PHYS/ASTR 8150
Introduction to probabilities and statistics

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The use of statistics and probabilities

- **Parameter estimation**: given some data, what is our best estimate of a particular parameter? What is the uncertainty in our estimate?
- Identify data **correlations** : are two variables we have measured correlated with each other, implying a possible physical connection?
- **Model/hypothesis testing** : given some data and one or more models, are our data consistent with the models? Which model best describes the data?

The use of statistics and probabilities (2)

Statistics are a mean to summarize concisely yet rather precisely some of the characteristics of our data, while probabilities are a way to understand how the data is likely to behave.

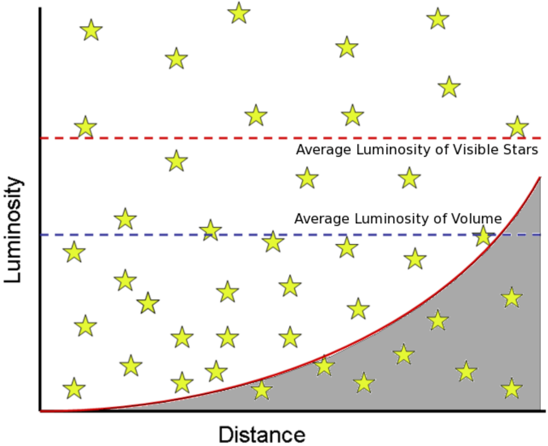
Both are used to state the uncertainties ("errors") in measurements:

- **Random errors**: always present in a measurement, inherently unpredictable fluctuations in the readings of a measurement apparatus or in the experimenter's interpretation of the instrumental reading (**stochastic** noise). Random errors show up as different noise occurrences and can be estimated by comparing multiple measurements, and reduced by averaging multiple measurements.
- **Systematic errors**: typically constant or proportional to the true value, caused by imperfect calibration of measurement instruments or imperfect methods of observation, or interference with the measurement process. Always affect the results of an experiment in a **predictable** direction. Systematic errors cannot be discovered or estimated by comparing/averaging occurrences, as they always push measurements in the same direction.

Biases

Statistics and probabilities can prevent us from being fooled by physical and psychological biases:

- Selection effects leading to spurious correlations, for example Malmquist bias



Biases (2)

- Confirmation bias : conclusions distorted by our preconceived idea about what the result should be

New light on old rays: N rays

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During the period 1903–1906, some 120 trained scientists published almost 300 articles on the origins and characteristics of a spurious radiation, the so-called N rays. Some new explanations are advanced for the extensive false observations and the deductions made from those observations. These are based on visits to Nancy, France, where the purported discovery was first announced and after which the rays were named, on an interview with a former assistant who knew some of the principals in the case, and on new archival information. Some of the misleading statements in the subsequent literature and oral history dealing with N rays are challenged, and additional information is provided on the original "discoverer," René Blondlot.

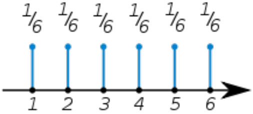
- Small samples: leading to noisy results
- A posteriori: using the same dataset which motivated a hypothesis to

Noise and probabilities

- Data is affected by noise, which prevents from getting to the exact mathematical laws, and behaves as a **random variable**
- Need to beat the noise: understanding the noise means we may get to the exact laws more easily
- Probabilities are the best tool to describe the noise **stochastic processes** or the data probability distribution
- Statistics cannot be understood if the noise **distribution** is unknown
- **Population**: the ensemble of all the samples with the characteristic one wishes to understand. A statistical population can be a group of actually existing objects (e.g. the set of all stars within the Milky Way galaxy) or a hypothetical and potentially infinite group of objects conceived as a generalization from experience (e.g. the set of all possible hands in a game of poker).
- **Sample**: a set of data collected and/or selected from a statistical population by a defined procedure, possibly repeated. It is a subset of the population, often chosen to represent the population in a statistical analysis.

Probability mass functions: discrete distributions

- **Discrete distribution**: data X is a discrete random variable, i.e. X takes integer values only.
- **Probability mass function** $f_X(x) = \Pr(X = x)$, gives the probability that X is exactly equal to some value x.
- Coin flip (**Rademacher distribution**): -1 to tails and 1 to heads, random variable X has a 50% chance of each,
$$f_X(x) = \begin{cases} 1/2 & \text{if } x = -1, \\ 1/2 & \text{if } x = +1, \\ 0 & \text{otherwise.} \end{cases}$$
- Uniform distribution for dices, e.g. for a 6-sided dice:



- A **discrete probability distribution** is a probability distribution characterized by a probability mass function with $\sum_x \Pr(X = x) = 1$

Probability density functions

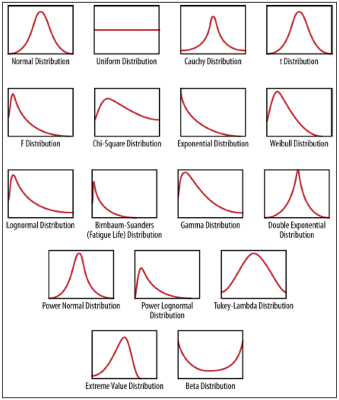


Figure 2-1. A bunch of continuous density functions (aka probability distributions)

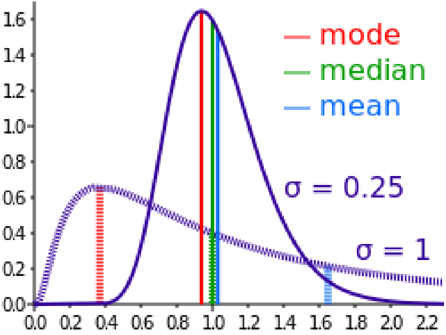
- Continuous case: if X a continuous random variable, the **probability density function** $f_X(X)$ is a continuous probability distribution
- **Support** of a probability function is the set of points where the probability density is not zero-valued
- The probability mass (not density) of getting any exact value is zero: $\Pr(X = a) = 0$
- In any interval $[a, b]$, $\Pr(a \leq X \leq b) = \int_a^b f_X(x)\, dx$

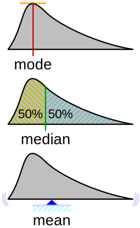
Measures of central tendency - Discrete case

Given a sample [1, 3, 6, 6, 6, 6, 7, 7, 12, 12, 17] with equal probabilities, find:

- **Mean**: $\bar{X} = \frac{1}{N} \sum_{i=0}^{N} x_i$. Note that $\bar{X}$ is the sample mean, as opposed to the the population mean/**expected value** $E[X]$; this latter often used for long-run/time averages, or Monte Carlo simulations.
- **Mode**: the element that occurs most often in the collection; if not unique, sample is said to be multimodal.
- **Median**: the element separating the higher half of a data sample from the lower half; arranging all the observations from lowest value to highest value and picking the middle one. If there is an even number of observations, then there is no single middle value; the median is then usually defined to be the mean of the two central values.

Measures of central tendency - Continuous





- Expected value: $\mu = \mathsf{E}[X] = \int x f(x)\,\mathrm{d}x$, over all the support of the distribution for the population.
- Mode: the peak value x where the probability density is maximum
- Median: x so that $\mathsf{P}(X \leq x) = \frac{1}{2}$ and $\mathsf{P}(X \geq x) = \frac{1}{2}$.

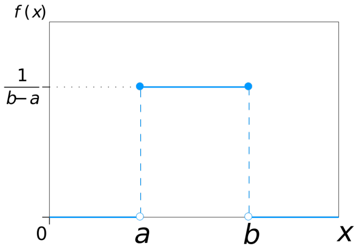
Variance and covariance

- If $\mu = \mathrm{E}[X]$, $\mathrm{Var}(X) = \mathrm{E}\left[(X-\mu)^2\right] = \mathrm{E}\left[X^2\right] - \mathrm{E}[X]^2$
- Continuous: $\mathrm{Var}(X) = \sigma^2 = \int (x-\mu)^2 f(x)\,dx = \int x^2 f(x)\,dx - \mu^2$
- Biased sample variance: $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2 = \left(\frac{1}{N}\sum_{i=1}^{N}x_i^2\right) - \mu^2$
- If the true (population) mean is unknown/computed as the sample mean, then the sample variance is a biased estimator: it underestimates the variance by the Bessel's correction factor $(N-1)/N$. **Homework 1 part 1: read on Bessel's correction.**
- Unbiased sample variance: $\sigma^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i-\mu)^2$

Cumulative distribution functions

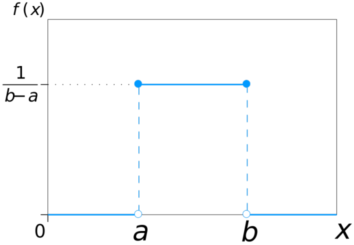
- The **cumulative distribution function** measures the probability that the variable takes a value less than or equal to x
- CDF: $F_X(x) = \mathrm{P}(X \leq x)$
- $\mathrm{P}(a < X \leq b) = F_X(b) - F_X(a)$
- In the continous case: $F_X(x) = \int_{-\infty}^{x} f_X(t)\, dt$

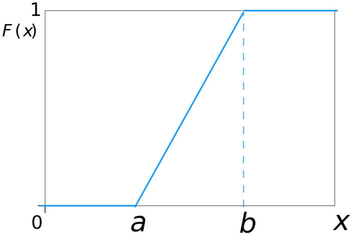
Examples of distributions: continuous uniform distribution



- Support ?
- Probability density function ?
- Cumulative distribution function ?
- Mean ?
- Median ?
- Mode ?
- Variance, and application to a randomly distributed variable in $[-\pi, +\pi]$?

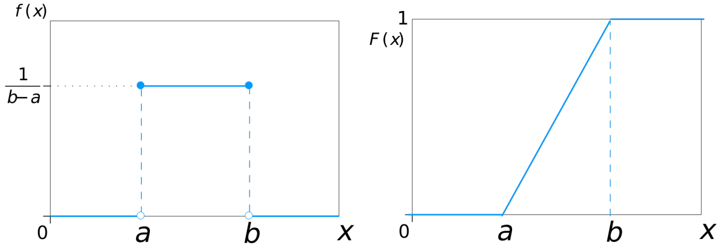
Examples of distributions: continuous uniform distribution





- Support $x \in [a, b]$
- Probability density function $f(x) = \begin{cases} \frac{1}{b-a} & \text{for } x \in [a, b] \\ 0 & \text{otherwise} \end{cases}$
- CDF $= \begin{cases} 0 & \text{for } x < a \\ \frac{x-a}{b-a} & \text{for } x \in [a, b) \\ 1 & \text{for } x \geq b \end{cases}$

Examples of distributions: continuous uniform distribution (2)



- Mean, Median $\frac{1}{2}(a+b)$, multimodal in (a, b)
- Variance $\frac{1}{12}(b-a)^2$, standard deviation is $\frac{b-a}{2\sqrt{3}}$
- Consequence: if data on an angle (by definition in $[-\pi, +\pi]$) has a standard deviation comparable to $\pi/\sqrt{3}\mathrm{rad} \simeq 104^o$, it is possibly completely random.

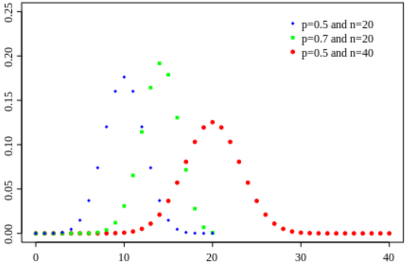
Variance computation and rolling statistics

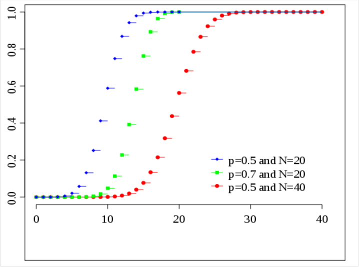
- Moving/rolling/running mean and variance are often used when dealing with streaming data
- Mean subject to issues with summation such as imprecision (research Kahan summation algorithm) or overfloat
- Algorithm 1: first compute the mean, then use it to compute the variance using classic expression. Two pass, and needs access to all the history of the data.
- Algorithm 2: accumulate sums of x_i and x_i^2. One pass only, does not need access to history.
- Welford's method: $(N-1)s_N^2 - (N-2)s_{N-1}^2 = (x_N - \bar{x}_N)(x_N - \bar{x}_{N-1})$, one pass and needs only updates.
- **Homework 1 part 2**: implement these three methods in Julia using for loops, then compare to native Julia functions for very large arrays (profile with @time or tic() and toc()).

Examples of distributions: Binomial distribution

- n **independent** trials of a random process with two mutually exclusive outcomes with probabilities p and $1 - p$, and k successes (occurences of p probability)
- Typical outcomes: detection or non-detection, belonging or not to a class of objects
- Special cases: tossing biased (Bernouilli) or unbiased coin (Rademacher distribution).

Examples of distributions: Binomial distribution





- Support: number of successes, $k \in 0, 1, 2 \ldots$
- PMF: $f(k; n, p) = \Pr(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$, $\binom{n}{k} = \frac{n!}{k!(n-k)!}$
- $E[X] = np$, $\mathrm{Var}\{X\} = np(1-p)$
- CDF:

$$\Pr(X \leq k) = \sum_{i=0}^{k} \binom{n}{i} p^i (1-p)^{n-i} = B_I(1-p, n-k, 1+k)/B(n-k, 1+k)$$

where B is the beta function and B_I the incomplete beta function.

Application of the Binomial distribution

Homework 1 part 3: do the following

- Professor Henry has a test with 10 multiple choice questions, with 5 possible answers per question. The right answer is unique for each question. Failing the test means getting less than 50% right answers (4 or less good answers in this case). For students that answer questions at random, Professor Baron wants to get the same failure rate with only 4 choices. How many questions are needed ?
- In the RECONS stellar catalog, 60% of stellar systems are binaries. How large should a stellar system sample be to have 99% or more chance of having at least two binary systems in the sample ?
- Find the probability of at least two students having the same birthday in a class of 25. Is the binomial distribution the right approach to the problem ? What would be the meaning of the binomial expectation here ?

Solution to the first two problems

- Failing the test: the events are independent with constant p, the binomial pdf applies:

$$\Pr(X \leq 4; n = 10; p = .2) \leq \Pr(X \leq \lceil \frac{n}{2} \rceil - 1; n; p = \frac{1}{4})$$

$$.967 \leq \left(\frac{3}{4}\right)^n + n\left(\frac{1}{4}\right)\left(\frac{3}{4}\right)^{n-1} + \ldots + \binom{n}{\lceil \frac{n}{2} \rceil - 1}\left(\frac{1}{4}\right)^{\lceil \frac{n}{2} \rceil - 1}\left(\frac{3}{4}\right)^{\lceil \frac{n}{2} \rceil}$$

$n \geq 16$ questions as $\Pr(X \leq 8; 8; p = .25) = .973$

- Binaries: binomial applies with $p = 0.6$, and we want the number of samples n to have the probability of finding LESS than 2 binaries (i.e. 0 or 1) below 100%-99%=1%.

$$\Pr(X = 0) + \Pr(X = 1) \leq 0.01$$

$$\binom{n}{0} p^0 (1-p)^{n-0} + \binom{n}{1} p(1-p)^{n-1} \leq 0.01$$

$$0.4^n + n \times 0.6 \times 0.4^{n-1} \leq 0.01 \rightarrow n \geq 8$$

Analyzing the birthday problem

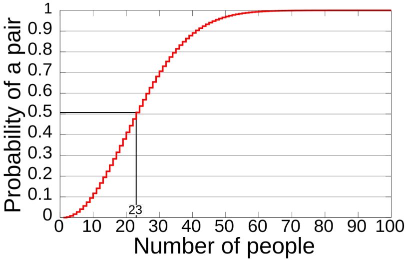
The binomial expected value (and standard deviation) should give you a strong clue something's amiss: $E[X] = np$ is n times the probability of a single event, reminding you it's treating the events as independent. Using the binomial probability distribution is **not** the right approach for this birthday problem, as the elementary events (having similar birthdays) are **not independent**. Let's look at the binomial expression terms:

- p^k: probability of having k independent successes.
- $(1-p)^{n-k}$: probability of having $(n-k)$ independent failures.
- $\binom{n}{k}$: number of possible ways to get k successes in n trials (e.g. success at first trial then third, or 4th and 6th, etc.).

There is no general formula to solve a problem with non-independent conditional probabilities (except Bayes theorem, later...).
The binomial distribution would only apply if you made a single student encounter 25 other students, and compare his birthday one by one. In this case the probability reaches $\sim 6.8\%$.

How to solve the birthday problem

- We want $1 - P(X = 0)$, where $P(X = 0)$ means $n = 25$ people with 0 common birthdays
- Easy (365 days) or hard problem (365.25 days, Feb 29th is counted)
- Classic way: first find the cardinal of the population ensemble, aka how many possible combination of birthdays can there be: 365^n.
- Then find how many possible ways of assigning birthdays without overlaps: $365 \times 364 \times \ldots \times (365 - n + 1) = 365!/(365 - n)!$.
- Therefore answer is $1 - P(X = 0) = 1 - 365!/(365^n(365 - n)!)$.



How to solve the birthday problem - Numerical method

- Using the classic formula has drawbacks: calculation of factorials can overfloat (Stirling and similar formula), and is undefined for non-integers (e.g. Mars year is 668.6 sols; would the gamma function solve this ? no). Solution = use **recursion**
- For 365 days, evaluate p(n) so that:

$$p(i) = \frac{365 - i + 1}{365} p(i-1) \quad \text{with} \quad p(1) = 1$$

For 365.25 days, $p_A(n)$ = prob. n different birthdays other than Feb 29, $p_B(n)$ = prob. n different birthdays, including one on Feb 29th. so that $p(i) = p_A(i) + p_B(i)$:

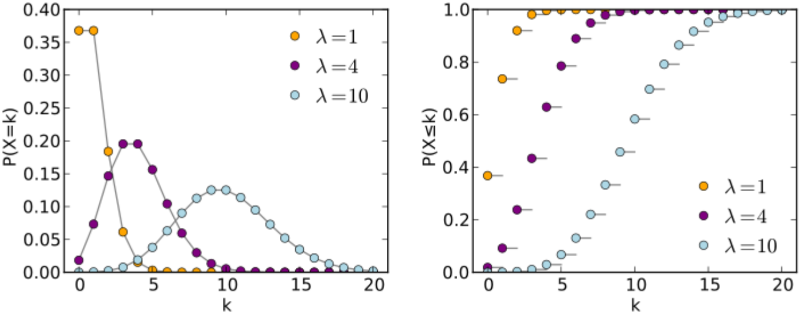
$$p_A(1) = \frac{365}{365.25}, \forall i > 1 : p_A(i) = \frac{365 - i + 1}{365} p_A(i-1)$$

$$p_B(1) = \frac{0.25}{365.25}, \forall i > 1 : p_B(i) = \frac{365 - i + 2}{365} p_B(i-1) + \frac{0.25}{365.25} p_A(i-1)$$

Examples of distributions: Poisson distribution

- **Discrete process**, measures number of events happening within a fixed interval of time if these events occur with a **known average rate** and **independently** of the time since the last event.
- Examples: junk mails per day, number of phone calls received by a call center per hour, decay events per second from a radioactive source, shot noise on cameras. Warning: the lapse of time between Poisson events does not follow a Poisson distribution, but an **exponential distribution** which is a continuous distribution.
- Shot noise caused by statistical quantum fluctuations in the number of photons sensed at a given exposure level. Noises at different pixels are independent of one another.
- Bad estimate of Poisson error: "Flux in pixel is k counts, therefore estimate of standard deviation $\sqrt{k}$ counts", assumes the mean count is the observed count, which is not true for low counts.

Examples of distributions: Poisson distribution



- PMF: $f(k;\lambda) = \Pr(X{=}k) = \frac{\lambda^k e^{-\lambda}}{k!}$, where λ the known average rate of occurrence, and k is the number of actual events observed.
- CDF: $F(k;\lambda) = \Pr(X \leq k) = e^{-\lambda} \sum_{i=0}^{k} \frac{\lambda^i}{i!}$
- $\mathrm{E}[X] = \lambda$, $\mathrm{Var}(X) = \lambda$.
- Poisson distribution does approach a normal distribution about its mean for large λ (typically $\lambda \geq 20$).

Application of the Poisson distribution

- The density of bugs in my code is 8 per 20,000 lines. How many lines should I read to ensure more than 50% chance of finding a bug ? What is the maximum number of lines I can have my boss read ensuring he will see less than 4 bugs ?

Solution

- We have a mean rate, so Poisson can be applied. Note we also have a true/false statement, so binomial could apply too.
- Expected number of bugs is $= \frac{8}{20000}n$

$$\Pr(X = 0) = \exp(-\frac{8}{20000}n) \leq 0.5$$
$$n \geq 1733$$

- What is the maximum number of lines I can have my boss read insuring he will see less than 4 bugs ? We need some additional information, i.e. acceptable probability. Otherwise there is always a probability, admittedly small, that there could be 5 bugs in the first line. We could set a threshold of 99%.

$$\Pr(X \leq 4) \geq 99\%?$$

Examples of distributions: Poisson and Binomial

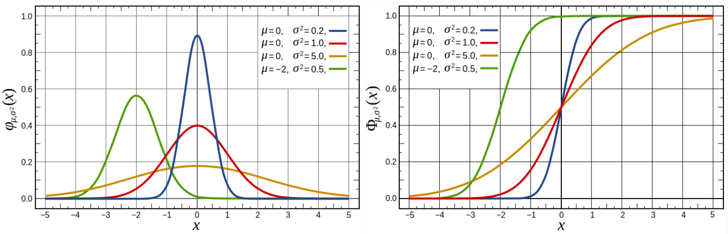
- **Law of rare events**: if $X \sim B(n,p)$, when $n \to \infty$ and $p \to 0$ and $\lim_{n\to\infty} np = \lambda$, then $X \sim P(\lambda)$. $p = \lambda/n$ is the probability of success of each of the k trial.

$$
\begin{aligned}
\lim_{n\to\infty} P(X=k) &= \lim_{n\to\infty} \binom{n}{k} p^k (1-p)^{n-k} \\
&= \lim_{n\to\infty} \frac{n!}{(n-k)!k!} \left(\frac{\lambda}{n}\right)^k \left(1-\frac{\lambda}{n}\right)^{n-k} \\
&= \lim_{n\to\infty} \left(\frac{\lambda^k}{k!}\right) && \to \frac{\lambda^k}{k!} \\
&\times \left(\frac{n}{n}\right)\left(\frac{n-1}{n}\right)\dots\left(\frac{n-k+1}{n}\right) && \to 1 \\
&\times \left(1-\frac{\lambda}{n}\right)^{-k} && \to 1 \\
&\times \left(1-\frac{\lambda}{n}\right)^{n} && \to e^{-\lambda}
\end{aligned}
$$

Examples of distributions: Poisson and Binomial (2)

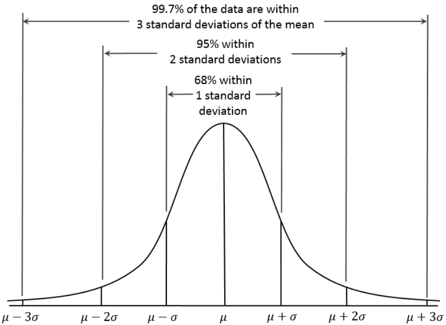
- **Poisson limit theorem**: another name for the law of rare events, if $n \to \infty$ and $p \to 0$ and $np \to \lambda$, then the binomial distribution tends to a Poisson distribution.
- Poisson distribution is the equivalent of a binomial law with a large number of attempts, each with with low probability, so that the expected average rate is a "reasonable" (not too low, not too high) number
- in practice, $n > 20$ and $p < 0.05$ works.

Examples of distributions: Gaussian/Normal distribution



- Notation: $X \sim \mathcal{N}(\mu, \sigma^2)$
- PDF: $f(x;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
- CDF: $F(x;\mu,\sigma) = \Pr(X \leq x) = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$, with $\operatorname{erf}(x) = \frac{1}{\sqrt{\pi}}\int_{-x}^{x} e^{-t^2}\, dt$
- $E[X] = \operatorname{Mode}(X) = \operatorname{Med}(X) = \mu$, $\operatorname{Var}(x) = \sigma^2$

Error bars and Gaussian/Normal distribution



- $X = \mu \pm \sigma$ means we assume X is a random variable normally distributed.
- Using the CDF we get:

$$\begin{aligned}&\Pr(\mu - n\sigma < X \leq \mu + n\sigma)\\ &= F(\mu + n\sigma) - F(\mu - n\sigma)\\ &= \operatorname{erf}\left(\frac{n}{\sqrt{2}}\right)\end{aligned}$$

- 68-95-99.7 or "3-sigmas" rule

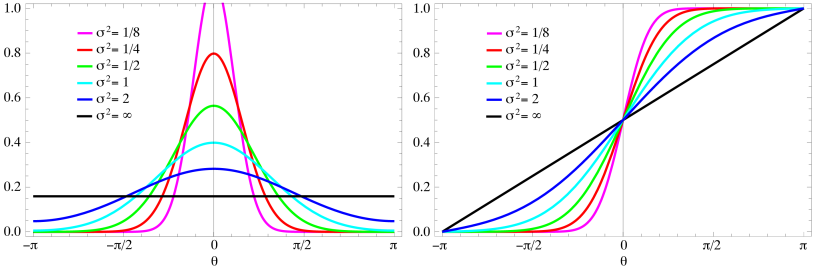
$$\begin{aligned}\Pr(\mu - \sigma \leq x \leq \mu + \sigma) &\approx 68.27\%\\ \Pr(\mu - 2\sigma \leq x \leq \mu + 2\sigma) &\approx 95.45\%\\ \Pr(\mu - 3\sigma \leq x \leq \mu + 3\sigma) &\approx 99.73\%\end{aligned}$$

Everything's normal, everything's fine...

Why is "everything" in papers normally distributed ?

- In the high "number of events" regime, Poisson for ($\lambda > 20$) and binomial distributions (very large n, De Moire-Laplace theorem) behave like Normal distributions.
- **Central limit theorem**: the mean of a large number of **independent and identically distributed** random variables, each with a well-defined expected value μ and well-defined variance σ, will be approximately normally distributed, **regardless of the underlying distribution**, as $\mathcal{N}(\mu, \sigma/\sqrt{N})$
- Take a large number of independent observations, and **average the results**; repeat this and note the distributions of theses averages: the central limit theorem says they will be normally distributed.
- The underlying distribution does not have to be unimodal !

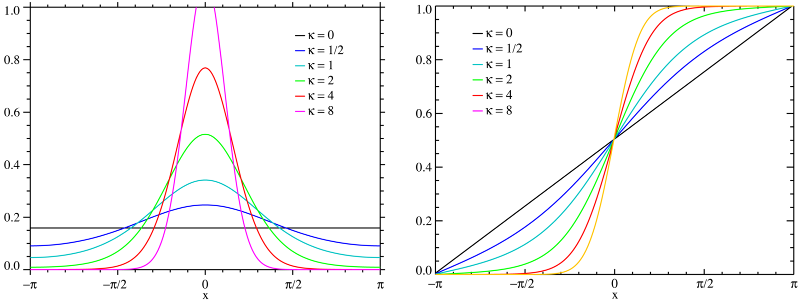
Wrapped normal distribution



Wrapped normal with $\mu = 0$ and support $[-\pi, +\pi]$

- PDF: $f_{WN}(\theta;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} \exp\left[\frac{-(\theta-\mu+2\pi k)^2}{2\sigma^2}\right]$
- Mean = Median = Mode = μ, circular variance $\text{Var}\{e^{i\theta}\} = 1 - e^{-\sigma^2}$
- A pain to deal with... No analytic CDF and tricky to manipulate.

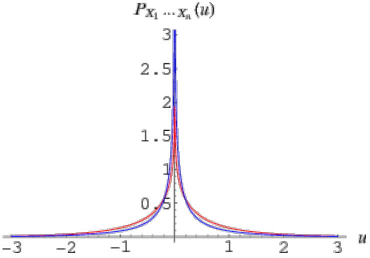
von Mises distribution

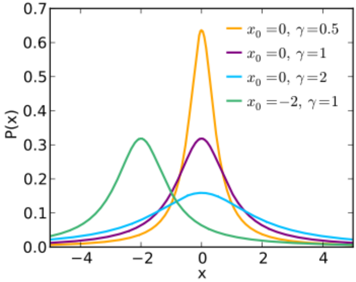


von Mises with $\mu = 0$ and support $[-\pi, +\pi]$

- A close approximation of the wrapped normal distribution PDF: $f_{WN}(\theta; \mu, \kappa) = \frac{e^{\kappa \cos(x-\mu)}}{2\pi I_0(\kappa)}$. $1/\kappa$ and σ^2 are related but not equal !
- Mean = Median = Mode = μ, $\mathrm{Var}\{e^{i\theta}\} = 1 - I_1(\kappa)/I_0(\kappa)$
- Still no analytic CDF.

Combination of normal variables





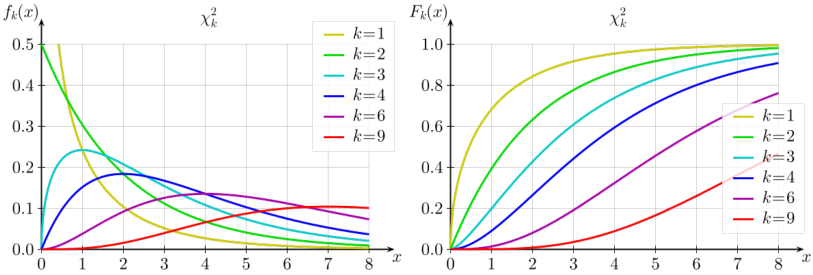
- If X and Y are independent normallly distributed random variables:
    - $Z = X + Y$ and $Z = X - Y$ are normally distributed.
    - $Z = XY$ follows a **normal product distribution** (above, left).
    - $Z = X/Y$ follows a **ratio distribution**. In the case where $X \sim \mathcal{N}(0, \sigma_X^2)$ and $Y \sim \mathcal{N}(0, \sigma_Y^2)$, it is a Cauchy distribution (above, right), else a Hinkley distribution. The mean and variance are in general undefined.
- If X is normallly distributed, X^2 follows a χ^2 distribution.

Examples of distributions: χ^2 distribution

- The chi-squared distribution with k degrees of freedom is the distribution of a sum of the squares of k independent standard normal random variables.
- This arises in particular when looking at:

$$\chi^2 = \sum_{i=1}^{k} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 = \sum_{i=1}^{k} X_i^2$$

- Each residual X_i (if the μ_i and σ_i are correct !) should be $X_i \sim \mathcal{N}(0, 1)$.
- For low k you may have bad deviations or outliers bogging down the χ^2. As k increases, you get more data and your estimate of the χ^2 get closer to its population mean.



- PDF: $f_k(x) = \frac{1}{2^{\frac{k}{2}}\Gamma\left(\frac{k}{2}\right)} \, x^{\frac{k}{2}-1} e^{-\frac{x}{2}}$
- CDF: $F_k(x) = \Pr(X \leq x; k) = \frac{1}{\Gamma\left(\frac{k}{2}\right)} \, \gamma\left(\frac{k}{2}, \, \frac{x}{2}\right)$
- $x = \chi^2$, Γ: Gamma function, γ: lower incomplete gamma function.
- $E[X] = k$, $\text{Mode}\{X\} = max(k-2, 0)$, $\text{Med}\{X\} = k(1 - \frac{2}{9k})^2$, $\text{Var}\{X\} = 2k$.
- For $k < 10$, distribution very skewed/non-Gaussian.
- For $k > 50$, central limit theorem implies $\chi^2 \sim \mathcal{N}(k, 2k)$.

Homework 2

- **Point of this homework**: learn to make publication-ready plots with a new language and learn about reduced χ^2 ...
- **Task**: imagine you're fitting N data samples, each normally distributed, using the χ^2 method. Let's define the reduced-χ^2 as $\chi_r^2 = \chi^2/N$. Plot the probability density distributions $\Pr(\chi_r^2 = x; N)$ on the continuous range $0 \leq x \leq 4$ for $N = 8, 36, 200, 1000$, each distribution being "renormalized" so that its maximum is 1. Add the corresponding legend and X and Y axis titles, and give the probability of getting $\chi_r^2 \leq 1$ for each case.

How a sample is approaching a population

- **Weak Law of Large Numbers/Bernouilli's theorem**: the sample mean converges towards the population mean for large samples (but only for distributions with existing means and variances). Example: coin flipping will average to 0.5 for probabilities of heads/tails.
- Let's suppose we made N **independent** observations of a random variable X from a Gaussian-distributed population with unknown parameters $\mathcal{N}(\mu, \sigma^2)$. The **standard error of the mean** is the standard deviation of the error in the sample mean with respect to the true (population) mean.
- We have $\bar{X} = \frac{1}{N}\sum_i X_i \sim \mathcal{N}(\mu, \sigma^2/N)$, or $\frac{\bar{X}-\mu}{\sigma/\sqrt{N}} \sim \mathcal{N}(0,1)$
- And: $S^2(X) = \frac{\sum_i (X_i - \bar{X})}{N-1} \sim \chi^2(N-1)$.
- $\frac{\bar{X}-\mu}{S/\sqrt{N}} \sim t(N-1)$: t-distribution with $N-1$ degrees of freedom, the distribution of the location of the sample mean relative to the true mean, divided by the sample standard deviation, after multiplying by the standardizing term $\sqrt{N}$.

Standard Errors on sample statistics (2)

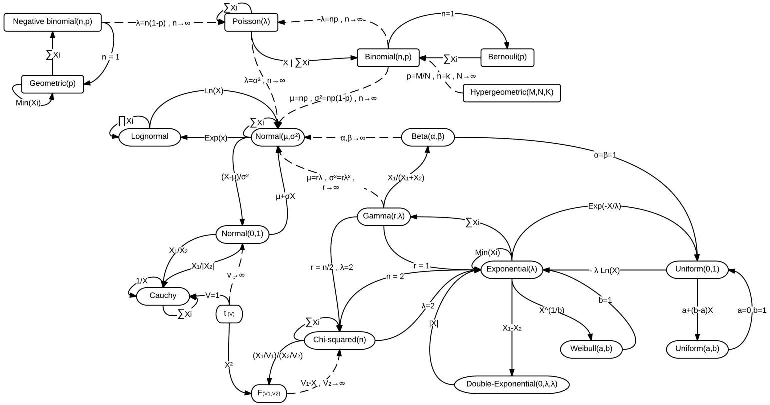
- **Student's t-distribution**: distribution of the mean of a normally distributed population in situations where the sample size is small and population standard deviation is unknown. Symmetric and bell-shaped, like the normal distribution, but has heavier tails, meaning that it is more prone to producing values that fall far from its mean. Often should use this instead of Normal distribution. In our example, the t-distribution can be used to estimate whether any given range would contain the true mean. When a true underlying distribution is known to be Gaussian, although with unknown σ, the resulting estimated distribution follows the Student t-distribution.
- A **standard error** of a statistic is the estimated standard deviation of this statistic. The standard error of the sample mean is the standard deviation of the Student t-distribution: $\mathrm{SE}(\bar{X}) = \sqrt{\mathrm{Var}(barX)} = \frac{S}{\sqrt{N}}$.
- Standard error on the sample median $\mathrm{SE}(\mathrm{Med}\{X\}) \simeq \sqrt{\frac{\pi}{2}}\frac{S}{\sqrt{N}}$: median more subject to sampling fluctuations than the mean.
- Standard error on sample standard deviation $\mathrm{SE}(S(X)) \simeq \frac{S}{\sqrt{2(N-1)}}$.

Other distributions

Less well-known, but of interest in physics and astronomy:

- Exponential distribution: measures the distribution of time intervals between Poisson events, i.e. a process in which events occur continuously and independently at a constant average rate. Length of time between phone calls, length of time until laptop failure, etc.
- lognormal distribution: distribution of a random variable whose logarithm is normally distributed

Relationships between distributions



- Even at low N, random variables following other distributions can often be transformed into normal variables. Anscombes transform $G(P) \mapsto 2\sqrt{P+\frac{3}{8}}$, P Poisson variable.

Generating random numbers following a given distribution

- All useful computer languages have an implementation of the uniform distribution (in Julia: `rand()`).
- To generate random numbers following a given distribution, the analytic expression of the inverse of the CDF then force $F(X)$ to follow a uniform distribution $U = F(X) \rightarrow X = F^{-1}(U)$.
- Proof:
  $F_X(x) = P(X \leq x) = P(F^{-1}(U) \leq x) = P(U \leq F(x)) = F(x)$
- When there is no analytic solution, the inverse may be found numerically since $P(X)$ is a increasing monotonic function of X.
- Exercice: try to generate random numbers following the exponential distribution which PDF is given here: $f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0, \\ 0 & x < 0. \end{cases}$

Distances between distributions - KS & Kuiper's tests

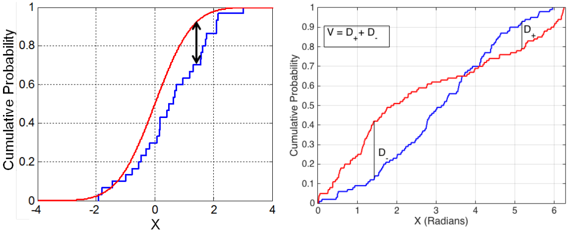
- You want to compare the distributions of two samples, $X_{1,i}$, $i = 1 \dots n_1$ and $X_{2,i}$, $i = 1 \dots n_2$.
- Empirical Distribution Functions: $F_1(x) = \frac{1}{n} \sum_{i=1}^{n} I(x_i \leq x)$ where I is the indicator function, here equal to 1 if $X_i \leq x$ and equal to 0 otherwise. For samples, $F_1(x) = n_1(x)/n$, $n_1(x)$ the number of X_1 values $\leq x$. Do the same for the second sample, $F_2(X_2)$.
- The Kolmogorov-Smirnov metric measures the distance between two distributions:

$$D_{\mathrm{KS}} = \max |F_1(X_1) - F_2(X_2)|$$

- Kuiper's test is a variant:

$$D_{\mathrm{Kuiper}} = \max(|F_1(X_1) - F_2(X_2)|) + max(|F_2(X_1) - F_1(X_2)|)$$

Distances between distributions - KS & Kuiper's tests



- Both tests are *frequentist* tests, testing the *null hypothesis* that the distributions are equal. They are often used to test versus a reference distribution. If $D_n > Q(\alpha)$, the hypothesis "x follows F_{test} distribution" fails at the confidence level $1 - \alpha$ (typically $\alpha = 1\%$ or 5%). Q(α) is gotten from tabulated values.
- For KS and $n > 10$, $Q(\alpha) \simeq 1.63/\sqrt{n}$ for $\alpha = 1\%$ and $Q(\alpha) \simeq 1.36/\sqrt{n}$ for $\alpha = 5\%$, where $n = \frac{n_1 n_2}{n_1 + n_2}$.

Distances between distributions - KS & Kuiper's tests

- Caveats: K-S test only applies to continuous distributions; if testing versus a reference distribution, it must be fully specified (i.e. parameters not fitted from data); the test is more sensitive near the center of the distribution than at the tail.
- Other tests exist: Lilliefors (derived from KS), Cramer-von Mises/Watson and Anderson-Darling (using quadratic distances), ShapiroWilk's test (specialized to test for Gaussianity).
- Some tests are tailored to compare only specific statistics of sample distributions (e.g. comparing the means): U test, Mann-Whitney-Wilcoxon test.
- Some tests are parametric: t test, f test.
- There is extensive litterature on the benefits/drawback of all these methods.

Thinking about probabilities...

- **Prosecutor's fallacy**: the murderer has a tatoo, there is a 1/1,000,000 chance of anyone having the same tatoo, therefore the accused (who has the tatoo) has 1/1,000,000 chances of being innocent.
- **Defense attorney's fallacy**: there are 320 millions people in the US, therefore around 320 matches for this tatoo, and my client has only 1/320 chance of being the murderer.

Frequentist approach to probabilities

- D: data
- M: Model
- Everything to the right of "$|$" means: "on the condition that these have occured", or "given these are true"
- Example: probability of $D = 5$ given $M = \mathcal{N}(3, 9)$
- Frequentist statistics assigns: $\Pr(D|M)$
- Frequentist probabilities are understood as though experiments where a population is repeatedly sampled and probabilities are used to express the proportions of outcomes.
- A model is rejected if $\Pr(D|M)$ is below a chosen threshold.

Bayesian approach to probabilities

- Bayesian statistics assigns probabilities to models given the data $\Pr(M|D)$ and to models and data themselves $\Pr(M)$ and $\Pr(D)$!
- Bayesian probabilities update model probabilities based on new data.
- Models are not rejected, just assigned low probabilities

Model-fitting: likelihood

- We obtain N data points through experiments $X = \{x_1, \ldots x_N\}$ with $S = \{\sigma_1, \ldots \sigma_N\}$ (heteroskedasticity)
- We have a model M based on parameters $\theta = \{\theta_1, \ldots \theta_p\}$, predicting values $\mu = \{\mu_1, \ldots \mu_N\}$.
- The **likelihood** of θ given the data is equal to the probability of the observed data given those parameter values

$$\mathcal{L}(\theta|X) = \Pr(X|\theta)$$

- The likelihood is a function of θ given X, i.e. **not** a probability density function (function of X given θ), i.e. it is not the probability that the model parameters are the right ones, given the data.
- Consequently the likelihood is generally unnormalized, i.e. $\int_\theta \mathcal{L}(\theta|X)d\theta \neq 1$, while $\int_X \mathcal{L}(\theta|X)dX = 1$

Model-fitting: likelihood and χ^2

- For independent data points,

$$\mathcal{L}(\theta|X) = \prod_{i}^{N} \Pr(x_i|M)$$

- The **log-likelihood** is

$$\log \mathcal{L}(\theta|X) = \sum_{i}^{N} \log \Pr(x_i|M)$$

- In particular if we assume the data normally distributed, the log-likelihoood is:

$$\sum_{i}^{N} \log \Pr(x_i|M) = \sum_{i}^{N} \log \frac{e^{-\frac{(x_i-\mu_i)^2}{2\sigma_i^2}}}{\sigma_i\sqrt{2\pi}} = \mathrm{cnst} - \frac{1}{2}\sum_{i}^{N}\left(\frac{x_i-\mu_i}{\sigma_i}\right)^2$$

Model-fitting and Maximum likelihood

- The most likely values for the model parameters μ are found by maximizing the likelihood.
- Maximizing the likelihood is minimizing the negative log-likelihood:

$$\begin{aligned}
\underset{\theta}{\operatorname{argmax}} \mathcal{L}(\theta|X) &= \underset{\theta}{\operatorname{argmin}} \{-\log \mathcal{L}(\theta|X)\} \\
&= \underset{\theta}{\operatorname{argmin}} \left(\mathrm{cnst} + \frac{1}{2} \sum_{i}^{N} \left(\frac{x_i - \mu_i(\theta)}{\sigma_i} \right)^2 \right) \\
&= \underset{\theta}{\operatorname{argmin}} \chi^2(\theta)
\end{aligned}$$

- χ^2 **minimization** results from applying the **maximum likelihood** approach to a model-fitting problem with normally-distributed data

χ^2 and reduced χ^2

- χ^2 is used for model-fitting (parameter estimation).

$$\chi^2 = \sum_{i=1}^{k} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 = \sum_{i=1}^{k} R_i^2$$

- Assuming Normal distribution or Poisson in the high count limit ($\sigma_i^2 \simeq \mu_i$), the residual $R_i = (x_i - \mu_i)/\sigma_i$ is $\mathcal{N}(0, 1)$.
- Such a χ^2 follows a χ^2 distribution with degrees of freedom k, i.e. $E\{\chi^2\} = k$ and $\mathrm{Var}\{\chi^2\} = 2k$.
- When fitting a model with p parameters on a sample of N independent data points, litterature often picks $k = N - p$ (we'll see later why this is not an optimal choice).
- Reduced χ^2: $\chi_r^2 = \chi^2/k \sim 1 \pm \sqrt{2/k} \xrightarrow{k\to\infty} 1$

Application of Maximum likelihood: Inverse variance weighting

- We attempt to **combine independent estimates** of a single quantity, using data x_i, σ_i^2, $i = 1 \ldots N$, x_i know to be normally distributed with variance σ_i^2. E.g. we could want to combine $T = 300 \pm 50K$ and $T = 326 \pm 12K$.

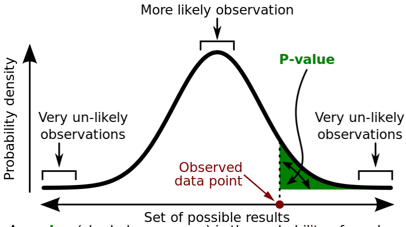
Application of Maximum likelihood: Inverse variance weighting

- We want to obtain the most probable estimate for our model value μ, plus an error bar. As χ^2 is a quadratic function of μ, $\tilde{\mu}$ can found by differentiation:

$$\tilde{\mu} = \underset{\mu}{\operatorname{argmin}} \sum_i \left(\frac{x_i - \mu}{\sigma_i} \right)^2 \implies 0 = \sum_i \frac{1}{\sigma_i^2} 2(x_i - \tilde{\mu}) \implies \tilde{\mu} = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}}$$

- The **inverse-variance weighted average** is $\mathrm{Var}\{\tilde{\mu}\} = \frac{1}{\sum_i 1/\sigma_i^2}$ and can be shown to have the least variance among all weighted averages.

Frequentist approach to hypothesis testing: p-value



A**p-value** (shaded green area) is the probability of an observed (ormore extreme) result assuming that the null hypothesis is true.

- p-value is the number one statistics used in "soft" sciences.
- **Null hypothesis**: default hypothesis (e.g. data originates from random noise, default distribution, etc.).
- **Alternative hypothesis**: any model different from the null hypothesis.
- p-value is the probability of getting our current result or an even less probable one if the null hypothesis were true.
- p-value is the **conditional probability** $\Pr(X \geq x | H_0)$
- X is often not an observation/measurement but a **test statistics**

More on p-value

- Example: what is the p-value of getting 5 heads in a row: what can we define as the test statistics ? Null hypothesis ? Alternative hypothesis ?

More on p-value

- Example: **Null hypothesis** H_0: a coin is fair, H: coin is not fair/ biased in some way. H and the null hypothesis H_0 are mutually exclusive and have to be the only possibilities. $\Pr(H) \neq \Pr(H_0)$ in general, but 50%-50% here.
- Applied to χ^2: we have a set of data at hand onto which we fitted a model, and found χ_0^2, then
p-value $= \Pr(\chi^2 \geq \chi_0^2 | H_0) = 1 - \Pr(\chi^2 < \chi_0^2 | H_0)$.
- Exercice: compute p-value at 5-sigma.
- The p-value is often compared to a significance level α, the proportion of false alarm or detection we are willing to tolerate. Typically $\alpha = 5\%$ or $\alpha = 1\%$. **We can only conclude one of two things**:
    - if $p > \alpha$, H_0 is rejected
    - if $p < \alpha$, H_0 cannot be rejected at that significance level (beware ! this not imply that H_0 is true).
- α gives the rate of falsely rejecting the null hypothesis
- The p-value is the lowest α for which the null hypothesis can be rejected for a given data set.

Frequent issue: misunderstanding the significance of p-value

- The p-value is a minefield, very easy to misunderstand unless studied properly.
- A p-value is a **frequentist** tool and **cannot be used to figure out the probability of any hypothesis being true** (including H and H_0).
- The p-value $p = \Pr(X \geq x|H_0)$ is not:
  - $\Pr(X)$: probability of getting the data we got
  - $\Pr(H_0)$: probability the null hypothesis is true
  - $\Pr(H)$: probability our hypothesis is true
  - $\Pr(H|X)$: probability our hypothesis is true given the data
  - $\Pr(X|H_0)$: the probability that a finding is "merely a fluke" or "the results are due to chance", i.e. that H_0 is correct.
  - the probability of falsely rejecting H_0
  - the probability that replicating the experiment would yield the same conclusion

Bayesian terms and Bayes' theorem

- The following equations are valid for any ensembles, but here I give them in the context of model-fitting
- $\Pr(M, D) = \Pr(M \cap D)$: joint probability (here of model and data)

$$\Pr(M, D) = \Pr(D)\Pr(M|D)$$

  but we also have

$$\Pr(M, D) = \Pr(M)\Pr(D|M)$$

- $\Pr(M|D)$: posterior probability of the model
- $\Pr(M)$: prior probability of model, sometimes written $\pi(M)$
- $\Pr(D|M)$ probability of the data given the model, or interpreted as likelihood of the model $\mathcal{L}(M|D)$
- $\Pr(D)$: evidence, marginal likelihood, "probability of the data"
- Bayes' theorem results from eq. (1) and (2)

$$\Pr(M|D) = \frac{\Pr(D|M)\Pr(M)}{\Pr(D)}$$

Thinking about probabilities with Bayes

- **Prosecutor's fallacy**: the murderer has a tatoo, there is a 1/1,000,000 chance of anyone having the same tatoo, therefore the accused who has the tatoo has 1/1,000,000 chances of being innocent.
- **Defense attorney's fallacy**: there are 320 millions people in the US, therefore around 320 matches for this tatoo, and my client has only 1/320 chance of being the murderer.
- Bayesian analysis: I = innocent, T =tatoo; the fallacies lie here:
    - Prosecutor: considers $\Pr(T|I) \lll 1$, and conflates it with $\Pr(I|T)$ or assume they are the same. If the accused was picked out of a database of people who have this tatoo, we have a data fishing issue.
    - Defense: forgot that the probability of anyone in the general population to be arrested in connection with the murder is likely to be low.

Marginalization of likelihood/evidence

- More generally, for mutually exclusive models/events M_i, $i = 1 \ldots N$, $M_i \cap M_j = \varnothing$, but exhaustive $M_1 \cup \ldots \cup M_N = \mathbb{U}$ then

$$\Pr(D) = \Pr\left((D \cap M_1) \cup \ldots \cup (D \cap M_N)\right) = \sum_i \Pr(D|M_i) \Pr(M_i)$$

- Very often applied to a continuous model parameter θ

$$\Pr(\theta|D) = \frac{\Pr(D|\theta) \Pr(\theta)}{\Pr(D)}$$

- The marginal likelihood $P(D)$ can be understood as a normalization factor, so that the posterior $\Pr(\theta|D)$ is normalized
- **Bayesian marginalization** of the likelihood over the parameter θ:

$$\Pr(D) = \int_\theta \Pr(D, \theta) d\theta = \int_\theta \Pr(D|\theta) \Pr(\theta) d\theta = \int_\theta \mathcal{L}(\theta|D) \pi(\theta) d\theta$$

- The parameter has been marginalized = "**integrated out**"

Evidence expression for mutually exclusive outcomes

- If there are only two possible models, M and $\bar{M}$ (e.g. a statement is true or false), then the marginalization gives:

$$\Pr(D) = p(M)p(D|M) + p(\bar{M})p(D|\bar{M})$$

- Bayes' equation becomes:

$$\Pr(M|D) = \frac{\Pr(D|M)\Pr(M)}{\Pr(M)\Pr(D|M) + \Pr(\bar{M})\Pr(D|\bar{M})}$$

Application of Bayes theorem: stellar survey

- Stellar survey in the neighborhood find only three types of stars:

Type	% total	Probability of multiplicity
F	0.45	0.10
G	0.15	0.45
K	0.40	0.20

- I randomly select a multiple star, what is the probability it is F-type ?

Application of Bayes theorem: stellar survey solution

Type	% total	Probability of multiplicity
F	0.45	0.10
G	0.15	0.45
K	0.40	0.20

- We want $\Pr(F|M)$ and we have $\Pr(M|F) = 0.1$ and $\Pr(F) = 0.45$.
- Bayes' theorem: $\Pr(F|M) = \frac{\Pr(M|F)\times\Pr(F)}{\Pr(M)}$
- We still need $\Pr(M)$, and we can marginalize over the stellar type to find it (as we know we only have 3 possibilities/types):
  $\Pr(M) = \Pr(M|G)\Pr(G) + \Pr(M|F)\Pr(F) + \Pr(M|K)\Pr(K) = .1925$
- So the answer is $\Pr(F|M) = \frac{.1\times.45}{.1925} = .23$

Bayesian statistics: the zombie disease example

- Only 1% of the population who participate to a zombie plague screening have the plague. 95% of plague carriers will get tested positive, and 10% of non-carriers also get tested positive. Fabien just got tested positive. What is the probability he is infected ?
- Sensitivity of the test: prob. of true positives
- Specificity of the test: prob. of true negatives, here $100\% - 10\% = 90\%$
- Type I errors: prob. of false positives, i.e. testing someone as positive who is in fact negative, given to be 10% here (other example: computer anti-virus flagging a safe file)
- Type II errors: prob. of false negatives, i.e. testing someone as negative who is in fact positive, here 100%-95% = 5% (example: computer anti-virus failing to detect actual viruses)

Bayesian statistics: the zombie disease example

- Only 1% of the population who participate to a zombie plague screening have the plague. 95% of plague carriers will get tested positive, and 10% of non-carriers also get tested positive. Fabien just got tested positive. What is the probability he is infected ?
- M: Fabien is infected, D: tested positive
- Prior probability $\Pr(M) = .01$, and $\Pr(\bar{M}) = .99$
- Sensitivity: $\Pr(D|M) = .95$, specificity: $\Pr(\bar{D}|\bar{M}) = 1 - \Pr(D|\bar{M}) = .9$
- Prob. type I: $\Pr(D|\bar{M}) = .1$, Prob. type II $\Pr(\bar{D}|M) = 1 - \Pr(D|M)$.

$$\Pr(M|D) = \frac{\Pr(D|M)\Pr(M)}{\Pr(M)\Pr(D|M) + \Pr(\bar{M})\Pr(D|\bar{M})} \simeq 8.8\%$$

- What is the probability he is infected if a second test also comes positive ?

Changing variables in a Bayesian context

- Changing variables requires using the **jacobian** modulus $\left|\frac{\partial Y}{\partial X}\right|$:

$$X \mapsto Y = f(X), \text{f monotonic} \implies \quad \Pr(X) = \Pr(Y)\left|\frac{\partial Y}{\partial X}\right|$$

- if $Y = f(X)$ is not a one to one transformation, $\Pr(X)$ is given by the sum over all values of Y which correspond to X.
- Generalization:

$$\Pr(X_i) = \Pr(Y_i) \times \left|\frac{\partial(Y_1, Y_2, \ldots Y_n)}{\partial(X_1, X_2, \ldots X_n)}\right|$$

- Multivariate **jacobian determinant**:

$$\left|\frac{\partial(Y_1, Y_2, \ldots Y_n)}{\partial(X_1, X_2, \ldots X_n)}\right| = \det\begin{bmatrix} \frac{\partial Y_1}{\partial X_1} & \cdots & \frac{\partial Y_1}{\partial X_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial Y_m}{\partial X_1} & \cdots & \frac{\partial Y_m}{\partial X_n} \end{bmatrix}$$

Changing variables in a Bayesian context: example

- Isotropic bivariate Gaussian given as a function of Cartesian coordinates (x, y)

$$\Pr(x, y) = \frac{1}{2\pi\sigma^2} \exp\left[-\frac{x^2 + y^2}{2\sigma^2}\right]$$

- We want it as a function of (r, θ)... and maybe just r ?

Changing variables in a Bayesian context: example

- Isotropic bivariate Gaussian given as a function of Cartesian coordinates (x, y)

$$\Pr(x, y) = \frac{1}{2\pi\sigma^2} \exp\left[-\frac{x^2 + y^2}{2\sigma^2}\right]$$

- We want it as a function of (r, θ).
- $x = r\cos\theta,\ y = r\sin\theta,\ \left|\frac{\partial(x,y)}{\partial(r,\theta)}\right| = \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix} = r$

$$\Pr(r, \theta) = \Pr(x, y) \left|\frac{\partial(x, y)}{\partial(r, \theta)}\right| = \frac{r}{2\pi\sigma^2} \exp\left[-\frac{r^2}{2\sigma^2}\right]$$

- Marginalization:

$$\Pr(r) = \int_0^{2\pi} \Pr(r, \theta) d\theta = \frac{r}{\sigma^2} \exp\left[-\frac{r^2}{2\sigma^2}\right]$$

Bayesian error propagation: $Z = f(X, Y)$

- Propagation of uncertainties, for $X = x_0 \pm \sigma_x$ and $Y = y_0 \pm \sigma_y$

$$
\begin{aligned}
\Pr(Z) &= \iint \Pr(Z|X, Y) \Pr(X, Y) dX dY \\
&= \iint \Pr(Z - f(X, y)) \Pr(X, Y) dX dY \\
&= \iint \Pr(X, Y) \delta(Z - f(X, Y)) dX dY
\end{aligned}
$$

- if X and Y are independent: $\Pr(X, Y) = \Pr(X) \Pr(Y)$

$$
\Pr(Z) = \int dX \Pr(X) \int \Pr(Y) \delta(Z - f(X, Y)) dY
$$

Error propagation: $Z = X + Y$

- For $Z = X + Y$

$$\begin{aligned}
\Pr(Z) &= \int \Pr(X)\Pr(Y = Z - X)dX \\
&= \frac{1}{2\pi\sigma_x\sigma_y}\int_{-\infty}^{+\infty} \exp\left[-\frac{(X-x_0)^2}{2\sigma_x^2}\right]\exp\left[-\frac{(Z-X-y_0)^2}{2\sigma_y^2}\right]dX \\
&= \frac{1}{\sqrt{2\pi}\sigma_z}\exp\left[-\frac{(Z-z_0)^2}{2\sigma_z^2}\right]
\end{aligned}$$

  with $z_0 = x_0 + y_0$ and $\sigma_z^2 = \sigma_x^2 + \sigma_y^2$.
- $Z = X - Y$ gives the same PDF, with $z_0 = x_0 - y_0$ and $\sigma_z^2 = \sigma_x^2 + \sigma_y^2$.
- This method is more general than "classic" error propagation

Classic error propagation

- For $Z = X - Y$, $\delta X = X - x_0$, $\delta Y = Y - y_0$, $(\delta_X)^2 = \sigma_x^2$, $(\delta_Y)^2 = \sigma_y^2$

$$\delta Z = \delta X - \delta Y$$

$$(\delta Z)^2 = (\delta X)^2 + (\delta Y)^2 - 2\delta X \delta_Y$$

$$< (\delta Z)^2 > = < (\delta X)^2 > + < (\delta Y)^2 > -2 < \delta X \delta Y >$$

$$\sigma_z^2 = \sigma_x^2 + \sigma_y^2 - 2\sigma_{xy}$$

- For $Z = X/Y$,

$$\delta Z = \frac{Y\delta X - X\delta Y}{Y^2}$$

$$\frac{\delta Z}{Z} = \frac{\delta X}{X} - \frac{\delta Y}{Y}$$

$$\frac{< (\delta Z)^2 >}{z_0^2} = \frac{< (\delta X)^2 >}{x_0^2} + \frac{< (\delta Y)^2 >}{y_0^2} - 2\frac{< \delta X >< \delta Y >}{x_0 y_0}$$

$$\frac{\sigma_z^2}{z_0^2} = \frac{\sigma_x^2}{x_0} + \frac{\sigma_y^2}{y_0} - 2\frac{\sigma_{xy}}{x_0 y_0}$$

The square modulus problem

- Classic error propagation two main drawbacks:
  - Relies on expansion around a center value which may sometimes fail when the function is submitted to constraints
  - Hides the fact that the PDF of the result often has changed nature (e.g. $Z = XY$ or $Z = X/Y$ are strongly non-Gaussian).
- Example of power spectrum measurement: $S = |X|^2$, $S = s_0 \pm \sigma_S$. S is normally distributed, and we know $X \geq 0$
- We would like to find the most probable distribution and give an answer under the form: $X_0 \pm \sigma_X$. How should we proceed ?

Failures of classic error propagation: square modulus

- We would like the most probable X, the classic analysis would set $X_0 = \sqrt{S_0}$ and

$$\begin{aligned} \delta S &= 2X_0 \delta X \\ < (\delta S)^2 > &= 4X_0^2 < (\delta X)^2 >= 4S_0 < (\delta X)^2 > \\ \sigma_S^2 &= 4S_0 \sigma_X^2 \end{aligned}$$

- This leads to $X = \sqrt{S_0} \pm \frac{\sigma_S}{2\sqrt{S_0}}$, which obviously will not work when $S_0 < 0$, e.g. $S = 8 \pm 5$ works but not $S = -1 \pm 4$
- We failed to express the problem in a Bayesian framework
- **Bayesian inference** encompasses all our knowledge of the problem by using as needed three tools: **Bayes' theorem, marginalization, and change of variables**

Success of Bayesian analysis: square modulus

- Given the data $D = \{S_0, \sigma_S\}$, we are looking at the most probable value for X, i.e. we are looking for $X_0 = \text{argmax}\, \Pr(X|D)$
- What we means by measurement $S = S_0 \pm \sigma_S$ is that as a function of S the probability of the data is Gaussian and expressed by:

$$\Pr(D|S) = \exp\left[-\frac{(S - S_0)^2}{2\sigma_S^2}\right] \quad (1)$$

- We also have a prior on S:

$$\Pr(S) = \begin{cases} 0 & S < 0 \\ \text{const} & S \geq 0 \end{cases} \quad (2)$$

- Due to the prior, central expansion (classic error propagation) fails in this case, but Bayesian change of variable still works
- Finally, Bayes equation allows us to express our whole knowledge of S:

$$\Pr(S|D) = \Pr(D|S)\,\Pr(S) \quad (3)$$

Success of Bayesian analysis: square modulus

- For $X < 0$, $\Pr(X|D) = 0$, and for $X \geq 0$:

$$\Pr(X|D) = \left|\frac{\partial S}{\partial X}\right| \Pr(S|D) = 2X \exp\left[-\frac{(X^2 - S_0)^2}{2\sigma_S^2}\right]$$

- This is a non-Gaussian function, and truncated for negative X !
- We want a **Gaussian approximation** so that $X_0 = \underset{X}{\operatorname{argmax}} \Pr(X|D)$:

$$\left.\frac{\partial \log \Pr(X|D)}{\partial X}\right|_{X_0} = 0 \implies X_0 = \left[\frac{S_0 + (S_0^2 + 2\sigma_S^2)^{\frac{1}{2}}}{2}\right]^{\frac{1}{2}}$$

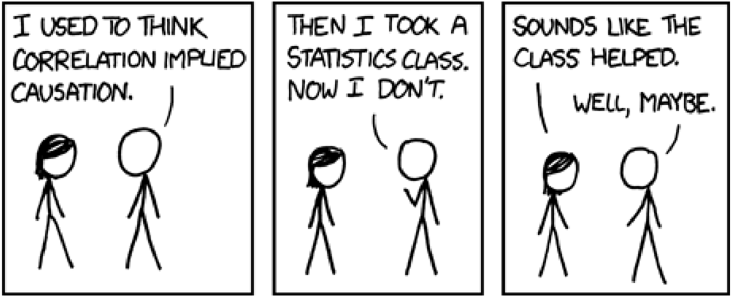
$$\left.\frac{\partial^2 \log \Pr(X|D)}{\partial X^2}\right|_{X_0} = -\frac{1}{\sigma_X^2} \implies \sigma_X = \left[\frac{1}{X_0^2} + \frac{2(3X_0^2 - S_0)}{\sigma_S^2}\right]^{-\frac{1}{2}}$$

Thinking with Bayes

True/false ?

- *Correlation is not evidence of causation*, Anonymous
- *Absence of evidence is not evidence of absence*, Martin Rees
- *Knowing that apples are green does not tells you anything about the color of ravens*, Bob the physicist

Demonstrate the following



These are **true** as Bayesian statements:

- *Correlation is not causation but it sure is a hint*, Edward Tufte
- *Absence of evidence is evidence of absence*
- *Knowing that apples are green provide evidential support to the proposition "All ravens are black"*, Carl Gustav Hempel
- Note that A is evidence of B if $Pr(B|A) > Pr(A)$, or if $Pr(B|A) > Pr(B|\bar{A})$.

Bayesian statistics and model-fitting: Maximum a posteriori

- Based on the same principle as Maximum likelihood
- At the root of many numerical methods we are going to see:
  - Monte Carlo Markov Chains
  - Error propagation
  - Optimization for model-fitting
  - Deconvolution
  - ...
- Maximum a posteriori (MAP) method: we want to find the most probable parameter θ of a model given the data, i.e. maximize $\Pr(\theta|D)$
- For a given data set, $\Pr(D)$ is constant:

$$\underset{\theta}{\operatorname{argmax}} \Pr(\theta|D) \propto \underset{\theta}{\operatorname{argmax}} \{\Pr(D|\theta)\Pr(\theta)\} = \underset{\theta}{\operatorname{argmax}} \{\mathcal{L}(\theta|D)\pi(\theta)\}$$

Examples of priors

- Prior knowledge about the problem: constraints or preferences on parameters, knowledge of their distribution, ...
- Contraints: positivity, specific bounds (e.g. ratio between 0 and 1)
- Preferences: smoothness, sparsity, correlation between parameters.
- Prior chosen as **non-committal** as possible in order not to bias the result. **Uninformative** priors express weak information about the problem
- An **improper prior** is not truly a prior, but a function that does not normalize to unity or only does so by assigning an infinitesimal probability to each value e.g. the scale $\pi(\theta) = \frac{1}{\theta}$. It can be made into a prior by normalizing it within reasonable bounds.
- Example: we measure $\theta = 40 \pm 10$ (normal distribution) and we know that $\Pr(\theta)$ follows $\pi(\theta) \propto \frac{1}{\theta}$, and that $1 \leq \theta \leq 100$. What is the most probable θ ?

Inverse problems and regularization

- **Inverse problem**: recovering a wanted set of parameters from noise-corrupted data (e.g. pixel fluxes in image reconstruction)
- **Ill-posed** inverse problem: when the effective number of parameters to recover is greater than the effective number of data points, the solution may not exist or may not be unique
- **Regularization**: introduction of priors (known as regularizers) which will try to compensate for our lack of data. As usual, the prior/regularizer expresses the *a priori* probability of an object when we have no data.
- Some regularizers can take the convenient form:

$$\Pr(\theta) \propto \exp\left[-R(\theta)\right] \implies -\log \Pr(\theta) = R(\theta)$$

- The solution $\tilde{\theta}$ of MAP for Gaussian-distributed data and N regularizers with weights $w_1, w_2, \ldots$ is found as:

$$\tilde{\theta} = \underset{\theta}{\operatorname{argmin}} \left[\chi^2(\theta) + \sum_{k=1}^{N} w_k R_k(\theta)\right]$$

Separable regularizers and ℓ_p norm

- For a set of independent parameters with identical priors (e.g. independent pixel fluxes with Poisson priors), the global regularizer is a **separable function**:

$$\Pr(\boldsymbol{\theta}) = \Pr(\theta_1) \times \Pr(\theta_2) \ldots \times \Pr(\theta_N) \implies R(\boldsymbol{\theta}) = \sum_i R(\theta_i)$$

- There are many classis regularizers. Amongst them, the ℓ_p norm of parameter set θ just penalize higher fluxes by using a power law:

$$\ell_p(\theta) = \left[\sum_{i=1}^{N} |\theta_i|^p \right]^{\frac{1}{p}}$$

- The ℓ_p norm penalizes parameters that depart from zero

Separable regularizers and ℓ_p norm: examples

- In practice for e.g. $\theta = [0, 3, 0, 4]$
- ℓ_0 is the number of non-zero θ_i, $\ell_0(\theta) = 2$.
- $\ell_1 = \sum_i |\theta_i|$ is the sum of moduli, $\ell_1(\theta) = 7$.
- $\ell_2 = (\sum_i |\theta_i|^2)^{\frac{1}{2}}$ is the square root of the sum of square moduli, $\ell_2(\theta) = \sqrt{3^2 + 4^2} = 5$.
- Different values of p penalize more or less higher vs lower fluxes.
- In MAP image reconstruction, when using ℓ_p regularizers in conjunction with χ^2, the higher p, the smoother and less noisy the resulting image will be. E.g. ℓ_2 give soft images, ℓ_1 sharp images, ℓ_0 very spiky images.
- $\ell_p(\theta - \gamma)$, where γ is a default expected level, expressing defaults values for parameter set θ, i.e. values that we would expect to be "normal" in absence of data. Example: the default expected flux level in a star field is zero in the absence of data, so the default image γ is an image with zero everywhere. But the default image for an image of the Sun is a mostly uniform disc, so γ would be this expected disc.

Maximum entropy method

- The Shannon entropy $S(\boldsymbol{\theta})$ is a **non-committal prior**. When used as regularizer, it expresses the expected absence of correlations between the parameters to recover (i.e. we expect θ_i and θ_j to be uncorrelated):

$$S(\boldsymbol{\theta}) = -\sum_i \theta_i \log \theta_i$$

- Maximum entropy is most often (but not exclusively) applied to a set of proportions, i.e. when $\sum \theta_i = 1$.
- In our Maximum a Posteriori framework, $R(\boldsymbol{\theta}) = -S(\boldsymbol{\theta})$ and so we actually want to maximize entropy S or minimize negentropy R.

Maximum entropy method

- Maximum entropy is based on the following principle: *If the proportion of some entity which has a given property is known to be p, then the most probable estimate of the proportion in some subclass which has that property is (in the absence of any information connecting the subclass with the property) the same number p*
- We all know that two thirds of physicists are right handed, and that only one in 10 physicists drink Coke (the remaining 9/10th preferring Pepsi). These are true facts. What is the probability that a randomly encountered physicist is a left-handed Coke drinker? Find a unique answer, show that it is equivalent to non-correlation between the parameters.
- What is the regularizer R that correspond to a prior Poisson distribution ? Conclusion ?

Maximum entropy method: solution 1

	Coke	Pepsi	
Left	p	$1/3 - p$	$\Pr(\text{Left}) = 1/3$
Right	$1/10 - p$	$2/3 - 1/10 + p$	$\Pr(\text{Right}) = 2/3$
	$\Pr(\text{Coke}) = 1/10$	$\Pr(\text{Pepsi}) = 9/10$	

- The table above is called a **contingency table**
- Method 1: non-correlation of handedness with soda: $\Pr(\text{Coke}|\text{Left}) = \Pr(\text{Coke}|\text{Right})$. We can express the joint probabilities as $\Pr(\text{Coke}, \text{Left}) = \Pr(\text{Coke}|\text{Left})\Pr(\text{Left})$ and $\Pr(\text{Coke}, \text{Right}) = \Pr(\text{Coke}|\text{Right})\Pr(\text{Right})$, leading to:

$$\frac{\Pr(\text{Coke}, \text{Left})}{\Pr(\text{Left})} = \frac{\Pr(\text{Coke}, \text{Right})}{\Pr(\text{Right})}$$

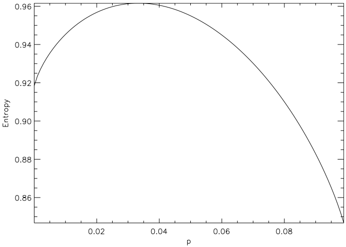
$$\implies \frac{p}{1/3} = \frac{1/10 - p}{2/3} \implies p = 1/30$$

Maximum entropy method: solution 1

- Method 2: express the entropy and maximize it

$$S = -\sum_i p_i \log p_i = -\Big[p \log p + (\frac{1}{3} - p)\log(\frac{1}{3} - p)$$
$$+(\frac{1}{10} - p)\log(\frac{1}{10} - p) + (\frac{2}{3} - \frac{1}{10} + p)\log(\frac{2}{3} - \frac{1}{10} + p)\Big]$$

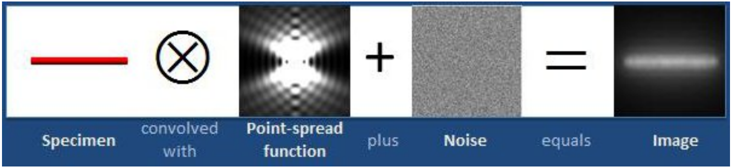
- $\frac{\partial S}{\partial p} = 0 \implies p = 1/30$



Sparsity, Compressed sensing, Total variation

- An object (image, array, vector) is said **sparse** in a basis ("dictionary") if it can be represented in this basis by a small number of non-zero coefficients
- The **impulsion dictionary** is the conventional grid of square pixels, an image is defined as $\boldsymbol{I} = \sum_i \theta_i \delta(x - x_i)\delta(y - y_i)$. An image with only unresolved (pointlike) stars is sparse in the impulsion basis.
- JPEG2000 stores the coefficients of images expressed in **wavelet dictionaries** that work well with most natural pictures
- **Compressed sensing theory** is a new mathematical paradigm from the 2000s that asserts that the optimal regularization can be obtained by imposing sparsity in the basis where the solution is the most sparse.
- Compressed sensing literature recommends using ℓ_0 and ℓ_1 on the sparsity basis as regularizers, in order to enforce **sparsity**.
- **Total variation** is $\ell_1(\nabla\boldsymbol{\theta})$, i.e. the ℓ_1 in the **spatial gradient** dictionary $\nabla\boldsymbol{\theta}$. In image reconstruction this regularizer favors patches of uniform flux with sharp transitions.

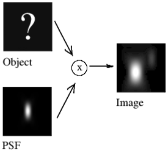
Application of MAP: Deconvolution



- Unknown object $\boldsymbol{o}$ is first blurred by instrument and then corrupted by additive Gaussian noise $\boldsymbol{n}$, resulting in the observed image $\boldsymbol{i}$. The **Point Spread Function** (PSF, here p) is the response to an impulsion (an unresolved object, a dirac).
- This is an inverse problem with unique solution
- The **direct model** is the model equation that transforms our unknown to data

$$\boldsymbol{i} = \boldsymbol{o} * \boldsymbol{p} + \boldsymbol{n} \tag{4}$$

Application of MAP: Deconvolution (2)



- The discrete convolution (noted $*$) in 2D is defined by:

$$(\boldsymbol{o} * \boldsymbol{p})[m,n] \stackrel{\text{def}}{=} \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \boldsymbol{o}[i,j]\, \boldsymbol{p}[m-i, n-j]$$
$$= \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \boldsymbol{o}[n-i, m-j]\, \boldsymbol{p}[i,j]$$

- Not to be confused with cross-correlation (similar but not identical definition).
- See `http://www.songho.ca/dsp/convolution/convolution2d_example.html`

Application of MAP: Deconvolution (3)

- We want to find the most probable image $\tilde{\boldsymbol{o}}$, i.e. we want:

$$\tilde{\boldsymbol{o}} = \operatorname*{argmax}_{\boldsymbol{o}} \Pr(\boldsymbol{o}|\boldsymbol{i}) \propto \operatorname*{argmax}_{\boldsymbol{o}} \Pr(\boldsymbol{i}|\boldsymbol{o}) \Pr(\boldsymbol{o}) \tag{5}$$

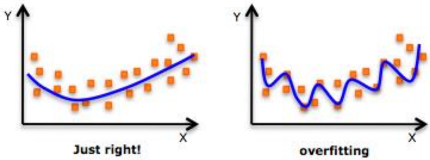
- For a given $\boldsymbol{o}$, the realization of the noise $n = \boldsymbol{i} - \boldsymbol{o} * \boldsymbol{p}$ depends on $\boldsymbol{i}$ and is normally distributed; the likelihood is:

$$\Pr(\boldsymbol{i}|\boldsymbol{o}) = \mathcal{L}(\boldsymbol{o}|\boldsymbol{i}) \propto \prod_n \exp\left[-\left(\frac{(\boldsymbol{i}_n - (\boldsymbol{o} * \boldsymbol{p})_n)^2}{2\sigma_n^2}\right)\right] \tag{6}$$

- Negloglikelihood is:

$$-\log \Pr(\boldsymbol{i}|\boldsymbol{o}) \propto \chi^2(\boldsymbol{o}) = \sum_n \frac{(\boldsymbol{i}_n - (\boldsymbol{o} * \boldsymbol{p})_n)^2}{2\sigma_n^2} \tag{7}$$

Application of MAP: Deconvolution (4)



- If we tried to minimize only $\chi^2(\boldsymbol{o})$, we might find we can achieve very low χ^2, yet the image will look poor.
- We are overfitting the model to the data, i.e. we are forcing pixels to take non-natural values negative: too low (negative !), too high (spurious peaks). We are trying to get too close to the actual measured image ! Regularization was invented to solve this issue.
- User can choose any "good" $R(\boldsymbol{o}) = -\log \Pr(\boldsymbol{o})$ to impose positivity, smoothness, sparsity, maximum entropy, etc.
- In the end we will be minimizing $\chi^2(\boldsymbol{o}) + \sum_i \mu_i R_i((\boldsymbol{o})$ with respect to $\boldsymbol{o}$ using an **optimization engine**