Experimental Methods Lecture 12

October 15th, 2020

Kramers-Kronig dispersion relations

- In conclusion, for a causal system

$$\mathrm{P}\int_{-\infty}^{\infty}\frac{\mathrm{h}(\omega')}{\omega-\omega'}\mathrm{d}\omega' \equiv \mathcal{H}(\mathrm{h}(\omega)) = \mathrm{i}\pi\mathrm{h}(\omega)$$

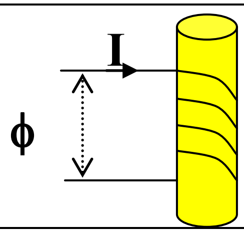
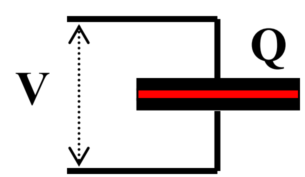
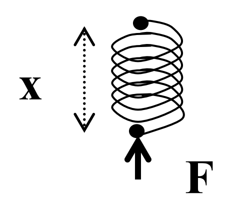
- or

$$Im\{h(\omega)\} = -\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{Re\{h(\omega')\}}{\omega-\omega'}d\omega' \equiv -\mathcal{H}(Re\{h(\omega)\}$$

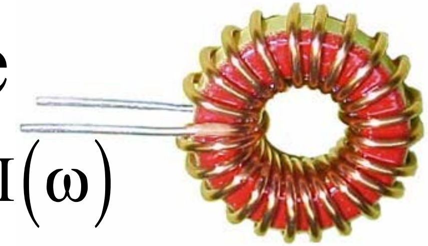
$$Re\{h(\omega)\} = \frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{Im\{h(\omega')\}}{\omega-\omega'}d\omega' \equiv \mathcal{H}(Im\{h(\omega)\}$$

One example from condensed matter

A general phenomenon in condensed matter
a frequency independent imaginary part in the "response" $\chi(\omega)$

	Magnetism	**Dielectrics**	**Mechanics**
Generalized response $\chi(\omega)$	**Inductance $L(\omega)$** $\phi(\omega) = L(\omega) I(\omega)$ $L(\omega) = L' - iL_o$	**Capacitance $C(\omega)$** $Q(\omega) = C(\omega) V(\omega)$ $C(\omega) = C'(\omega) - iC_o$	**Spring constant $k(\omega)$** $F(\omega) = -k(\omega) x(\omega)$ $k(\omega) = k'(\omega) + ik_o$
Nyquist formula	$S_\phi(\omega) = 4k_B T \frac{L_o}{\omega}$	$S_Q(\omega) = 4k_B T \frac{C_o}{\omega}$	$S_F(\omega) = 4k_B T \frac{k_o}{\omega}$
			

Consider the magnetic case



the magnetic flux-current relation: $\phi(\omega) = L(\omega) I(\omega)$

- The magnetic susceptibility χ of the core material is connected to inductance thru:

$$L(\omega) = \chi(\omega) L_o$$

- Magnetic susceptibility of real material is complex:

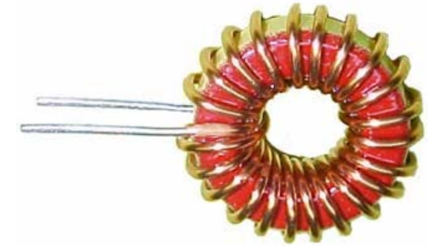
$$\chi(\omega) = \chi'(\omega) - i\chi''(\omega)$$

- Notice that impedance $Z(\omega)=i\omega L(\omega)$ acquires a real part, i.e. a resistive component

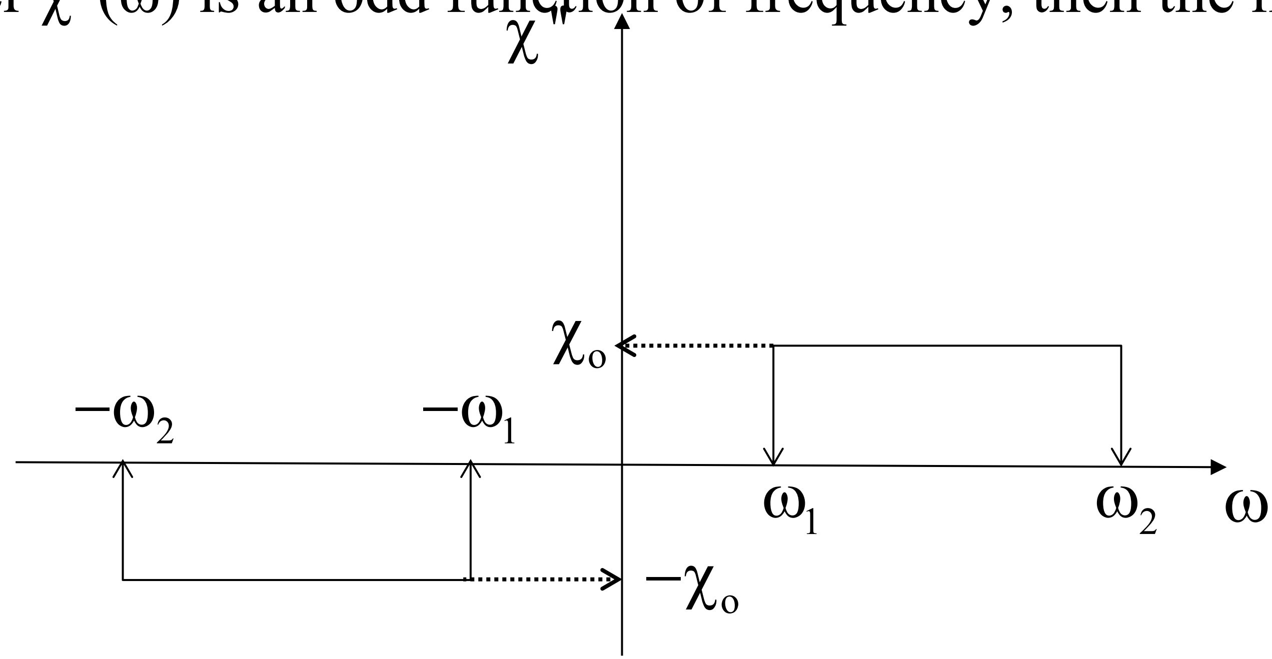
$$\mathrm{Re}\left\{Z(\omega)\right\} = \omega\chi''(\omega) L_o$$

- At low frequency $\chi''(\omega) \simeq \chi_o$ in many materials

A popular model



- $\chi''(\omega) \simeq \chi_o$. Assume this is true in some decade-wide frequency interval, outside which $\chi''(\omega)=0$. (Can't be infinite otherwise there is no Fourier transform in strict sense)
- Remember $\chi''(\omega)$ is an odd function of frequency, then the model is:



Characteristic Function $\chi_{[a,b]}(t)$	$\frac{1}{\pi}\ln\left\|\frac{t-a}{t-b}\right\|$

Real part from Kramers Kronig

Characteristic Function $\chi_{[a,b]}(t)$	$\frac{1}{\pi}\ln\left\vert\frac{t-a}{t-b}\right\vert$

- Use Hilbert transform

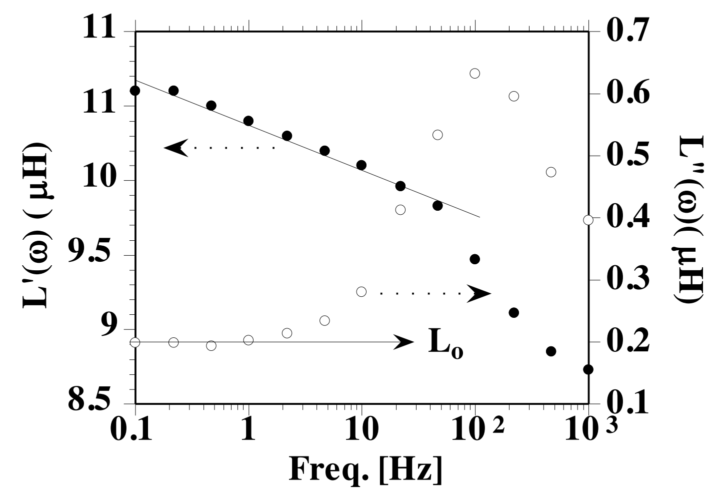
$$\chi'(\omega) = \mathcal{H}\{-\chi''\} = -\frac{\chi_o}{\pi} ln\left|\frac{\omega-\omega_1}{\omega-\omega_2}\right| + \frac{\chi_o}{\pi} ln\left|\frac{\omega+\omega_2}{\omega+\omega_1}\right| = -\frac{\chi_o}{\pi} ln\left|\frac{\omega^2-\omega_1^2}{\omega^2-\omega_2^2}\right|$$

- For $\omega_1 \ll \omega \ll \omega_2$

$$\chi'(\omega) = -\frac{2\chi_o}{\pi}(\ln(\omega) - \ln(\omega_2))$$

- Notice

$$\frac{1}{\chi''}\frac{d\chi'}{dln(\omega)} = -\frac{2}{\pi}$$



(Vitrovac @ 4,2 K)

G.A. Prodi & al. J. Appl. Phys. **66** 5984 (1989) double emission at 589.29 nm wavelength.

The variation of refractive index with wavelength for various glasses.

Complex index of refraction and absorption [edit]

See also: Mathematical descriptions of opacity

When light passes through a medium, some part of it will always be absorbed. This can be conveniently taken into account by defining a complex index of refraction,

$$\tilde{n} = n + i\kappa.$$

Here, the real part of the refractive index n indicates the phase speed, while the imaginary part κ indicates the amount of absorption loss when the electromagnetic wave propagates through the material.

That κ corresponds to absorption can be seen by inserting this refractive index into the expression for electric field of a plane electromagnetic wave traveling in the z-direction. We can do this by relating the wave number to the refractive index through $k = \frac{2\pi n}{\lambda_0}$, with λ_0 being the vacuum wavelength. With complex wave number $\tilde{k}$ and refractive index $n + i\kappa$ this can be inserted into the plane wave expression as

$$\mathbf{E}(z,t) = \mathrm{Re}(\mathbf{E}_0 e^{i(\tilde{k}z-\omega t)}) = \mathrm{Re}(\mathbf{E}_0 e^{i(2\pi(n+i\kappa)z/\lambda_0-\omega t)}) = e^{-2\pi\kappa z/\lambda_0}\mathrm{Re}(\mathbf{E}_0 e^{i(kz-\omega t)}).$$

Here we see that κ gives an exponential decay, as expected from Beer–Lambert law.

κ is often called the **extinction coefficient** in physics although this has a different definition within chemistry. Both n and κ are dependent on the frequency. In most circumstances $\kappa > 0$ (light is absorbed) or $\kappa = 0$ (light travels forever without loss). In special situations, especially in the gain medium of lasers, it is also possible that $\kappa < 0$, corresponding to an amplification of the light.

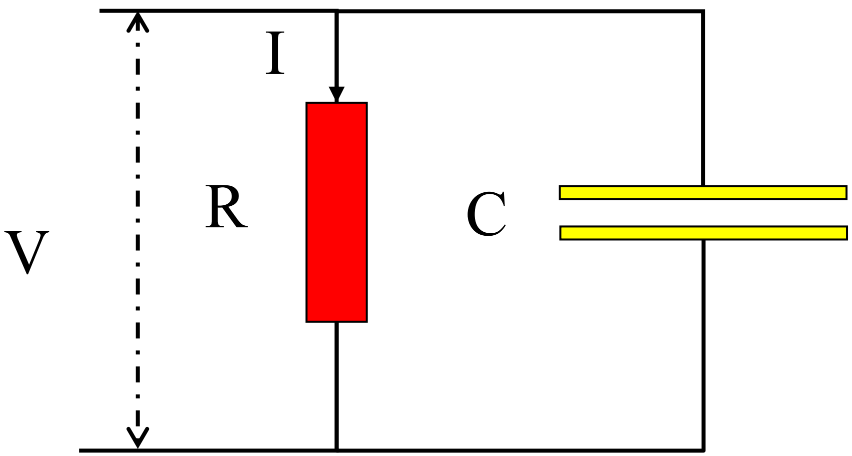
An alternative convention uses $\tilde{n} = n - i\kappa$ instead of $\tilde{n} = n + i\kappa$, but where $\kappa > 0$ still corresponds to loss. Therefore these two conventions are inconsistent and should not be confused. The difference is related to defining sinusoidal time dependence as $\mathrm{Re}(e^{-i\omega t})$ versus $\mathrm{Re}(e^{+i\omega t})$. See Mathematical descriptions of opacity.

Dielectric loss and non-zero DC conductivity in materials cause absorption. Good dielectric materials such as glass have extremely low DC conductivity, and at low frequencies the dielectric loss is also negligible, resulting in almost no absorption ($\kappa \approx 0$). However, at higher frequencies (such as visible light), dielectric loss may increase absorption significantly, reducing the material's transparency to these frequencies.

The real and imaginary parts of the complex refractive index are related through the Kramers–Kronig relations. For example, one can determine a material's full complex refractive index as a function of wavelength from an absorption spectrum of the material.

For X-ray and extreme ultraviolet radiation the complex refractive index deviates only slightly from unity and usually has a real part smaller than 1. It is therefore normally written as $\tilde{n} = 1 - \delta + i\beta$ (or $\tilde{n} = 1 - \delta - i\beta$).[14]

Exercise: verify that



$$Z(\omega) = \frac{V(\omega)}{I(\omega)}$$

$$Z(\omega) = \frac{R/i\omega C}{R + 1/i\omega C} = \frac{R}{1 + i\omega\tau} \qquad \tau = RC$$

Fulfils Kramers-Kronig

What should you know on systems

- Impulse response
- Step response
- Frequency response and transfer function
- Role of free evolution
- Linear damped oscillator, simple pole (low pass) and archetypal transfer functions
- Feedback, stability and linearization
- Dispersion relations

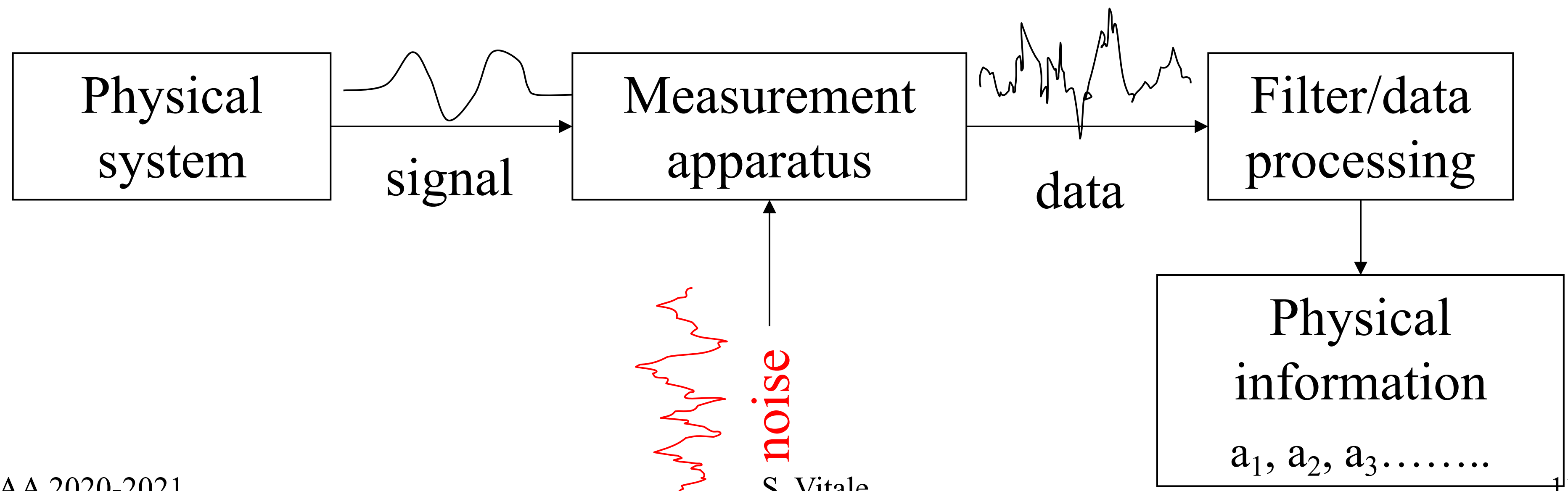
Noise in physical systems

- This part describes disturbances of statistical nature in physical measurements.
- To describe noise we are going to set up the basis of the mathematical theory of *stochastic processes*.
- A good reference text for this part is “Probability, random variables, and stochastic processes” / Athanasios Papoulis, 4. ed Boston, Mass. [etc.] : McGraw-Hill, c2002. (available in Italian)

Noise

Noise in physical experiments is described as a random signal x(t):

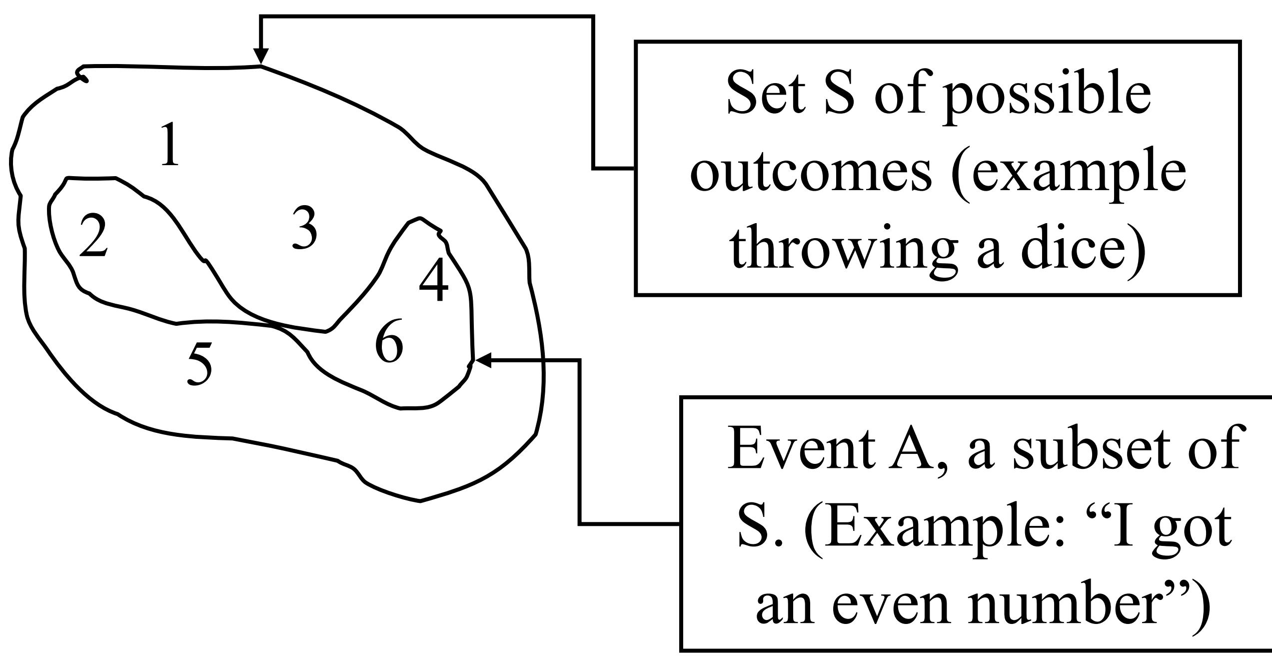
Independent repetitions of the same experiment produce different functions of time x(t)



What you should know about probability

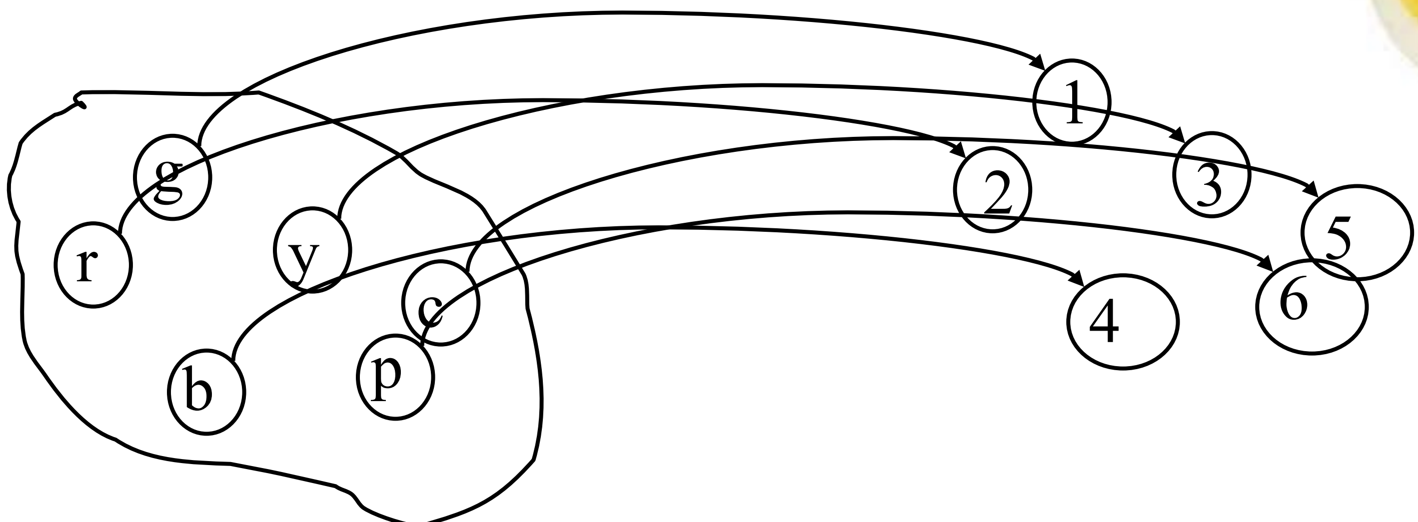
1. The concept of experiment:
   a. A set S of all possible results
   b. A class of subsets of S called “the events”
   c. A probability P(A) associated to events

1. Various constraints hold
   a. $0 \leq P(A) \leq 1$
   b. S is an event (certain)
   c. Ø is an event (impossible)
   d. Etc……..



What you should know about probability

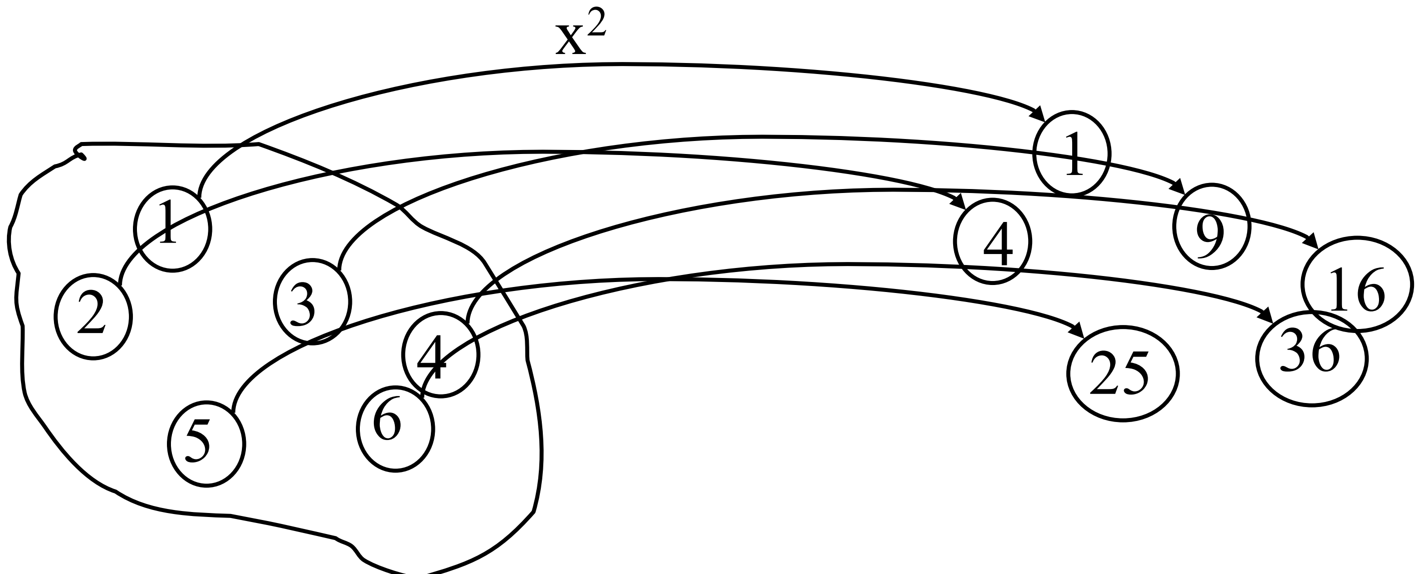
- Random variable (rv): a rule that associates numbers to experiment outcomes



- For each outcome the rv takes one value and only one

What you should know about probability

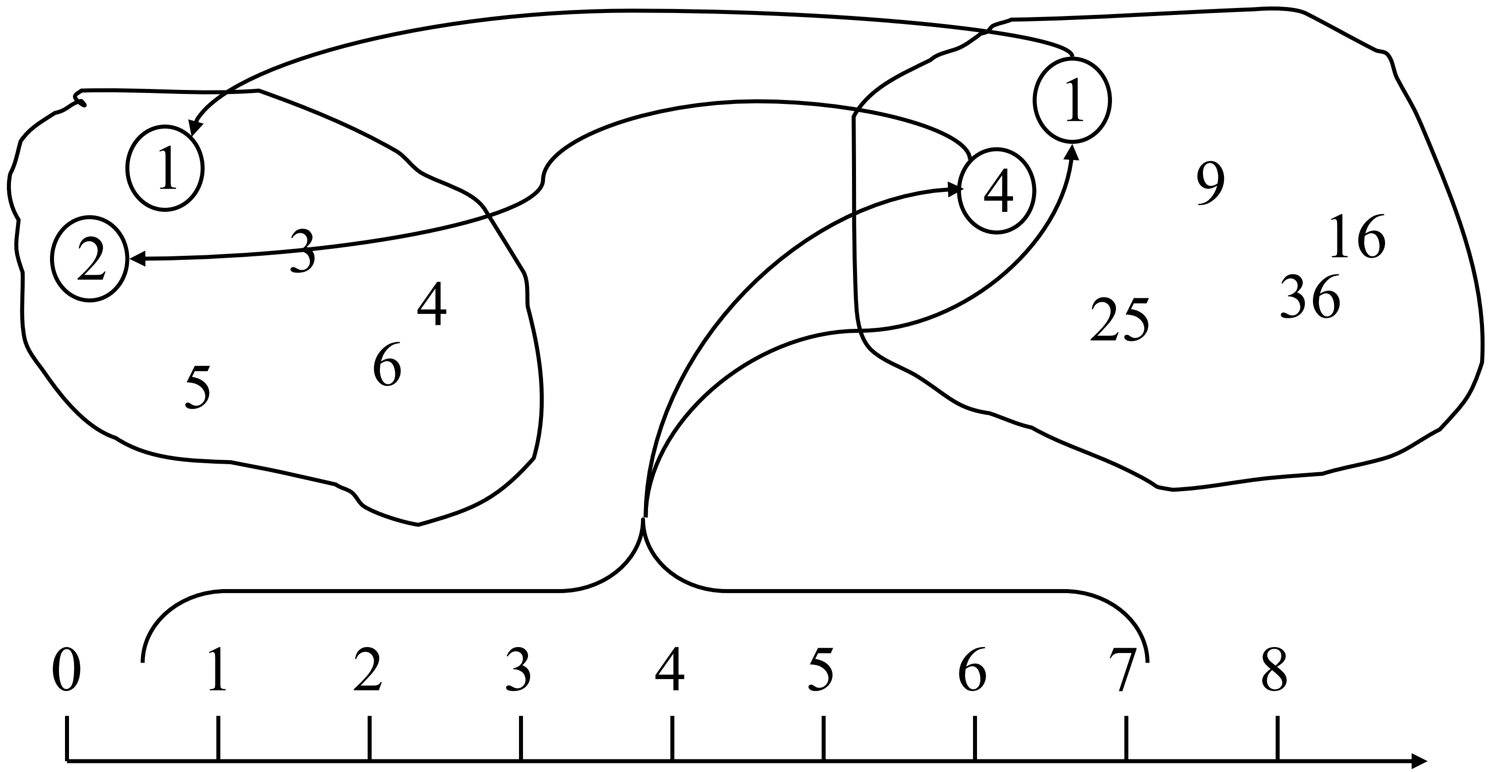
- Random variable (rv): a rule that associates numbers to experiment outcomes



- For each outcome the rv takes one value and only one

What you should know about probability

- The rv associates real intervals to events



- Thus a probability value is associated to each interval of the real axis

What you should know about probability

- Probability of the event corresponding to outcomes for which the random variable takes a value $x_o \le x \le x_1$.

$$P\left\{x_o \le x \le x_1\right\} = \int_{x_o}^{x_1} f(x)\,dx$$

- f(x) is the *probability density*
- Notice, as for each possible outcome the rv associates a number, the event $-\infty \le x \le \infty$ is certain.

$$P\left\{-\infty \le x \le \infty\right\} = \int_{-\infty}^{\infty} f(x)\,dx = 1$$

- For continuous variables

$$P\left\{x \equiv x_o\right\} = \int_{x_o}^{x_o} f(x)\,dx = 0$$

- In discrete experiments (like coin tossing), finite probability may be associated to single numbers. Around one of these numbers, x_o, f(x) is

$$f(x) = P\left\{x_o\right\}\delta(x - x_o)$$

What you should know about probability

- From the probability density function

$$P\{x_o \le x \le x_1\} = \int_{x_o}^{x_1} f(x)\,dx$$

- One can define the *cumulative distribution function*

$$P\{-\infty \le x \le x_o\} = \int_{-\infty}^{x_o} f(x)\,dx \equiv F(x_o)$$

- You can easily demonstrate that

$$f(x) = \frac{dF(x)}{dx}$$

What you should know about probability

- Basic parameters of distribution. Let's call x the random variable and $f_x(\chi)$ its probability density
  - Mean value

$$\langle x\rangle = \int_{-\infty}^{\infty} \chi f_x(\chi)\,d\chi$$

  - Mean value of any function of the g(x) of the x

$$\langle g(x)\rangle = \int_{-\infty}^{\infty} g(\chi) f_x(\chi)\,d\chi$$

  - Variance

$$\sigma^2 \equiv \left\langle \left(x-\langle x\rangle\right)^2 \right\rangle = \int_{-\infty}^{\infty} \left(\chi-\langle x\rangle\right)^2 f_x(\chi)\,d\chi$$

  - A classical result:

$$\sigma^2 = \int_{-\infty}^{\infty} \chi^2 f_x(\chi)\,d\chi + \langle x\rangle^2 \int_{-\infty}^{\infty} f_x(\chi)\,d\chi - 2\langle x\rangle \int_{-\infty}^{\infty} \chi f_x(\chi)\,d\chi$$

  - then

$$\sigma^2 = \langle x^2\rangle + \langle x\rangle^2 - 2\langle x\rangle^2 = \langle x^2\rangle - \langle x\rangle^2$$

What you should know about probability

- In general
  - Moment of order m

$$\mu'_m = \left\langle x^m \right\rangle = \int_{-\infty}^{\infty} \chi^m f_x(\chi) d\chi$$

  - Central moment of order m

$$\mu_m = \left\langle \left(x - \langle x \rangle \right)^m \right\rangle = \int_{-\infty}^{\infty} \left(\chi - \langle x \rangle \right)^m f_x(\chi) d\chi$$

  - Mean value is equal to μ_1’, variance is equal to μ_2
  - If all moments are known $f_x(\chi)$ is also known

Key distributions

- Normal
  - Density

$$f(x)=\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-x_o)^2}{2\sigma^2}}$$

  - Cumulative distribution

$$F(x)=\mathrm{Erf}\left[\frac{x-x_o}{\sigma}\right]$$

  - Mean

$$\int_{-\infty}^{\infty}\frac{x}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-x_o)^2}{2\sigma^2}}dx=x_o$$

  - Variance

$$\int_{-\infty}^{\infty}\frac{(x-x_o)^2}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-x_o)^2}{2\sigma^2}}dx=\sigma^2$$

Key distributions

- Rectangular
  - Density

$$f(x)=\Pi(x)$$

  - Cumulative distribution

$$F(x)=(x+1/2)\Pi(x)+\Theta(x-1/2)$$

  - Mean

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} x\,dx=0$$

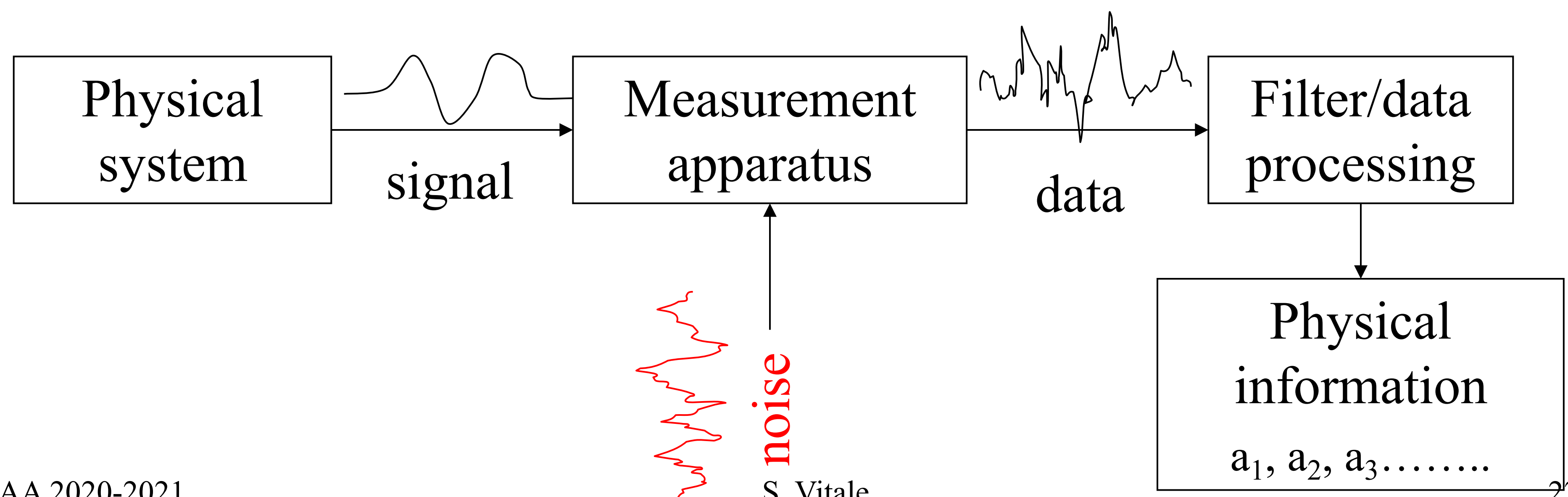
  - Variance

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} x^2\,dx=\frac{1}{12}$$

Noise

Noise in physical experiments is described as a random signal x(t):

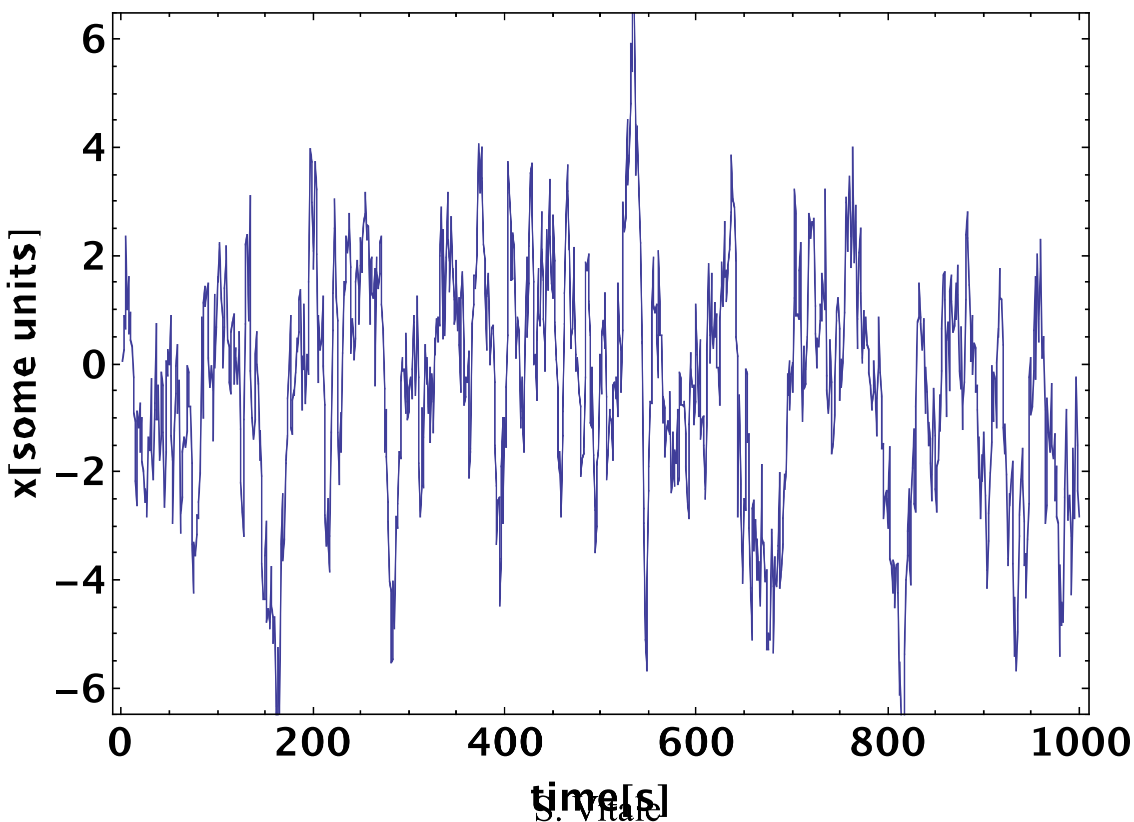
Independent (ensemble) repetitions of the same experiment produce different functions of time x(t)



Random signals

- At each repetition of a given experiment I get a different function of time x(t)

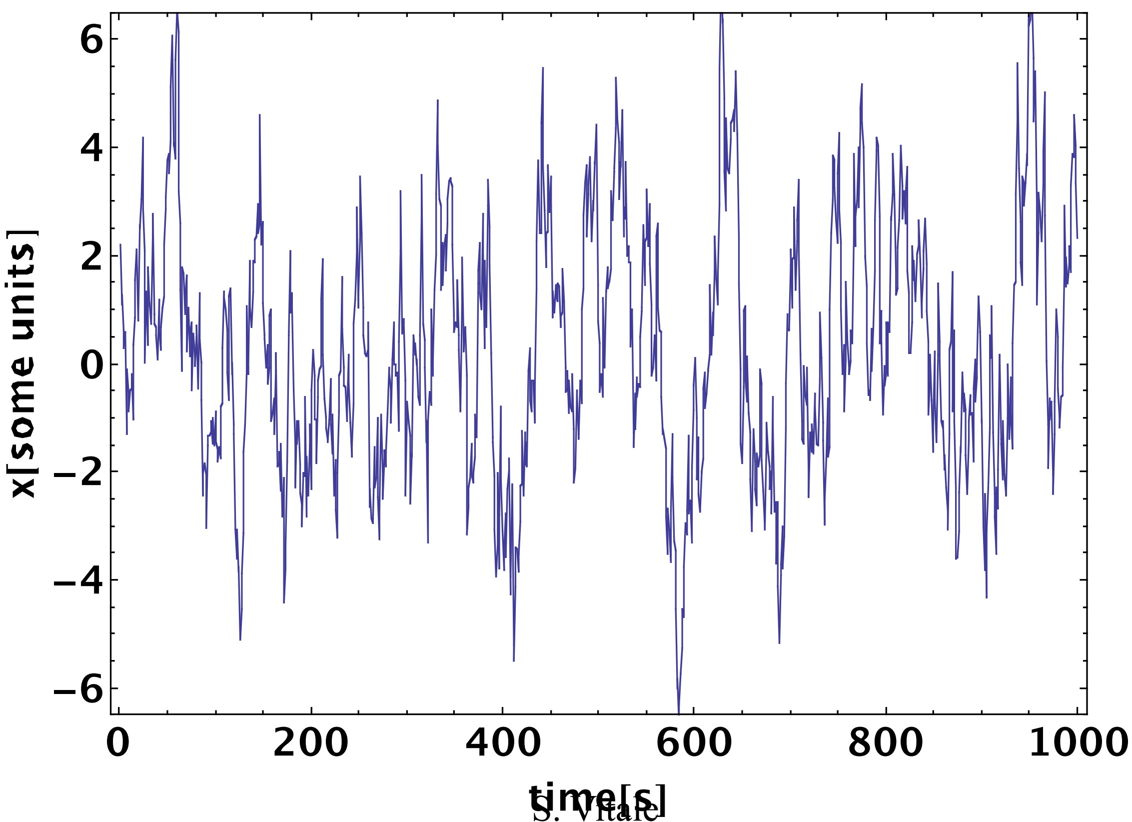
Trial 1



Random signals

- At each repetition of a given experiment I get a different function of time x(t)

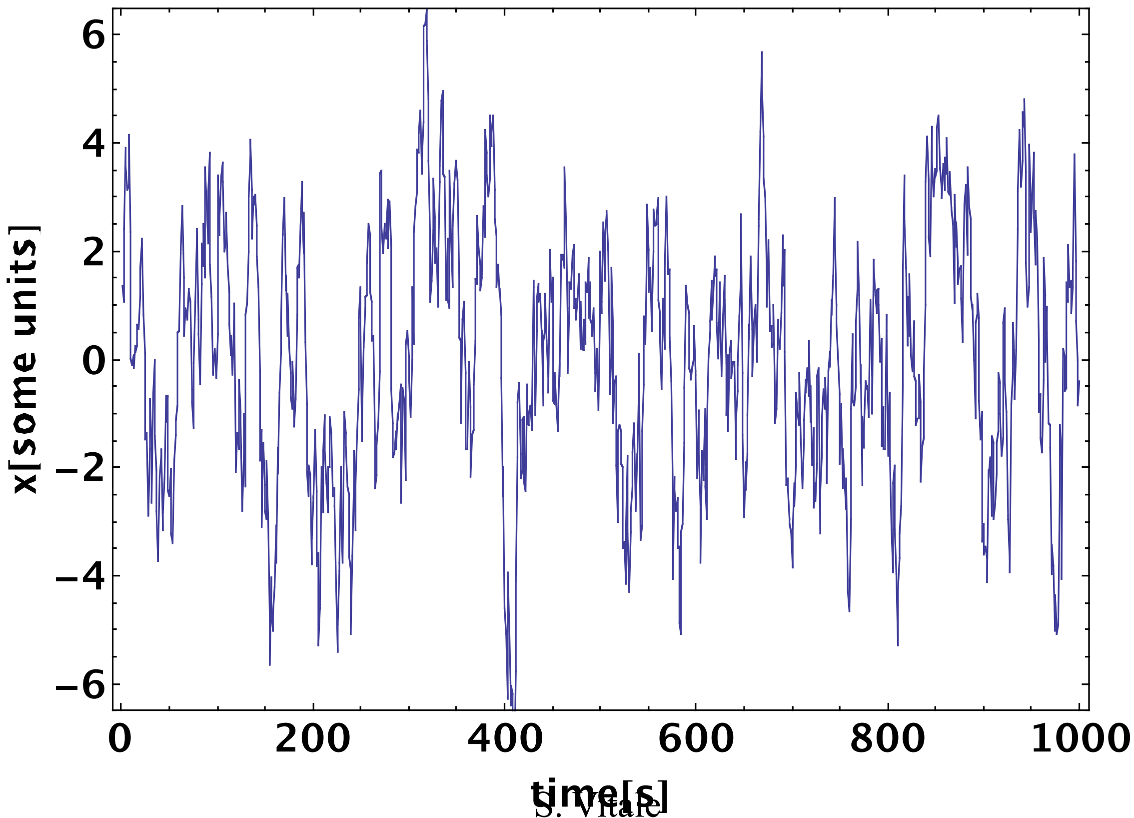
Trial 2



Random signals

- At each repetition of a given experiment I get a different function of time x(t)

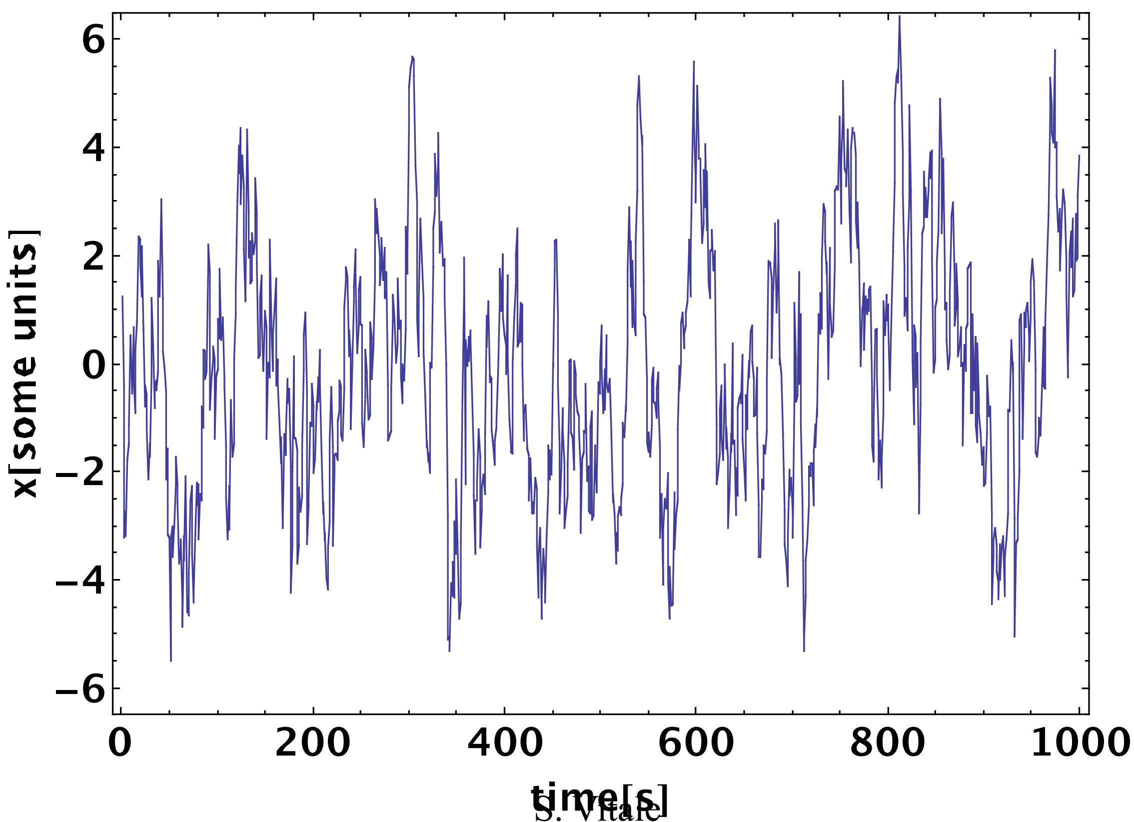
Trial 3



Random signals

- At each repetition of a given experiment I get a different function of time x(t)

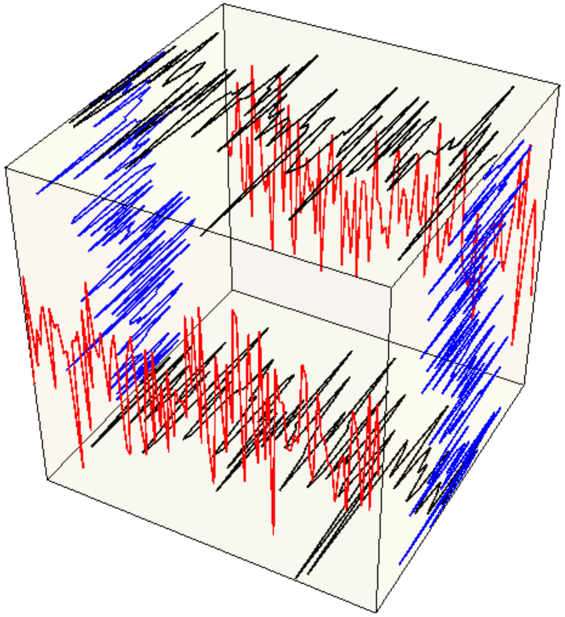
Trial 4



A stochastic process

- At each outcome of an experiment I get a function of time x(t)

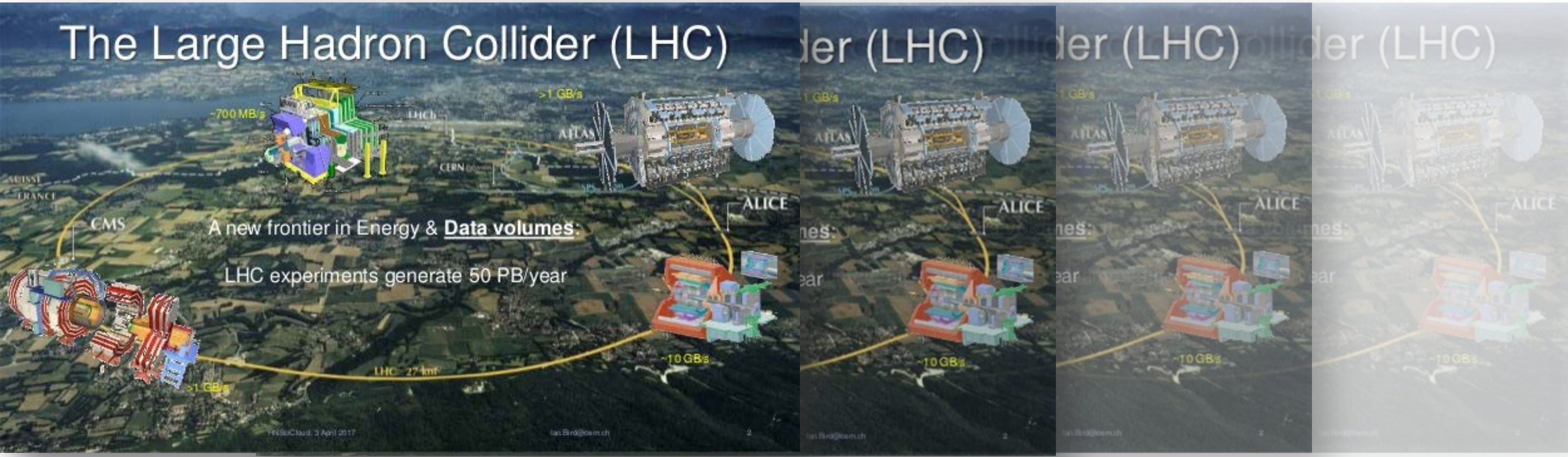
dice



Stochastic dice

Probability ensemble and repetitions

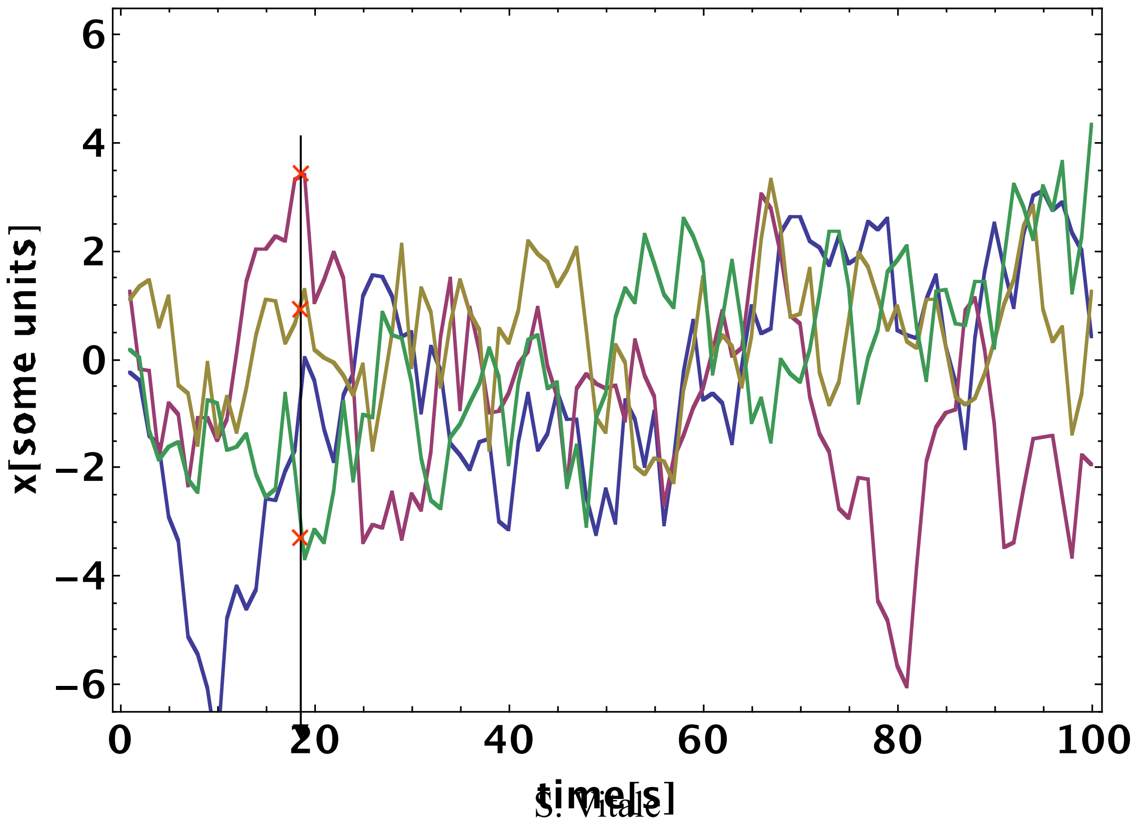
- The theory of probability describes only one experiment at the time



- Probability: prediction on the frequency of occurrence of same experiment in another “universe” (ensemble element)
- Not a prediction on frequency of occurrence in multiple repetitions over time
- An experiment repeated in time is a new single experiment

A stochastic process

- For each outcome a function of time x(t)
- For each time t: a random variable



A stochastic process

- As $x(t_1)$, $x(t_2)$, $x(t_3)$….. are all different rv, a stochastic process defines infinite many rv.
- Each rv will have its own density function

$$f_{x(t)}(\chi)$$

- With mean value

$$\eta(t) \equiv \langle x(t) \rangle = \int_{-\infty}^{\infty} \chi f_{x(t)}(\chi) d\chi$$

- This is called the mean value of the process and is in general a function of time.
- Same for the variance of the process

$$\sigma^2(t) \equiv \langle x^2(t) \rangle - \eta(t)^2 = \int_{-\infty}^{\infty} \chi^2 f_{x(t)}(\chi) d\chi - \eta(t)^2$$

Multiple random variables

- The statistical properties of multiple random variables like the $x(t_1)$, $x(t_2)$, $x(t_3)$…… are described by joint probabilities. Take two rv x and y. Their joint probability density $f_{x,y}$ is defined by:

$$P\left\{x_o \le x \le x_1 \text{ and } y_o \le y \le y_1\right\} = \int_{x_o}^{x_1}\int_{y_o}^{y_1} f_{x,y}(\chi,\psi)\,d\chi\,d\psi$$

- Also this density needs to be normalized

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_{x,y}(\chi,\psi)\,d\chi\,d\psi = 1$$

- The relation between the joint density $f_{x,y}$ and the marginal densities f_x and f_y is

$$\int_{x_o}^{x_1} f_x(\chi)\,d\chi = P\left\{x_o \le x \le x_1\right\} =$$

$$= P\left\{x_o \le x \le x_1 \text{ and } -\infty \le y \le \infty\right\} = \int_{x_o}^{x_1}\int_{-\infty}^{\infty} f_{x,y}(\chi,\psi)\,d\chi\,d\psi$$

- Then: $f_x(\chi) = \int_{-\infty}^{\infty} f_{x,y}(\chi,\psi)\,d\psi \qquad f_y(\psi) = \int_{-\infty}^{\infty} f_{x,y}(\chi,\psi)\,d\chi$