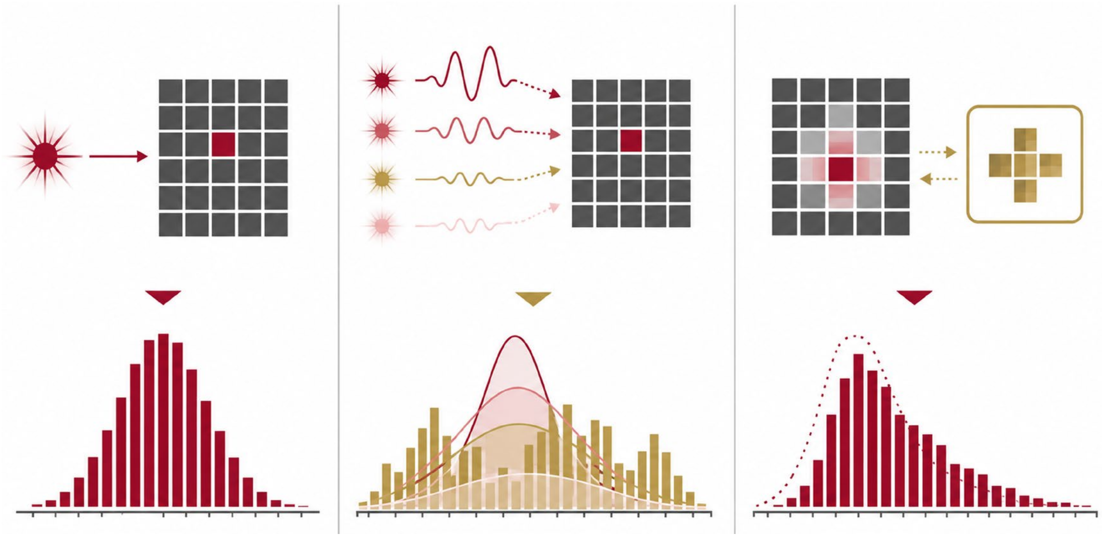
Free electron laser, XPCS

When detecting individual photons, tread carefully

Measured signal always comes from many factors

Signal statistics ≠ just photon shot noise!

$$P(I):\ P(source) \otimes P(sample) \otimes P(detector)$$



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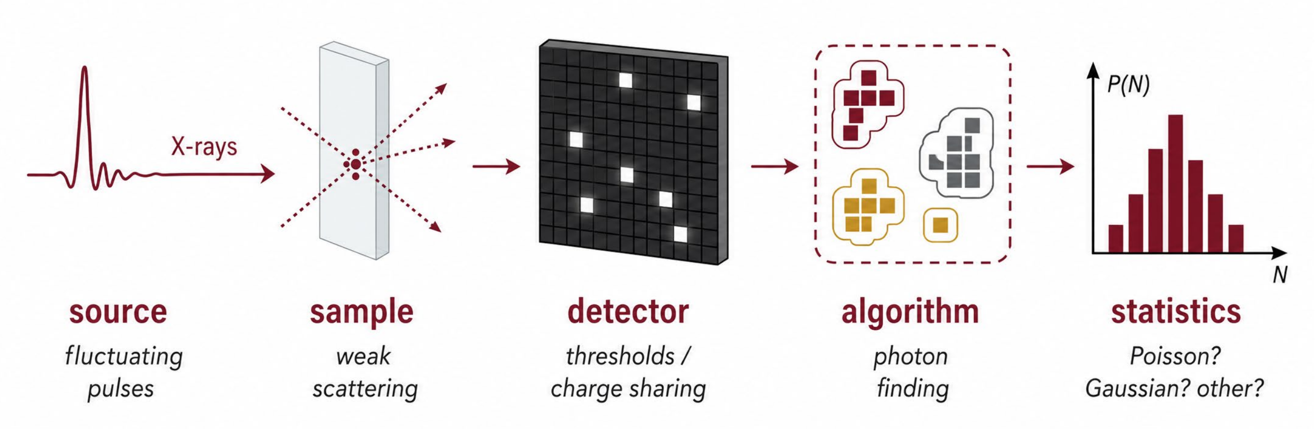
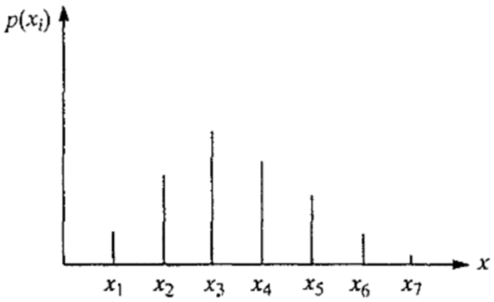


What is a random variable?

Random variable: numerical outcome of an experiment

For a discrete variable x_n

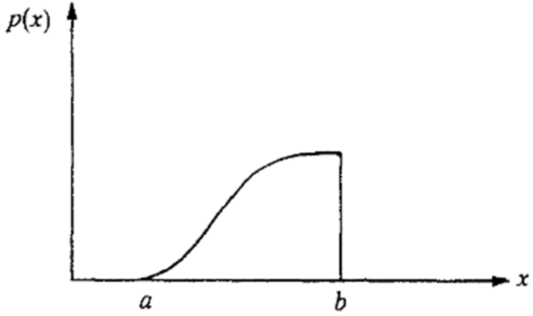
$$\sum_n P(n) = 1$$



$$\langle f(n)\rangle = \sum_n f(n)P(n)$$

For a continuous variable x

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



$$\langle f(x)\rangle = \int f(x)p(x)\, dx$$

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Moments of a distribution

Moments of a distribution (generally) characterize it. The r-th moment:

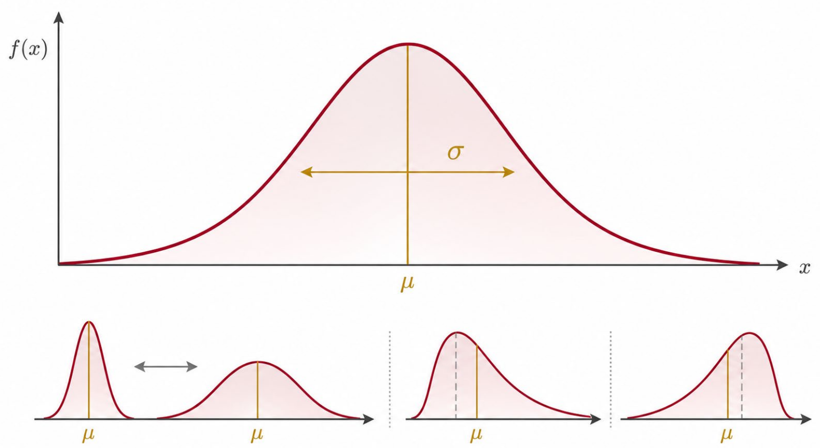
$$\nu_r \equiv \langle x^r \rangle = \int x^r p(x)\, dx \qquad \text{or discrete} \qquad \nu_r \equiv \langle n^r \rangle = \sum_{n=0}^{\infty} n^r P_n$$

First moment: mean

Second moment: variance

$$\mu = \langle X \rangle$$

$$\sigma^2 = \langle (X-\mu)^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2$$



Generally you **can not** (!) express higher moments through lower

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Linear combination of independent variables

Let

$$y = \sum_i a_i x_i$$

Then

$$\langle y \rangle = \sum_i a_i \langle x_i \rangle$$

And

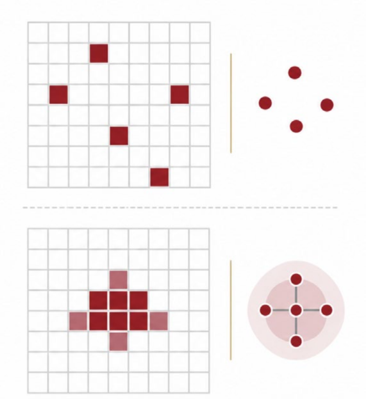
$$\langle (\Delta y)^2 \rangle = \sum_i \sum_j a_i a_j \langle \Delta x_i \Delta x_j \rangle$$

If the variables are statistically independent

$$\langle \Delta x_i \Delta x_j \rangle = 0 \qquad i \neq j$$

so

$$\langle (\Delta y)^2 \rangle = \sum_i a_i^2 \sigma_i^2$$



But signal in e. g. different pixels can be correlated!

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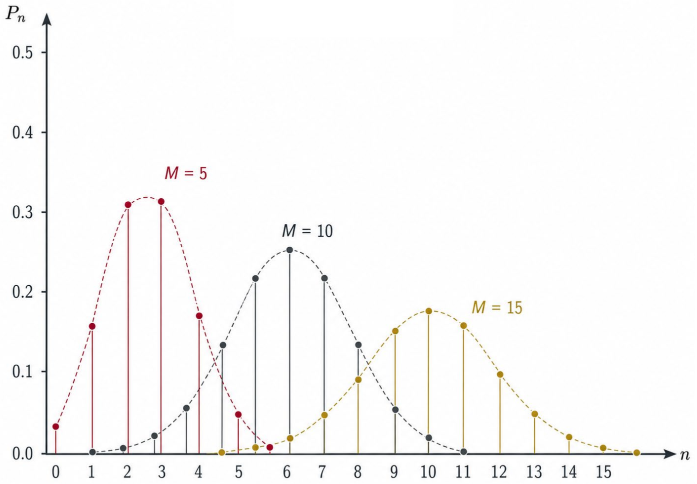
Common distributions: binomial

M independent trials, success or failure.

Success probability in each p.

Probability of specific n successes and $M-n$ failures is $p^n(1-p)^{M-n}$.



But there are $\binom{M}{n} = \frac{M!}{n!(M-n)!}$ arrangements.

$$P_n = \binom{M}{n} p^n (1-p)^{M-n}, \qquad n = 0, 1, \ldots, M \qquad \bar{n} = \langle n \rangle = Mp \qquad \langle (\Delta n)^2 \rangle = Mp(1-p)$$

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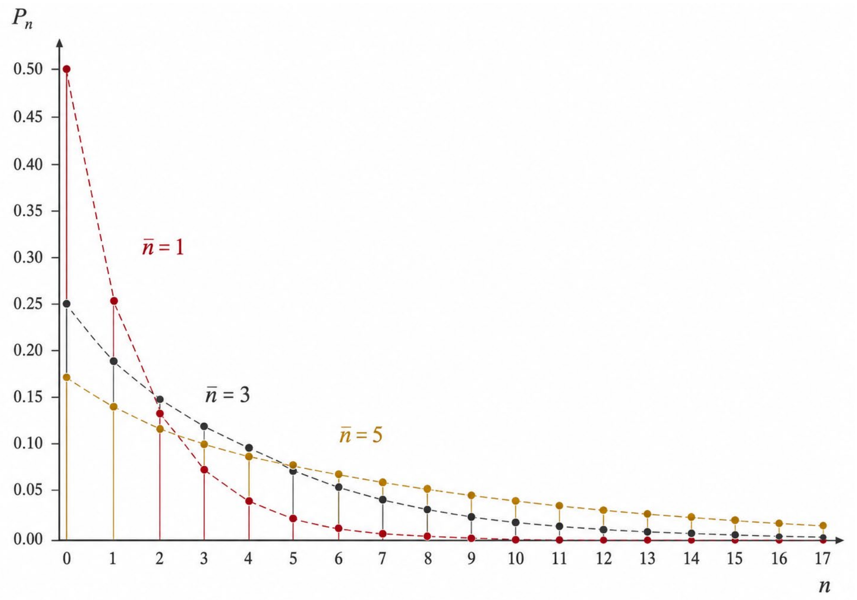
Common distributions: Bose-Einstein distribution

Let the outcomes be indistinguishable and $M \to \infty$, and $p/(1-p) = q < 1$.

Then through sequence summation we arrive at



$$P_n = (1-q)q^n \qquad \bar{n} = \langle n \rangle = \frac{q}{1-q} \qquad \langle (\Delta n)^2 \rangle = \bar{n}(1+\bar{n})$$

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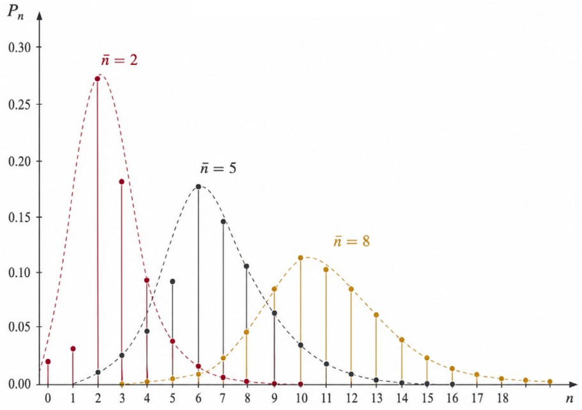
Common distributions: Poisson distribution

Let us take a different limit from binomial distribution keeping the expectation of success constant

$$M \to \infty, \qquad p \to 0, \qquad Mp = \bar{n}$$



Distribution and moments:

$$P_n = \frac{\bar{n}^n}{n!} e^{-\bar{n}}$$

$$\langle n \rangle = \bar{n}$$

$$\langle (\Delta n)^2 \rangle = \bar{n}$$

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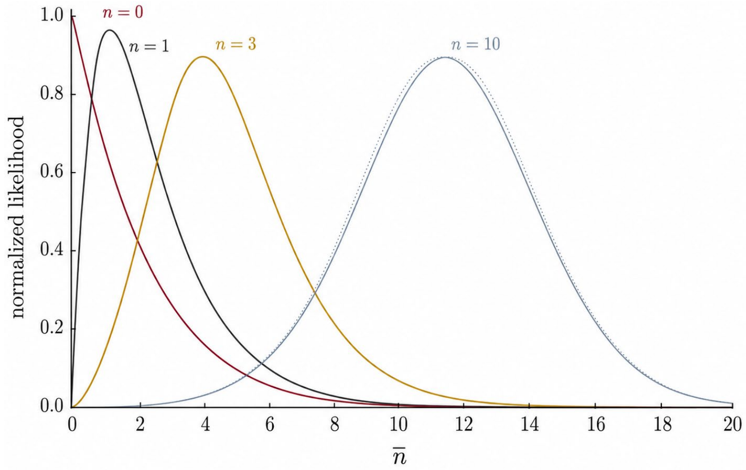
Poisson distribution: “error bars” at low counts

A signal 0 or 1 doesn‘t mean the average is 0 or 1

$n \pm \sqrt{n}$ is a high count approximation $\quad 0 \pm 0$ is wrong

„Error bars“ are not symmetric for Poisson distribution at low counts.

Likelihood $\quad \mathcal{L}(\bar{n}|n) \propto \bar{n}^n e^{-\bar{n}}$



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Photon shot noise

Poisson distribution commonly comes from „photon shot noise“

Particle nature of light → if counting photons in a certain time window, „random“ distribution

Shot noise is only one of the fluctuation sources! Real life example:

Chaotic light source, 1 mode (e. g. FEL):

$$p(I) = \frac{1}{\bar{n}} \exp\left(-\frac{I}{\bar{n}}\right)$$

$\otimes$

Shot noise:

$$P_n(I) = \frac{I^n e^{-I}}{n!}$$

Result:

$$P_n = \int_0^\infty \frac{I^n e^{-I}}{n!} \frac{1}{\bar{n}} e^{-I/\bar{n}}\, dI$$

$$P_n = \frac{\bar{n}^n}{(1+\bar{n})^{n+1}}$$

Bose-Einstein!

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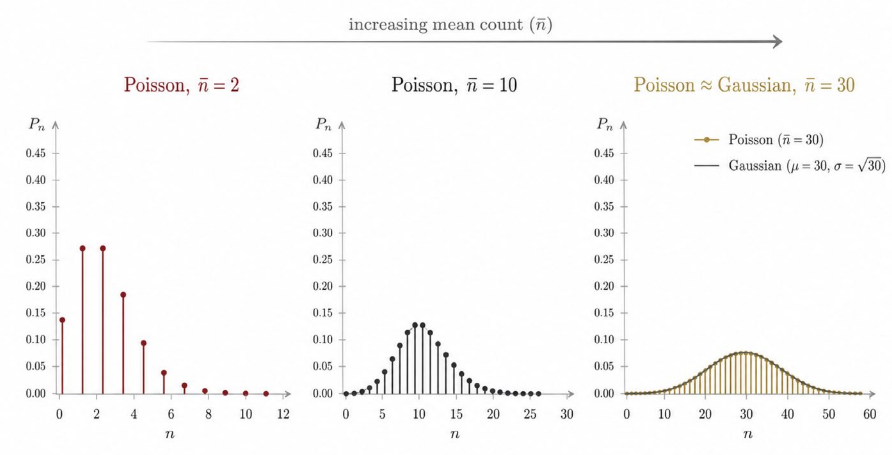
Gaussian distribution

Poisson distribution when $\bar{n} \to \infty$:

$$x = \frac{(n - \bar{n})}{\sqrt{\bar{n}}}$$

General form:

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



$$\mu = \langle x \rangle \qquad \sigma^2 = \langle (x-\mu)^2 \rangle$$

Distribution is defined by just the first 2 moments!

Stronger statement is true: if you can define a distribution by 2 moments, IT IS Gaussian!

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Central limit theorem

Important!

Take arbitrary **independent (!)** random variables

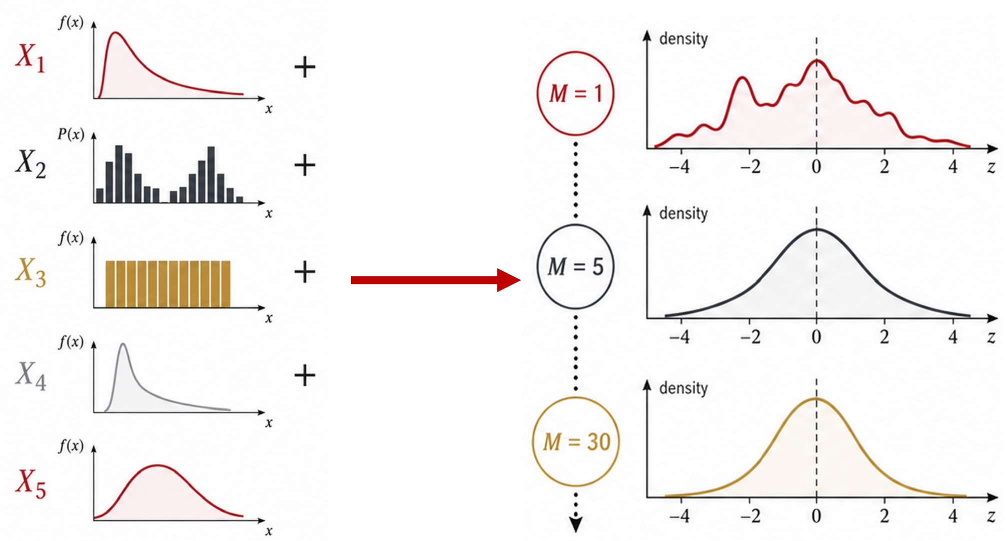
$$X_1, X_2, \ldots, X_M$$

For a large M the sum

$$S_M = \sum_{i=1}^{M} X_i$$

behaves as a Gaussian

Why do Gaussians suddenly appear
Every time probability is near?



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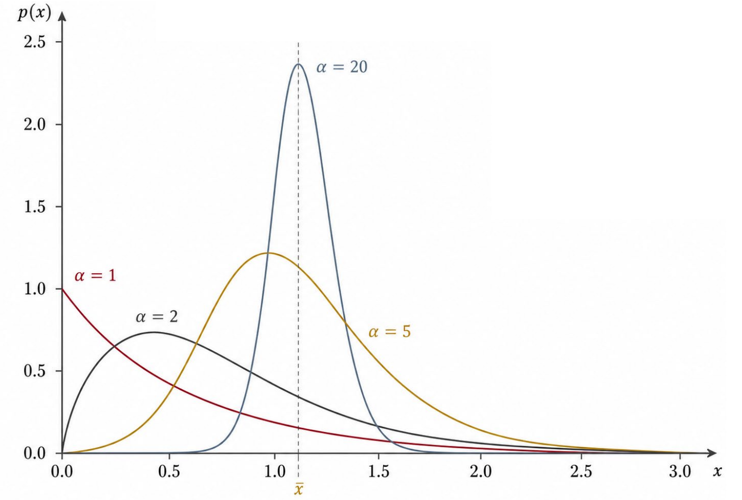
Gamma distribution

Another distribution of positive x

$$p(x) = \frac{1}{\Gamma(\alpha)} \left(\frac{\alpha}{\bar{x}}\right)^{\alpha} x^{\alpha-1} \exp\left(-\frac{\alpha x}{\bar{x}}\right), \qquad x \geq 0$$



Moments

$$\langle x \rangle = \bar{x}$$

$$\langle (\Delta x)^2 \rangle = \frac{\bar{x}^2}{\alpha}$$

Gamma function

$$\Gamma(\alpha) = \int_0^{\infty} t^{\alpha-1} e^{-t}\, dt$$

For integer α=m: $$p_m(x) = \frac{1}{(m-1)!} \left(\frac{m}{\bar{x}}\right)^{m} x^{m-1} \exp\left(-\frac{m x}{\bar{x}}\right) \qquad \Gamma(m) = (m-1)!$$

This is NOT a Poisson distribution despite form!

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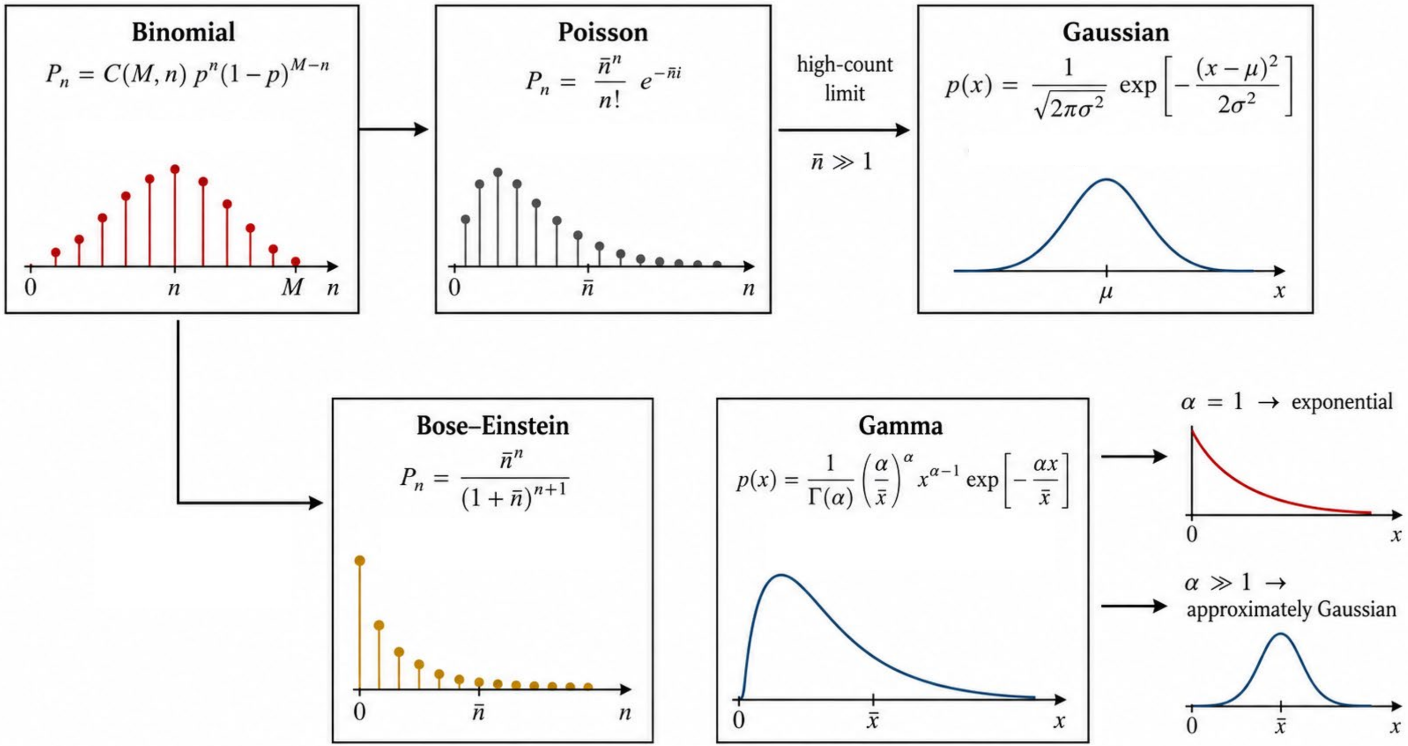
Distribution relationships



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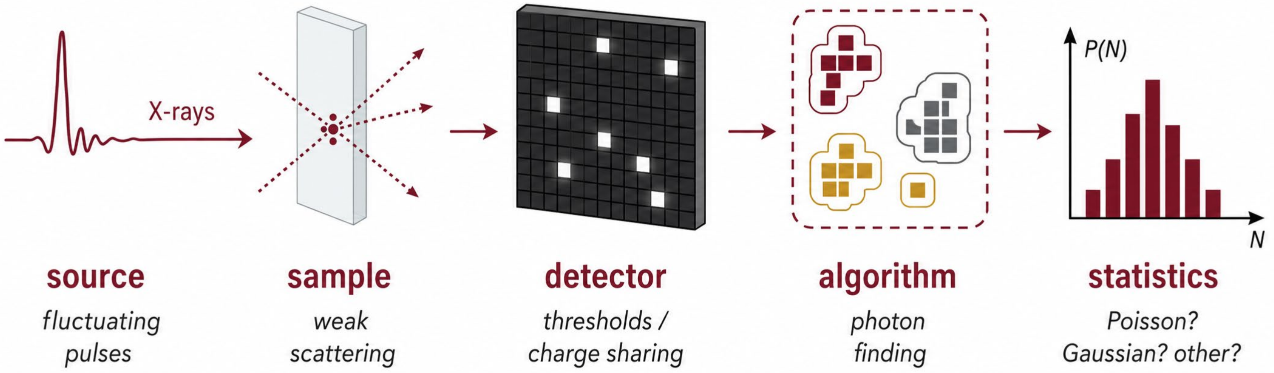
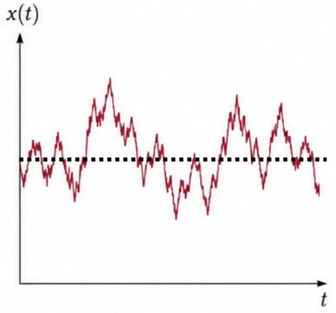


Random processes

A random process is a family of random variables $X(t)$ or $X_i, \quad i = 1, 2, \ldots$

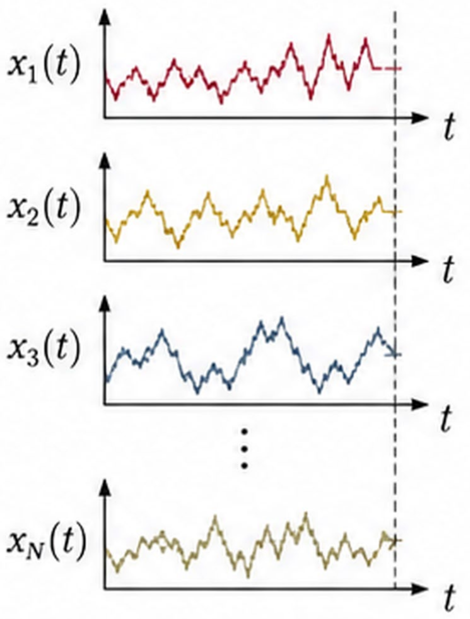
Continuous process can be averaged over *time*:

$$\overline{X}_T = \frac{1}{T}\int_0^T X(t)\,dt$$



Or over different realizations – over *ensemble*:

$$\langle X(t)\rangle = \lim_{N\to\infty}\frac{1}{N}\sum_{r=1}^{N} {}^{(r)}X(t)$$



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Stationarity and ergodicity

A process is *stationary* if its statistical properties does not change over time

Weak stationarity: $\langle X(t)\rangle = \text{const.}$ and $C(\tau) = \langle \Delta X(t)\Delta X(t+\tau)\rangle$

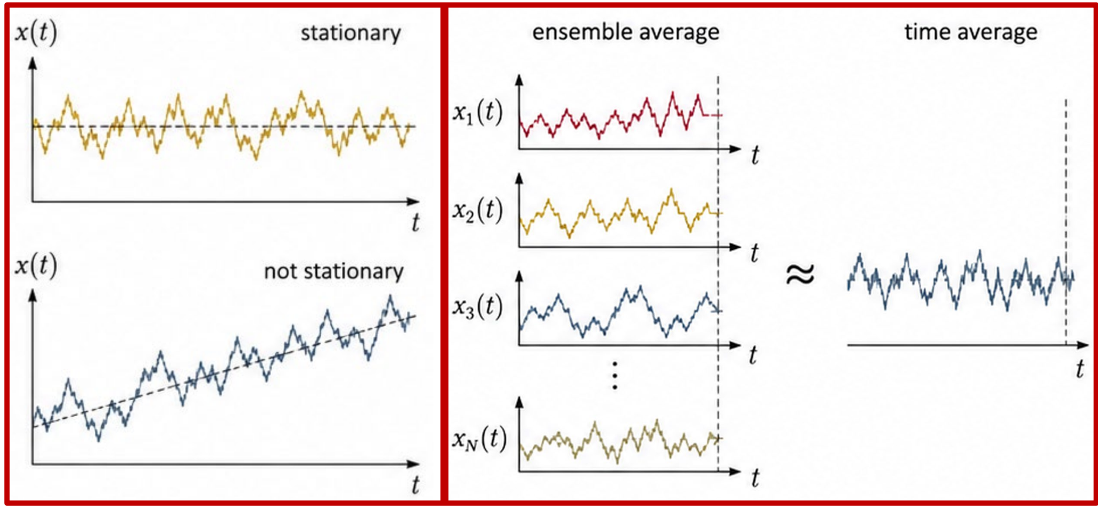
depends only on time difference τ

A process is *ergodic* if time average equals ensemble average:

$$\overline{X}_T = \frac{1}{T}\int_0^T X(t)\,dt \approx \langle X\rangle$$

$$\overline{X}_T \to \langle X\rangle \qquad T \to \infty.$$

When we measure multiple times, we rely on ergodicity and/or stationarity!



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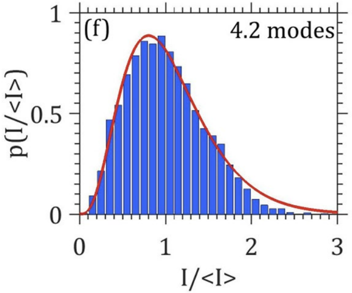
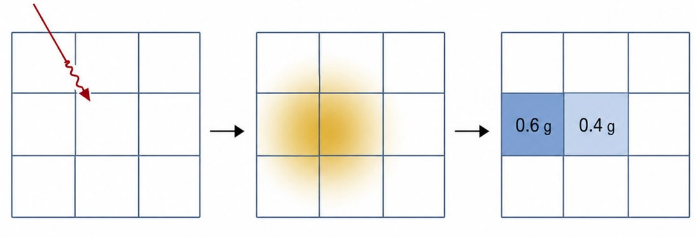
When to be careful with real random processes

- When source statistics are not “normal”, such as coherent sources: free electron lasers, advanced synchrotron sources...



- When individual photons need to be counted: detector physics and algorithms get involved

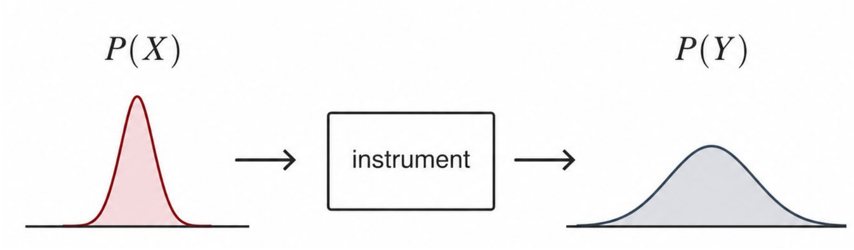


- When additional fluctuations are involved

- In general when counts are low

Note on “instrumental” and “statistical” errors

Sometimes separated:
- Statistical error describes randomness in the value
- Instrumental error describes how the instrument changes observation

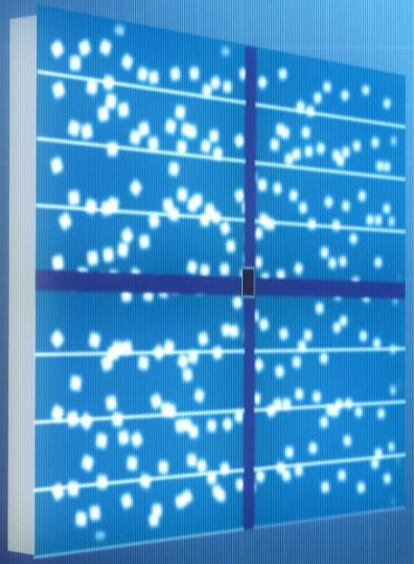


In real experiments, we sample a running random process with complex instrumentation, it‘s hard to decouple:

Finite sampling, shot noise, source fluctuations, readout noise, drift, et cetera…

Summary

- Errors are commonly calculated assuming normal or Poisson distributions, but other possibilities exist
- Probability distributions encode different assumptions about the physics of measurement
- Source statistics, detector physics, and even processing algorithms can affect the statistics of results
- At low counts, it can be difficult to distinguish distribution properties – be careful!



European XFEL