From probabilistic inference to ‘Bayesian’ unfolding

(passing through a toy model)

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Helmholtz School “Advanced Topics in Statistics”

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Preamble

“Advanced topics”: ?

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- Don’t expect fancy tests with Russian names

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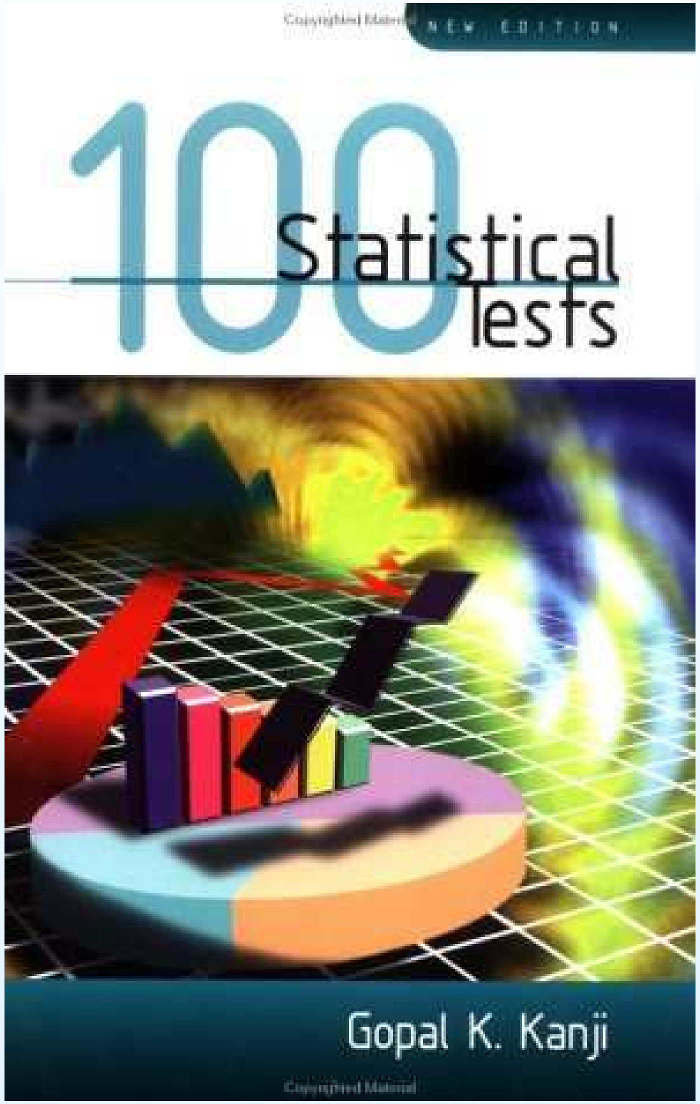

Not exhaustive compilation. . .

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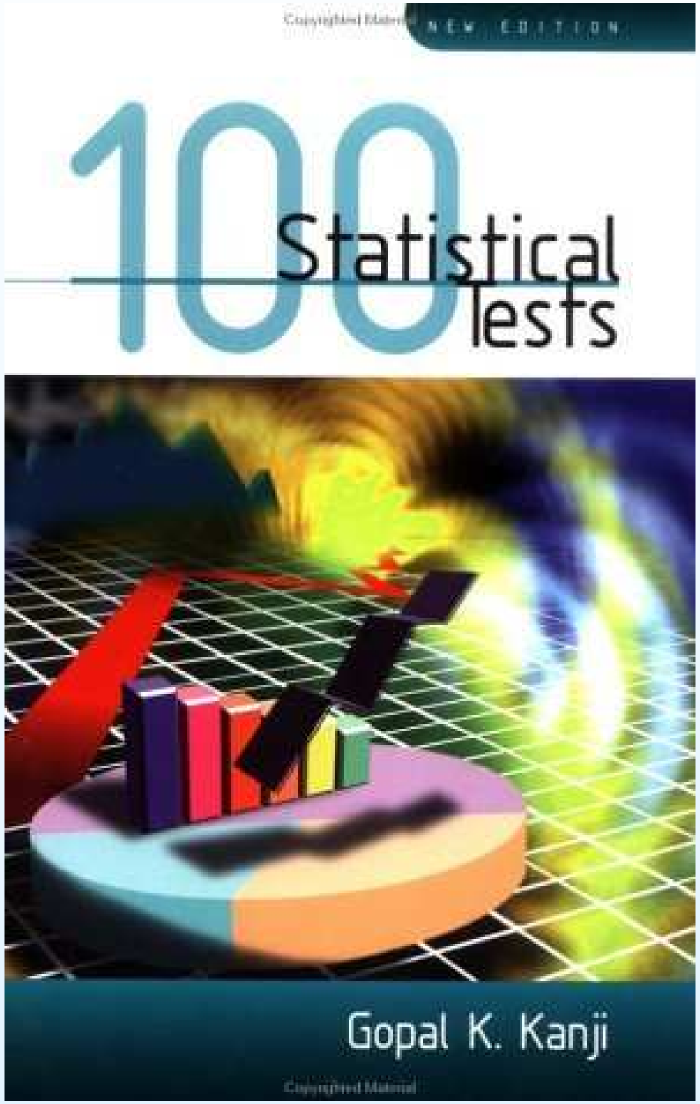

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⇒ wikipedia.org/wiki/P-value#Frequent_misunderstandings

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$\Rightarrow$ An invitation to (re-)think on foundamental aspects, that help in developping applications

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⇒ An invitation to (re-)think on foundamental aspects, that help in developping applications

⇒ 'Forward to past'

Good and sane probabilistic reasoning
by Gauss, Laplace, etc.
(in contrast with XX century statisticians)

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"The celebrated Monsieur Leibnitz *has observed it to be a defect in the common systems of logic, that they are very copious when they explain the operations of the understanding in the forming of demonstrations, but are too concise when they treat of probabilities, and those other measures of evidence on which life and action entirely depend, and which are our guides even in most of our philosophical speculations."* (D. Hume)

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⇒ Message to young people: improve quality of the teaching of probabilistic reasoning, recognized since centuries to be a weak point of the scholar system:

  ⇒ Not (magic) ad-hoc formulae, but a consistent probabilistic framework, capable to handle a large varity of problems

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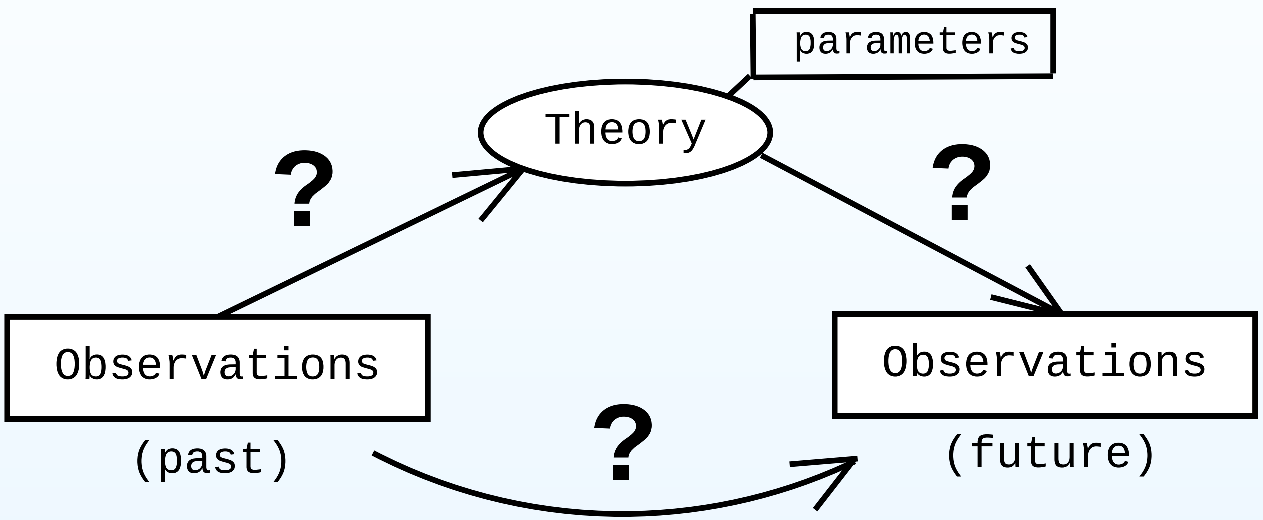
  that I will try to complement,
  before moving to a particular application.

Outline

- Learning from data the probabilistic way
  - Causes $\longleftrightarrow$ Effects

    "The essential problem of the experimental method" *(Poincaré)*.
  - Graphical representation of probabilistic links
  - Learning about causes from their effects
  - Playing with 6 boxes and 30 balls
- Parametric inference Vs unfolding
- From principles to real life... [the iteration 'dirty trick']
- The old code and its weak point
- Improvements:
  - use (conjugate) pdf's insteads of just 'estimates'
  - uncertainty evaluated by general rules of probability (instead of 'error propagation' formulae)
- Some examples on toy models

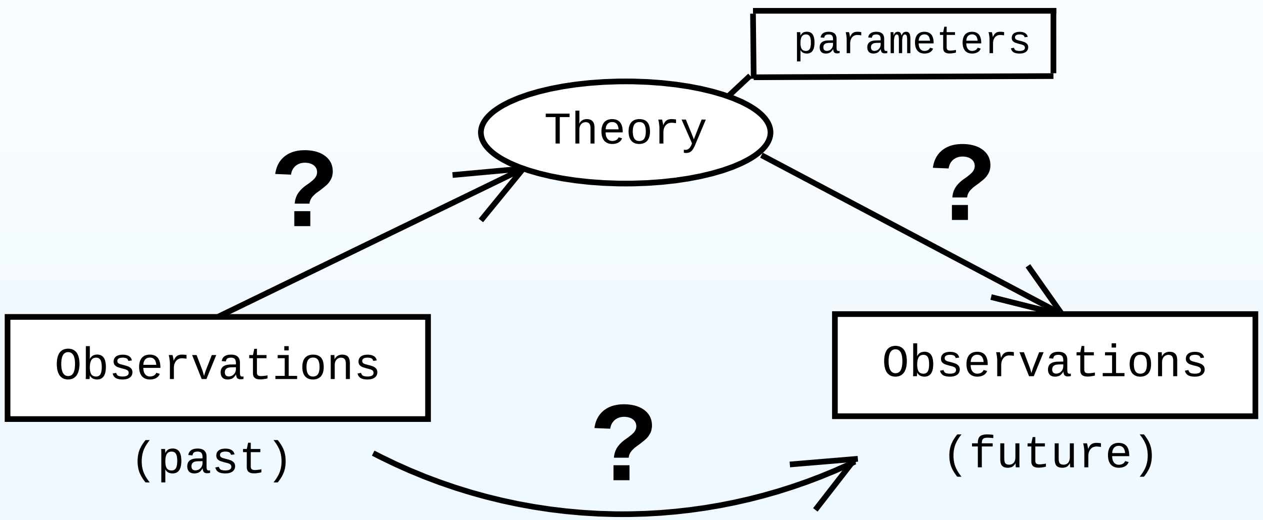
Learning from experience and source of uncertainty



Uncertainty:

Theory	—?⟶	Future observations
Past observations	—?⟶	Theory
Past observations	—?⟶	Future observations

Learning from experience and source of uncertainty



Uncertainty:

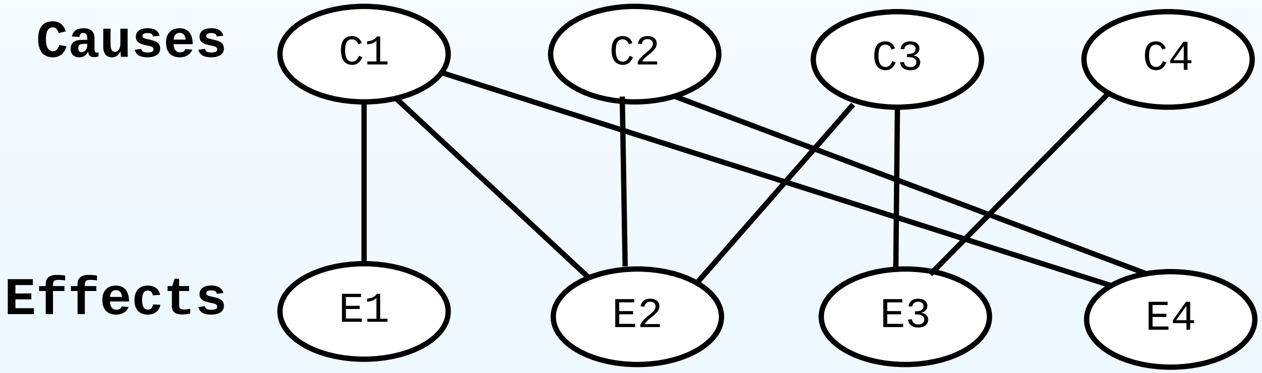
Theory	— ? ⟶	Future observations
Past observations	— ? ⟶	Theory
Past observations	— ? ⟶	Future observations

$\Longrightarrow$ **Uncertainty about causal connections**

CAUSE $\Longleftrightarrow$ **EFFECT**

Causes $\longrightarrow$ effects

The same *apparent* cause might produce several,different effects



Given an observed effect, we are not sure about the exact cause that has produced it.

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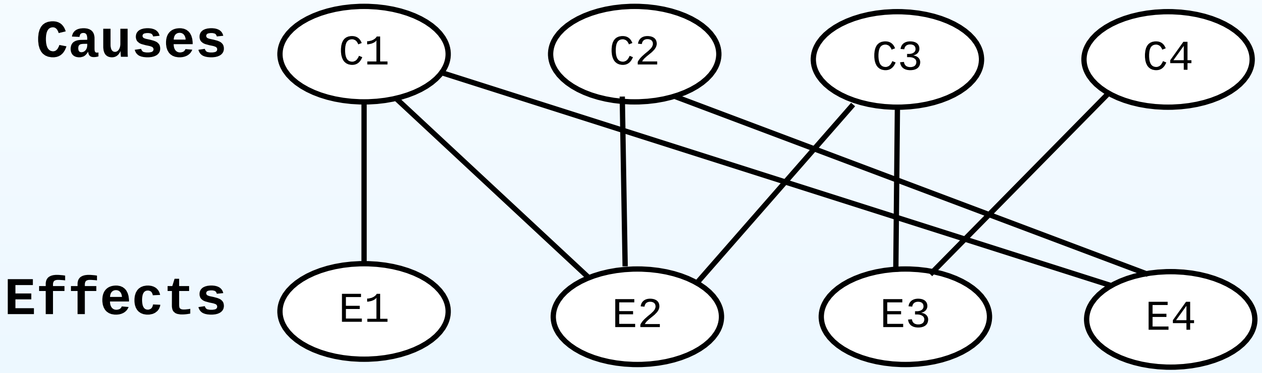

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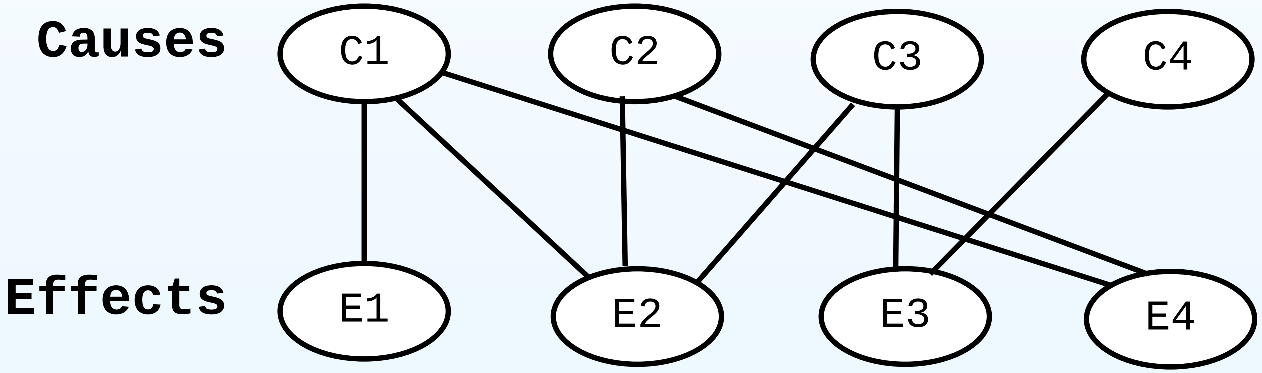

Given an observed effect, we are not sure about the exact cause that has produced it.

$$\mathbf{E_2} \Rightarrow \{C_1,\, C_2,\, C_3\}?$$

The essential problem of the experimental method

"Now, these problems are classified as *probability of causes*, and are most interesting of all their scientific applications. I play at *écarté* with a gentleman whom I know to be perfectly honest. What is the chance that he turns up the king? It is 1/8. This is a problem of the *probability of effects*.

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I play with a gentleman whom I do not know. He has dealt ten times, and he has turned the king up six times. What is the chance that he is a sharper? This is a problem in the probability of causes. It may be said that it is the essential problem of the experimental method."

(H. Poincaré – *Science and Hypothesis*)

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(H. Poincaré – *Science and Hypothesis*)

- An essential problem of the experimental method would be expected to be thaught with special care in the first years of the physics curriculum. . .

Uncertainties in measurements

Having to perform a measurement:

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> Which numbers shall come out from our device?

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> What have we learned about the value of the quantity of interest?

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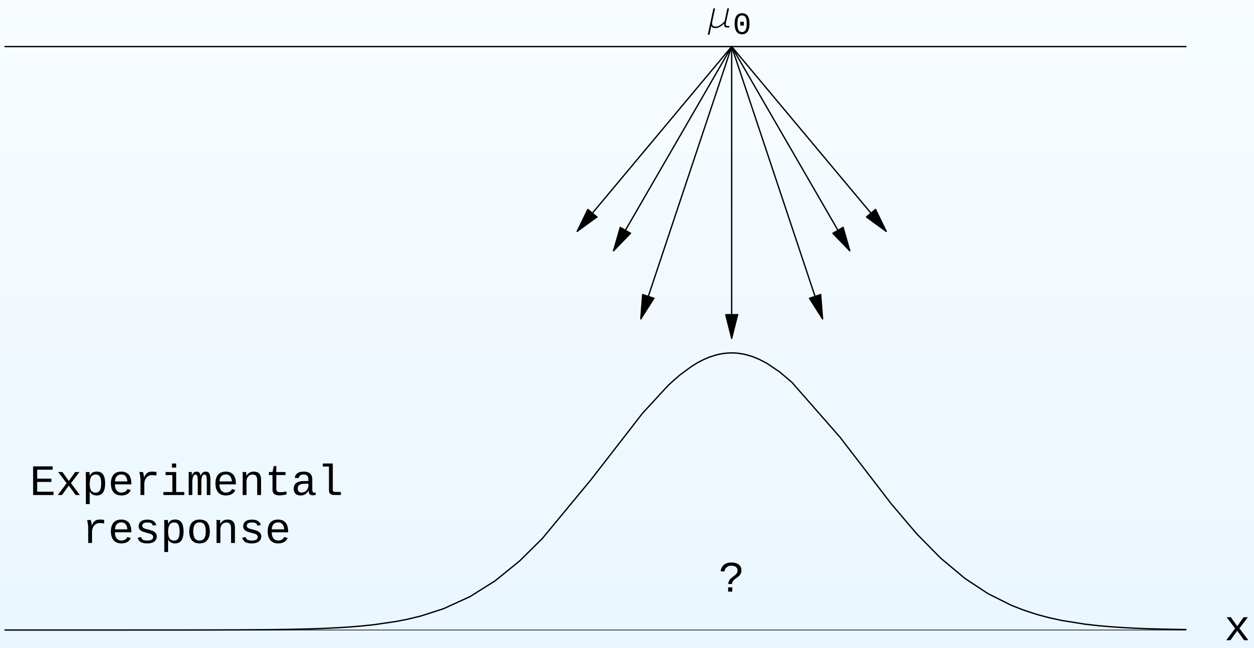
Under well controlled conditions (calibration) we can make use of past frequencies to evaluate 'somehow' the detector response $P(x \mid \mu)$.

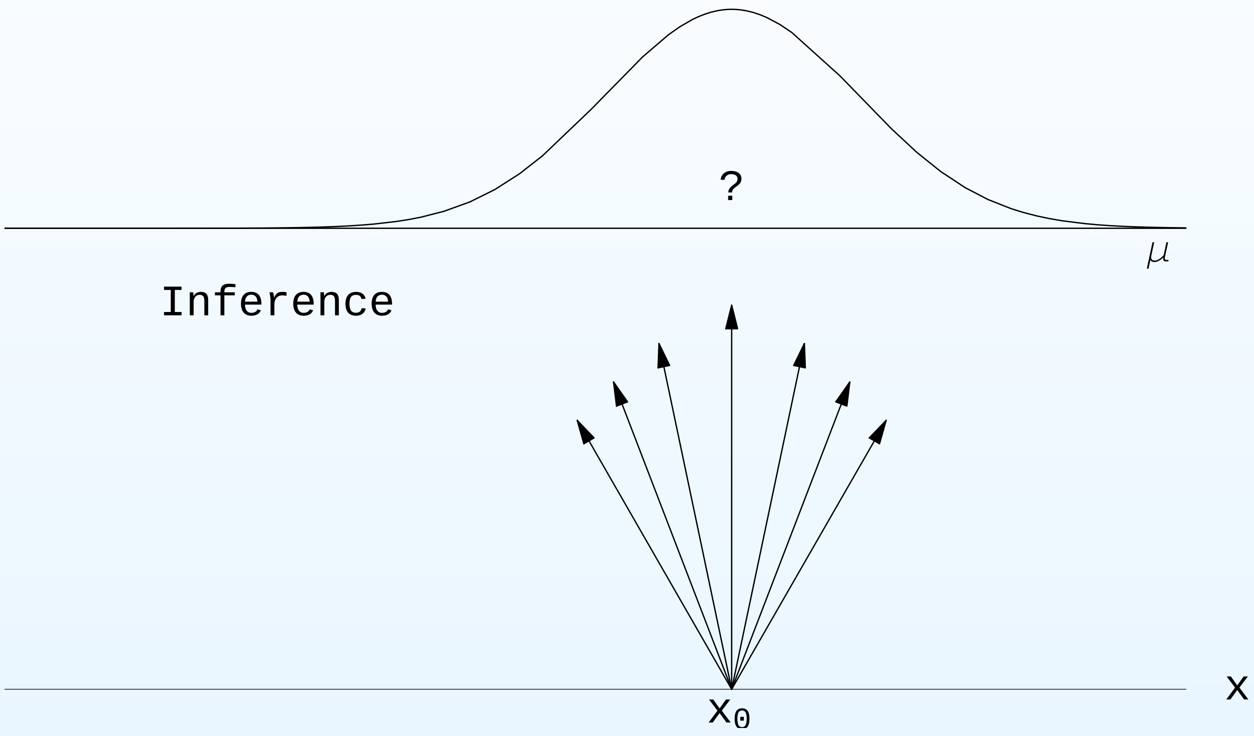
There is (in most cases) no way to get *directly* hints about $P(\mu \mid x)$.

Uncertainties in measurements



$P(x \mid \mu)$ experimentally accessible (though 'model filtered')

Uncertainties in measurements



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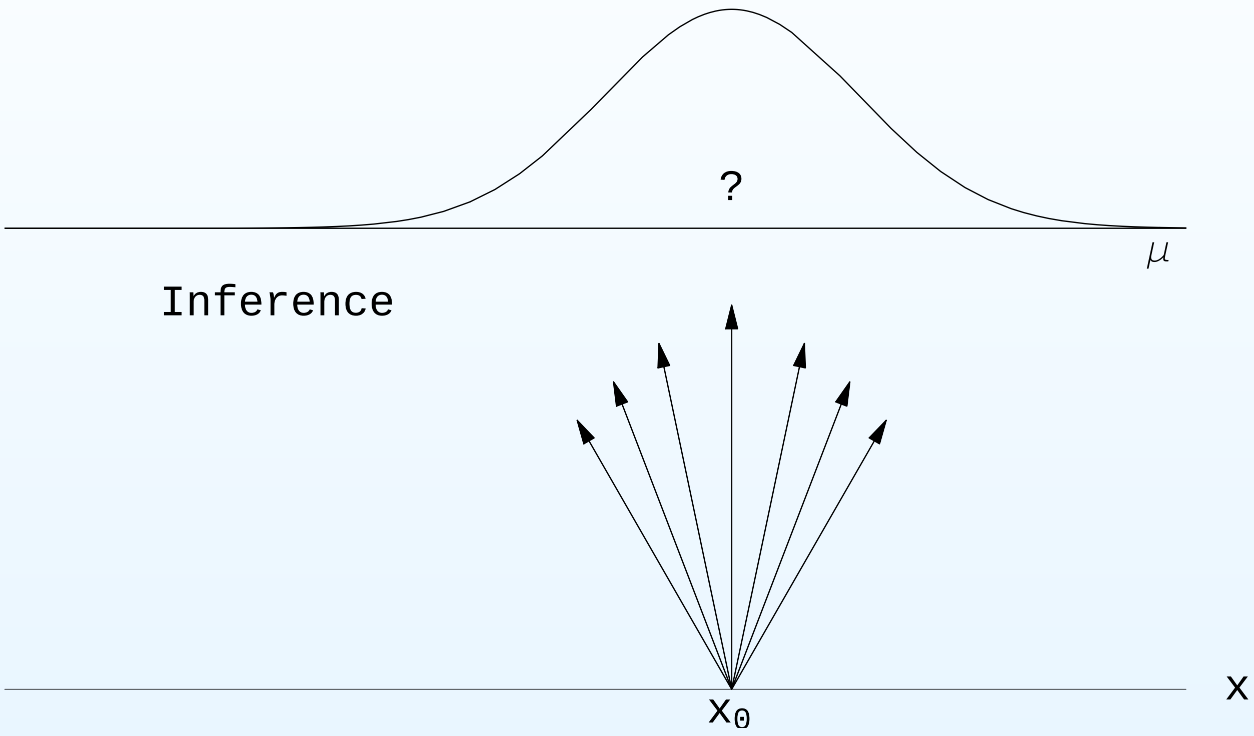
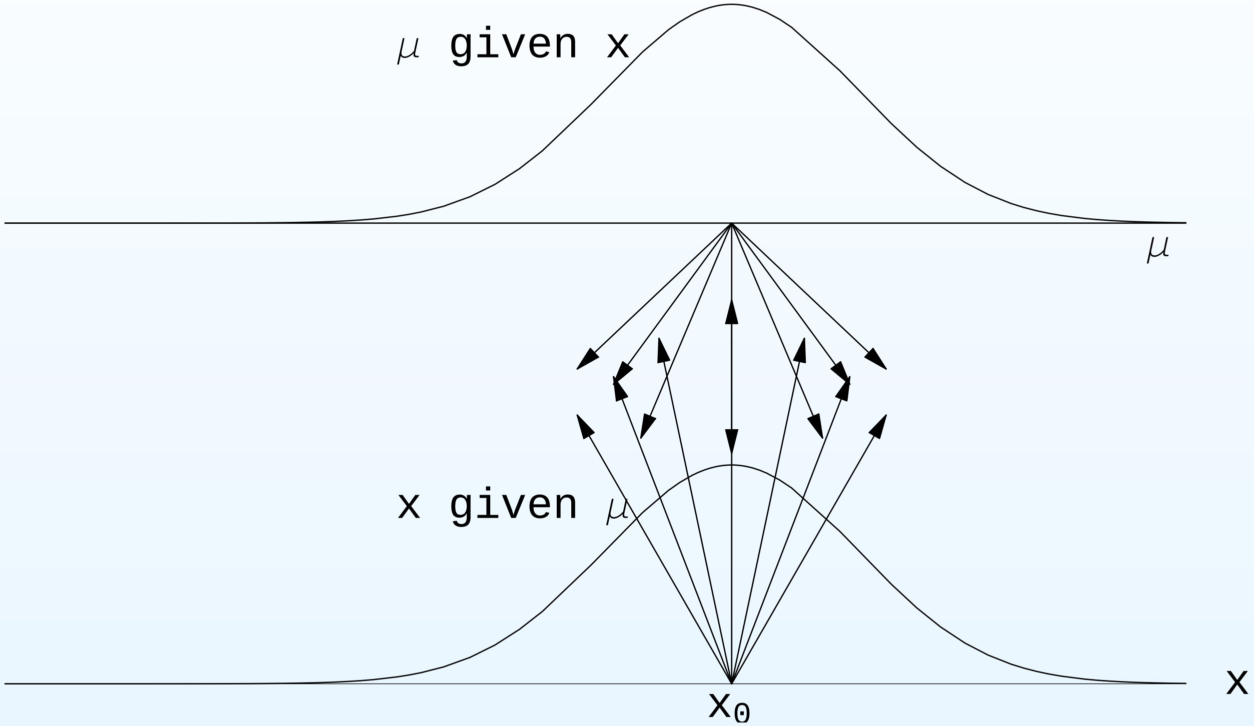


$P(\mu \mid x)$ experimentally inaccessible

but logically accessible!

$\longrightarrow$ we need to learn how to do it

Uncertainties in measurements



Symmetry in reasoning!

Uncertainty and probability

We, as physicists, consider absolutely natural and meaningful statements of the following kind

- $P(-10 < \epsilon'/\epsilon \times 10^4 < 50) >> P(\epsilon'/\epsilon \times 10^4 > 100)$
- $P(170 \le m_{top}/\text{GeV} \le 180) \approx 70\%$
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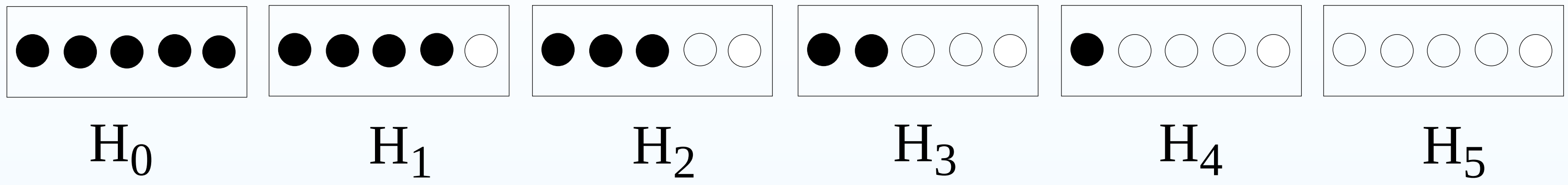
I stick to common sense (and physicists common sense) and assume that probabilities of causes, probabilities of of hypotheses, probabilities of the numerical values of physics quantities, etc. are sensible concepts that match the mind categories of human beings

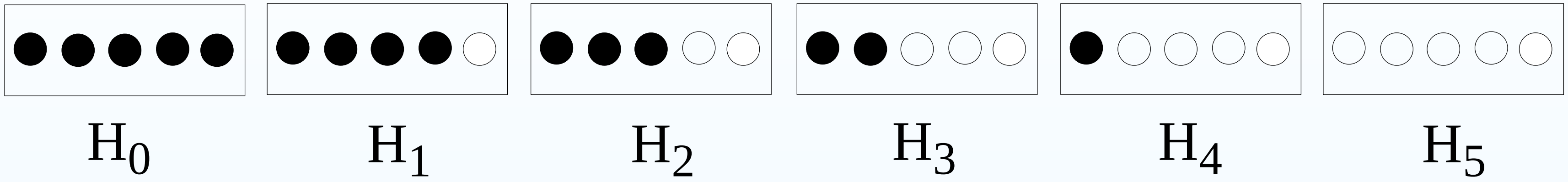
(see D. Hume, C. Darwin + modern researches)

The six box problem



Let us take randomly one of the boxes.

The six box problem



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We are in a state of uncertainty concerning several *events*, the most important of which correspond to the following questions:

(a) Which box have we chosen, $H_0, H_1, \ldots, H_5$?

(b) If we extract randomly a ball from the chosen box, will we observe a white ($E_W \equiv E_1$) or black ($E_B \equiv E_2$) ball?

Our certainty:

$$\begin{aligned} \cup_{j=0}^{5} H_j &= \Omega \\ \cup_{i=1}^{2} E_i &= \Omega\,. \end{aligned}$$

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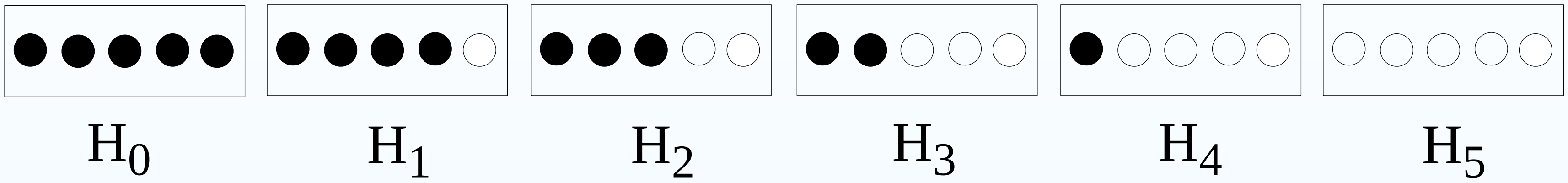

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  - Intuitively we now how to roughly change our opinion.
  - Can we do it quantitatively, in an objective way?

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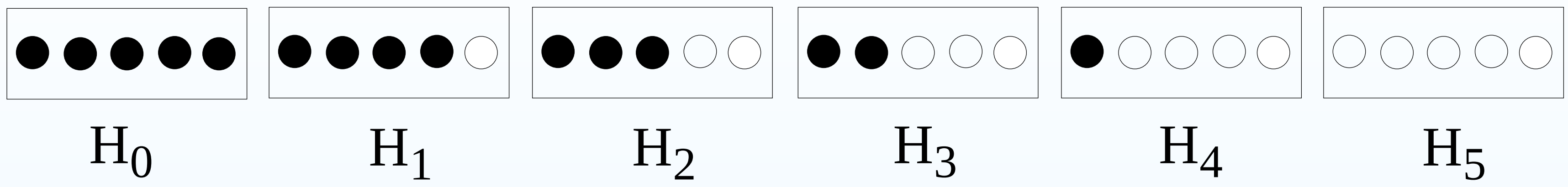

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  - Can we do it quantitatively, in an objective way?
- And after a sequence of extractions?

Predicting sequences

Side remark/exercise

Imagine the four possible sequences resulting from the first two extractions from the misterious box:

BB, BW, WB and WW

- How likely do you consider them to occur?
  [$\longrightarrow$ If you could win a prize associated with the occurrence of one of them, on which sequence(s) would you bet?]

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- **No, they are not equally likelly!**

  Laplace new perfectly why
  $\longrightarrow$ If our logical abilities have regressed it is not a good sign!
  (Remember Leibnitz/Hume quote)

The toy inferential experiment

The aim of the experiment will be to guess the content of the box without looking inside it, only extracting a ball, recording its color and reintroducing it into the box

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This toy experiment is conceptually very close to what we do in Physics

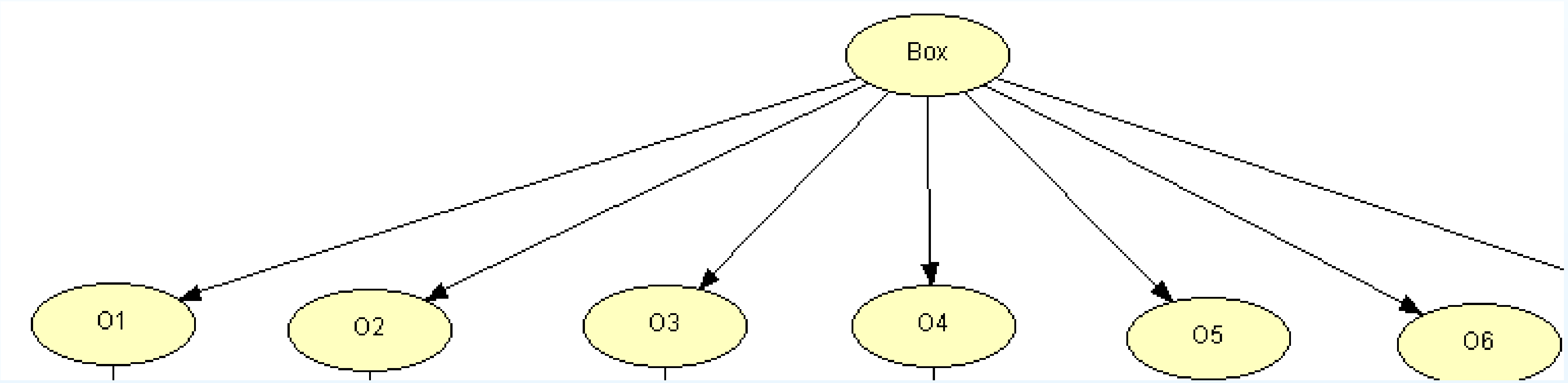
- try to guess what we cannot see (the electron mass, a branching ratio, etc)

  . . . from what we can see (somehow) with our senses.

The rule of the game is that we are not allowed to watch inside the box! (As we cannot open and electron and read its properties, like we read the MAC address of a PC interface)

Cause-effect representation

box content → observed color



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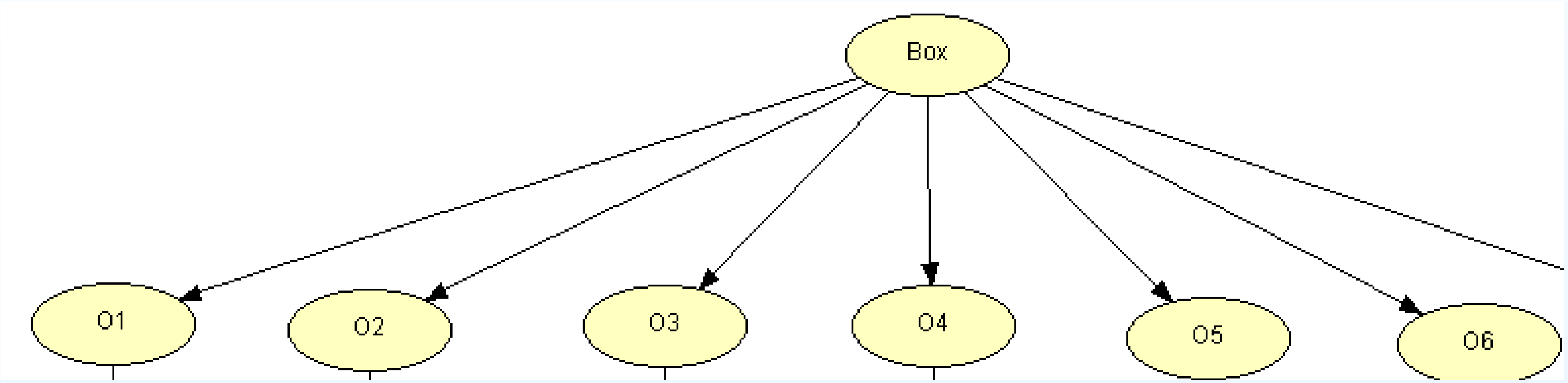
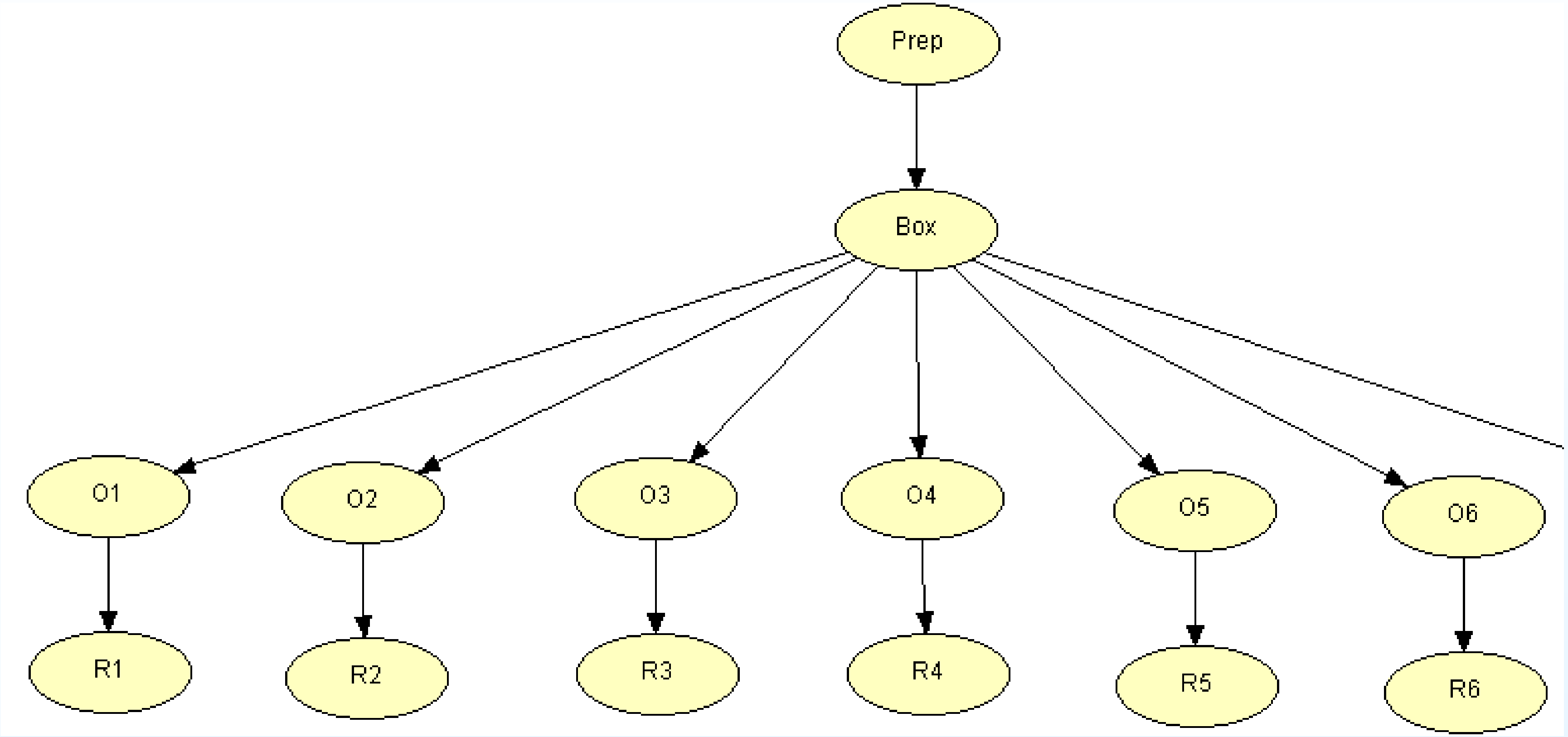
box content $\longrightarrow$ observed color



An effect might be the cause of another effect $\longrightarrow$

A network of causes and effects



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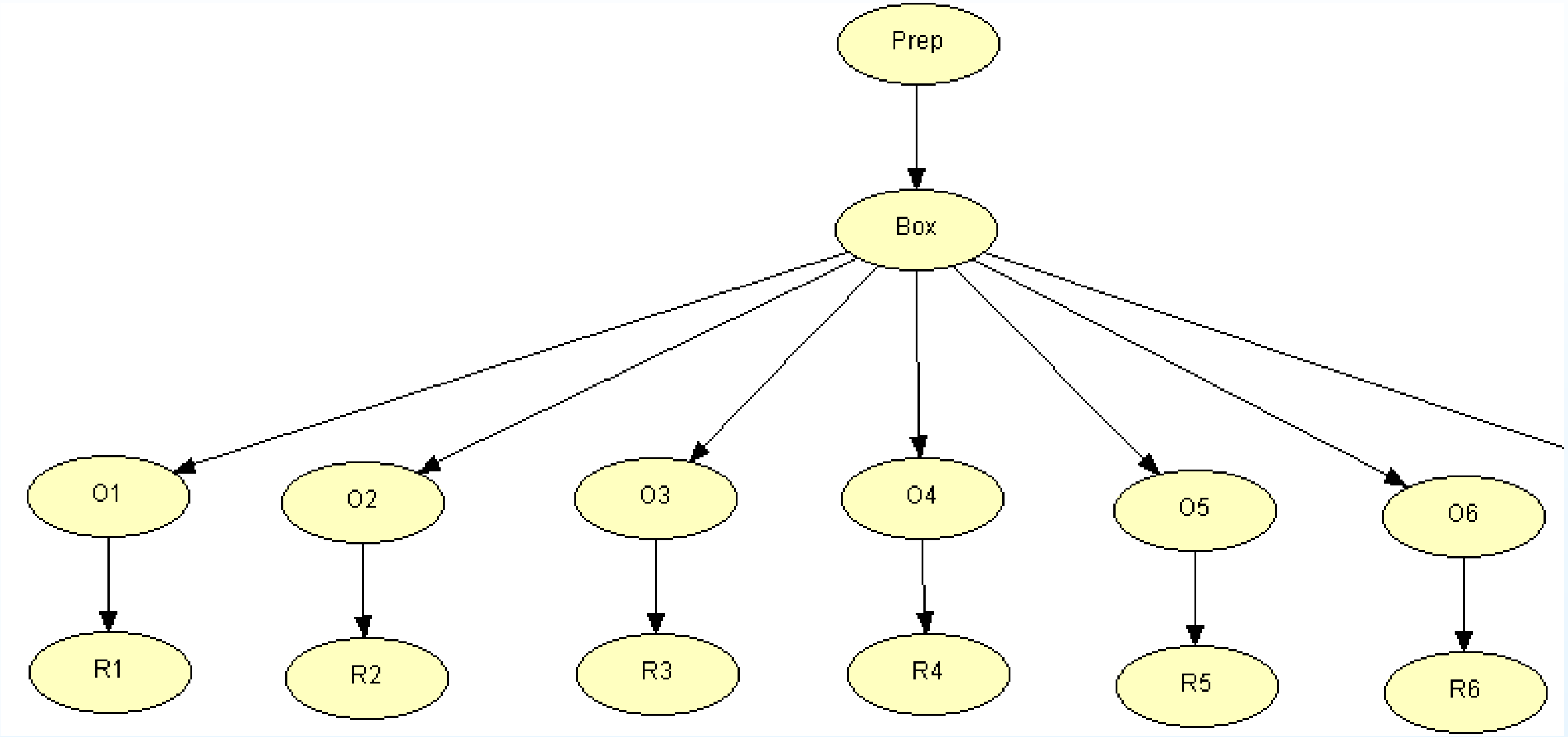
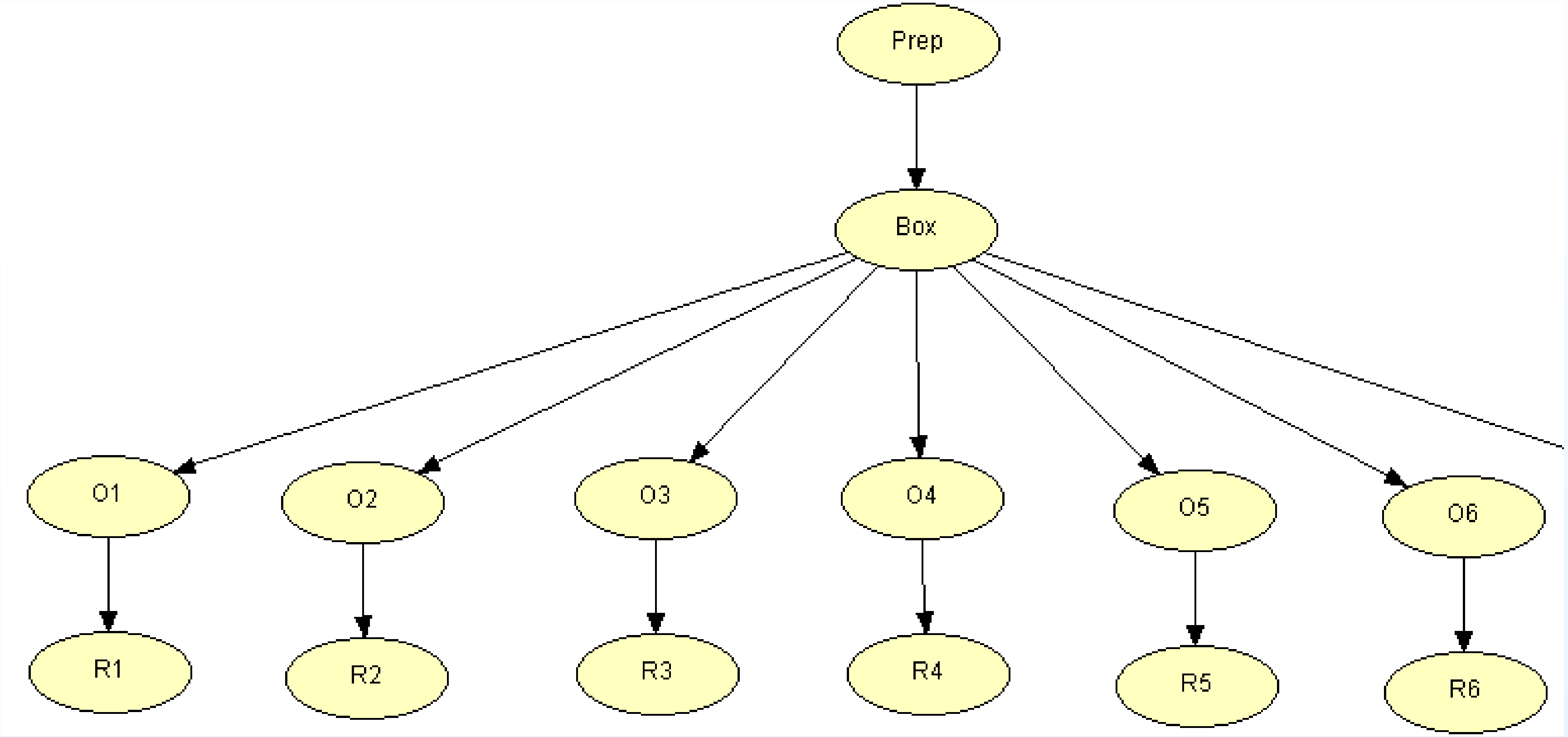


A report (R_i) might not correspond exactly to what really happened (O_i)

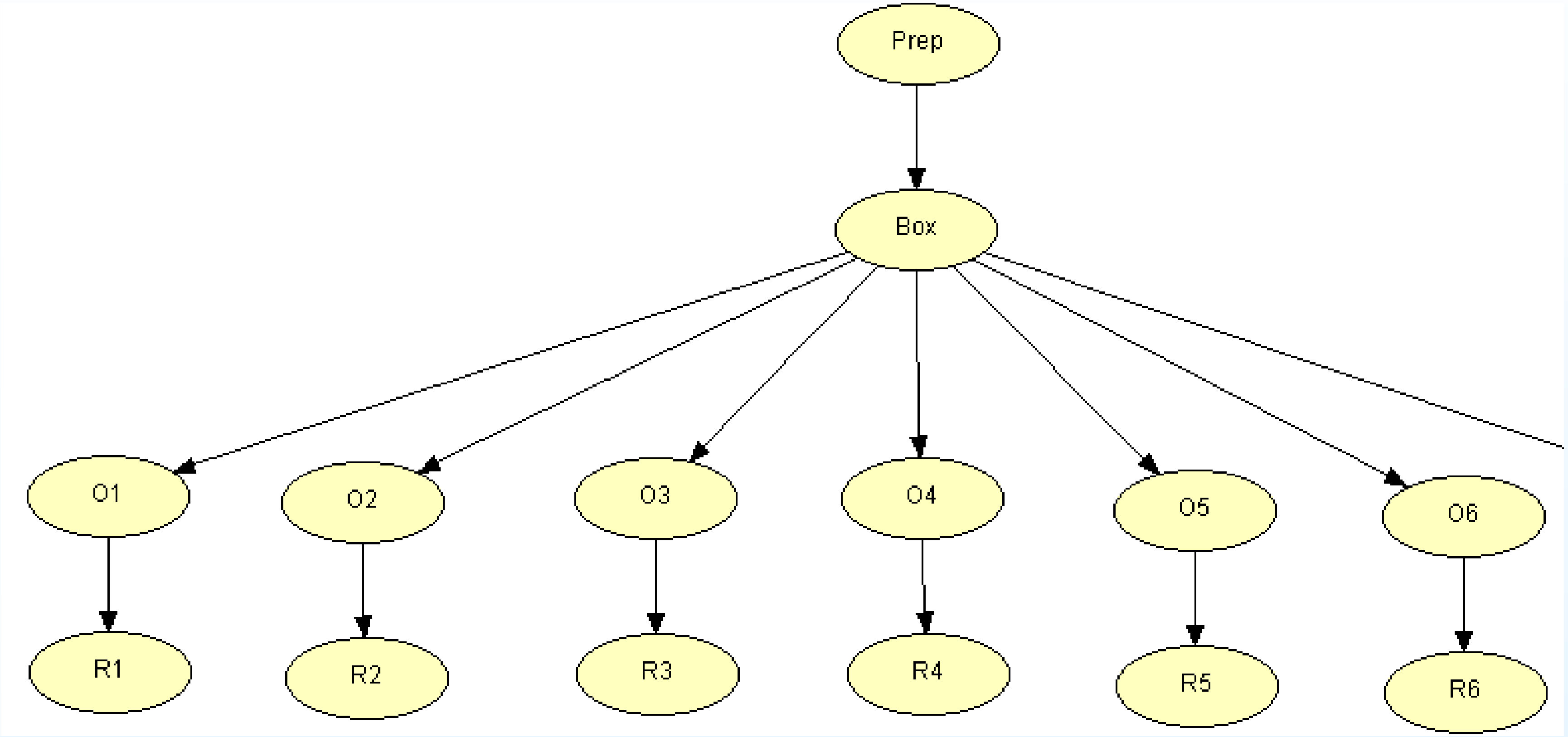
A network of causes and effects



Of crucial interest in Science!

$\Rightarrow$ Our devices seldom tell us 'the truth'.

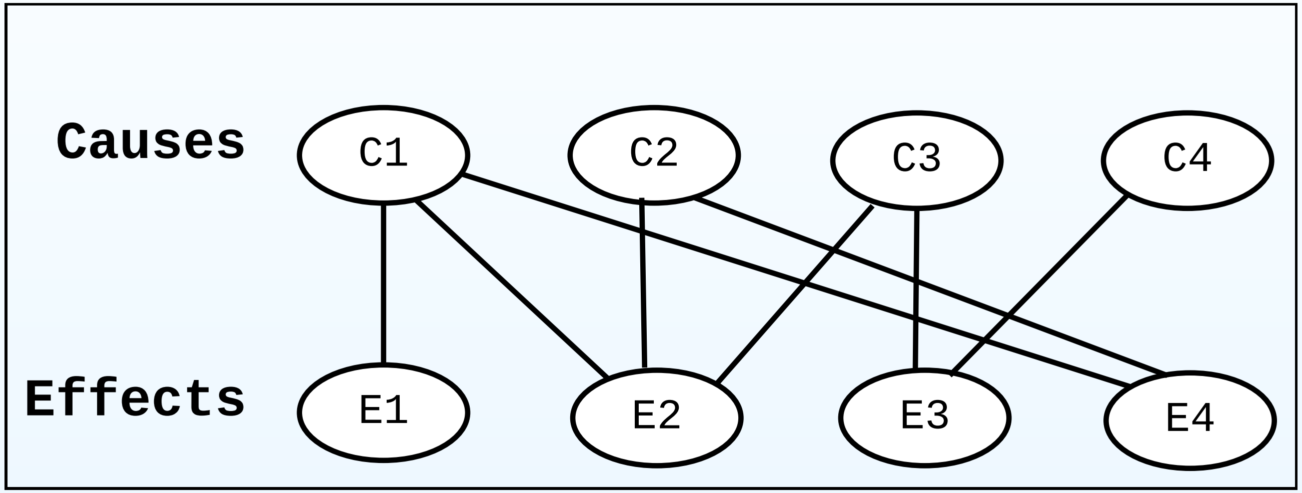
A network of causes and effects



$\Rightarrow$ Belief Networks (Bayesian Networks)

From causes to effects and back

Our original problem:



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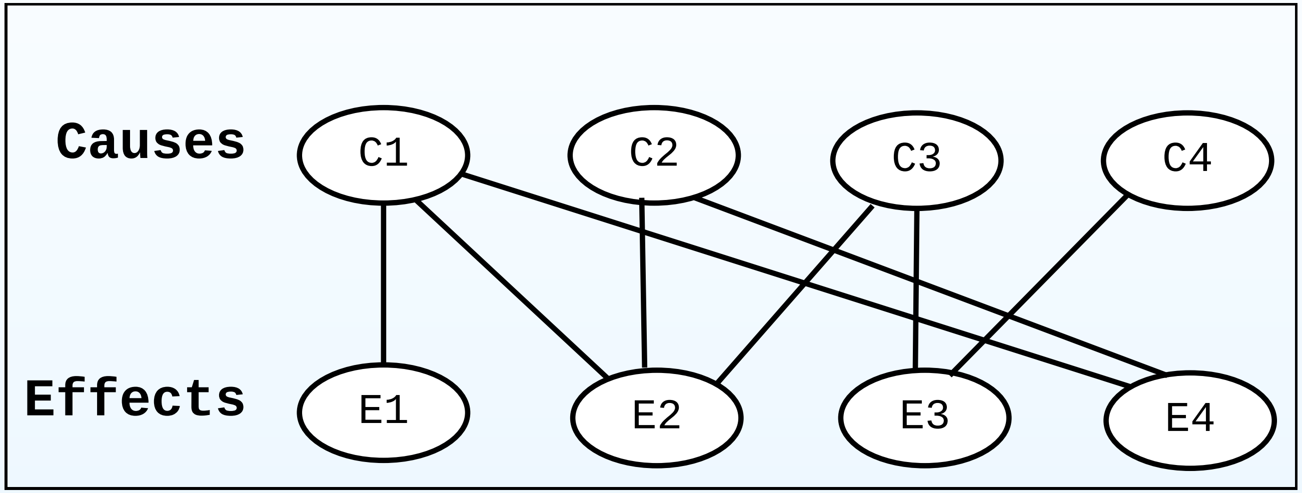

Our conditional view of probabilistic causation

$$P(E_i \,|\, C_j)$$

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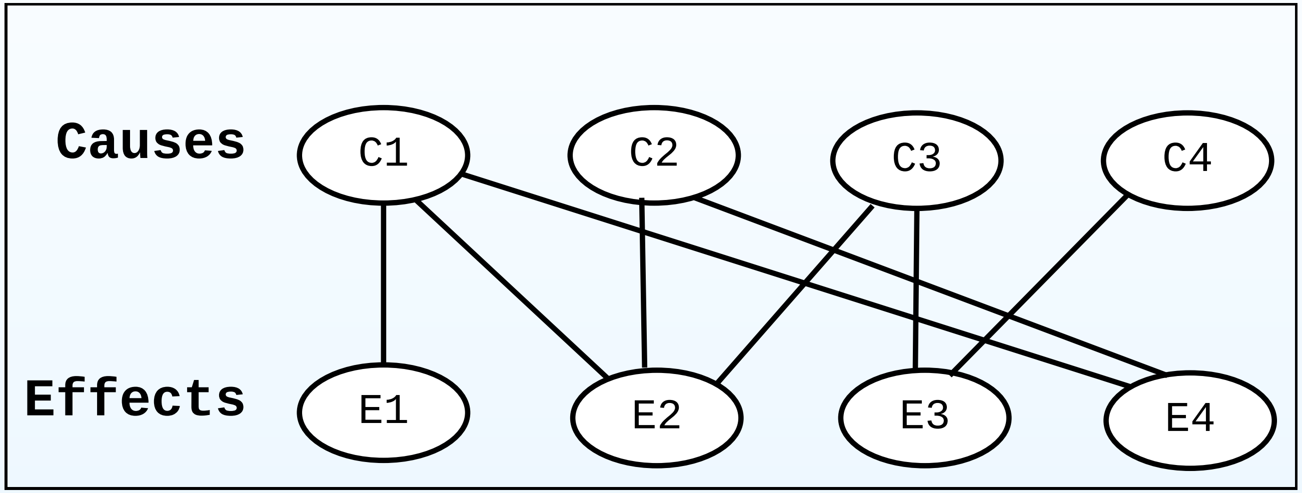

Our conditional view of probabilistic causation

$$\boxed{P(E_i \,|\, C_j)}$$

Our conditional view of probabilistic inference

$$\boxed{P(C_j \,|\, E_i)}$$

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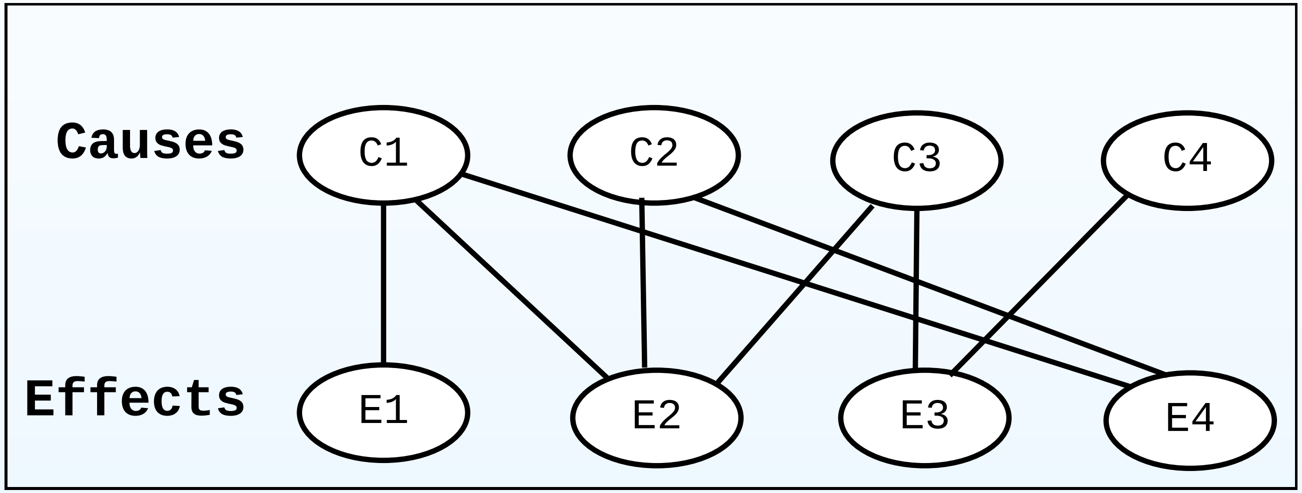

Our conditional view of probabilistic causation

$$P(E_i \,|\, C_j)$$

Our conditional view of probabilistic inference

$$P(C_j \,|\, E_i)$$

The fourth basic rule of probability:

$$P(C_j, E_i) = P(E_i \,|\, C_j)\, P(C_j) = P(C_j \,|\, E_i)\, P(E_i)$$

Symmetric conditioning

Let us take basic rule 4, written in terms of hypotheses H_j and effects E_i, and rewrite it this way:

$$\frac{P(H_j\,|\,E_i)}{P(H_j)} = \frac{P(E_i\,|\,H_j)}{P(E_i)}$$

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Got 'after' Calculated 'before'

(where 'before' and 'after' refer to the knowledge that E_i is true.)

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"post illa observationes" *"ante illa observationes"*

(Gauss)

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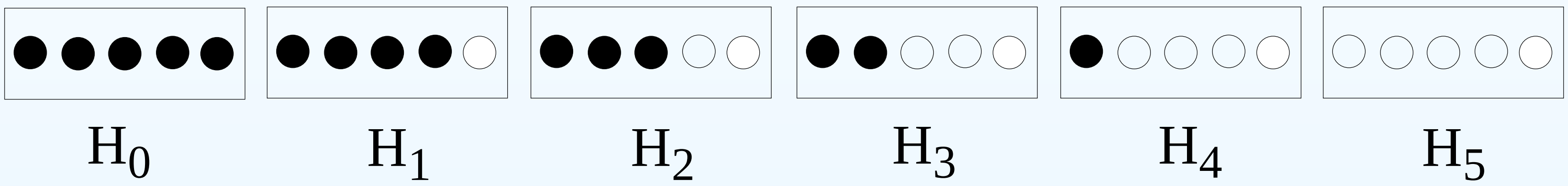
$\Rightarrow$ Bayes theorem

Application to the six box problem



Remind:

- $E_1 =$ White
- $E_2 =$ Black

Collecting the pieces of information we need

Our tool:

$$P(H_j \,|\, E_i, I) = \frac{P(E_i \,|\, H_j, I)}{P(E_i \,|\, I)} \, P(H_j \,|\, I)$$

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- $P(H_j \,|\, I) = 1/6$

Collecting the pieces of information we need

Our tool:

$$P(H_j \mid E_i, I) = \frac{P(E_i \mid H_j, I)}{P(E_i \mid I)} P(H_j \mid I)$$

- $P(H_j \mid I) = 1/6$
- $P(E_i \mid I) = 1/2$

Collecting the pieces of information we need

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$$P(H_j \,|\, E_i, I) = \frac{P(E_i \,|\, H_j, I)}{P(E_i \,|\, I)} \, P(H_j \,|\, I)$$

- $P(H_j \,|\, I) = 1/6$
- $P(E_i \,|\, I) = 1/2$
- $P(E_i \,|\, H_j,\, I)$:

$$\begin{aligned} P(E_1 \,|\, H_j,\, I) &= j/5 \\ P(E_2 \,|\, H_j,\, I) &= (5-j)/5 \end{aligned}$$

Collecting the pieces of information we need

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Our prior belief about H_j

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Probability of E_i under a well defined hypothesis H_j
It corresponds to the 'response of the apparatus in measurements.
→ likelihood (traditional, rather confusing name!)

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$\rightarrow$ How much we are confident that E_i will occur.

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Probability of E_i taking account all possible H_j
$\rightarrow$ How much we are confident that E_i will occur.
Easy in this case, because of the symmetry of the problem.
But already after the first extraction of a ball our opinion about the box content will change, and symmetry will break.

Collecting the pieces of information we need

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But it easy to prove that $P(E_i \,|\, I)$ is related to the other ingredients, usually easier to 'measure' or to assess somehow, though vaguely

'decomposition law': $P(E_i \,|\, I) = \sum_j P(E_i \,|\, H_j, \, I) \cdot P(H_j \,|\, I)$

($\rightarrow$ Easy to check that it gives $P(E_i \,|\, I) = 1/2$ in our case).

Collecting the pieces of information we need

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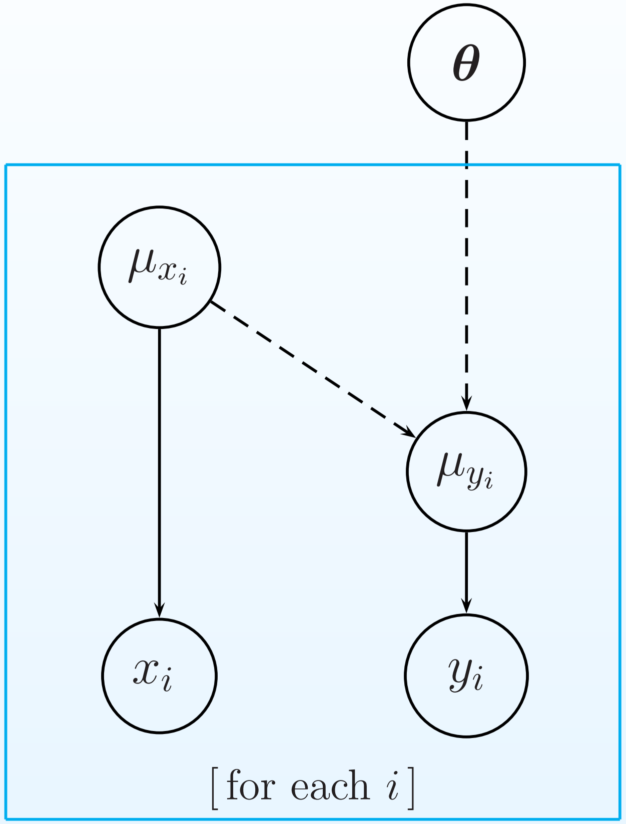
We are ready

$\longrightarrow$ Let's play!

A different way to view fit issues



- Determistic link μ_x's to μ_y's
- Probabilistic links $\mu_x \longrightarrow x$, $\mu_y \longrightarrow y$

$\Rightarrow$ aim of fit: $\{\boldsymbol{x}, \boldsymbol{y}\} \longrightarrow \boldsymbol{\theta} \Rightarrow f(\boldsymbol{\theta}\,|\,\{\boldsymbol{x}, \boldsymbol{y}\})$

Parametric inference Vs unfolding

$f(\boldsymbol{\theta}\,|\,\{\boldsymbol{x},\boldsymbol{y}\})$:

Parametric inference Vs unfolding

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probabilistic parametric inference
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$\Rightarrow$ Unfolding (deconvolution)

Smearing matrix $\longrightarrow$ unfolding matrix

Invert smearing matrix?

Smearing matrix $\longrightarrow$ unfolding matrix

Invert smearing matrix?

In general is a bad idea:

not a rotational problem

but an inferential problem!

Smearing matrix $\longrightarrow$ unfolding matrix

Imagine $S = \begin{pmatrix} 0.8 & 0.2 \\ 0.2 & 0.8 \end{pmatrix}$: $\longrightarrow U = S^{-1} = \begin{pmatrix} 1.33 & -0.33 \\ -0.33 & 1.33 \end{pmatrix}$

Let the true be $s_t = \begin{pmatrix} 10 \\ 0 \end{pmatrix}$: $\longrightarrow s_m = S \cdot s_t = \begin{pmatrix} 8 \\ 2 \end{pmatrix}$;

If we measure $s_m = \begin{pmatrix} 8 \\ 2 \end{pmatrix} \longrightarrow S^{-1} \cdot s_m = \begin{pmatrix} 10 \\ 0 \end{pmatrix}$ $\surd$

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BUT

if we had measured $\begin{pmatrix} 9 \\ 1 \end{pmatrix} \rightarrow S^{-1} \cdot s_m = \begin{pmatrix} 11.7 \\ -1.7 \end{pmatrix}$

if we had measured $\begin{pmatrix} 10 \\ 0 \end{pmatrix} \rightarrow S^{-1} \cdot s_m = \begin{pmatrix} 13.3 \\ -3.3 \end{pmatrix}$

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Indeed, matrix inversion is recognized to producing ‘crazy spectra’ and even negative values (unless such large numbers in bins such fluctuations around expectations are negligeable)

Bin to bin?

En passant:

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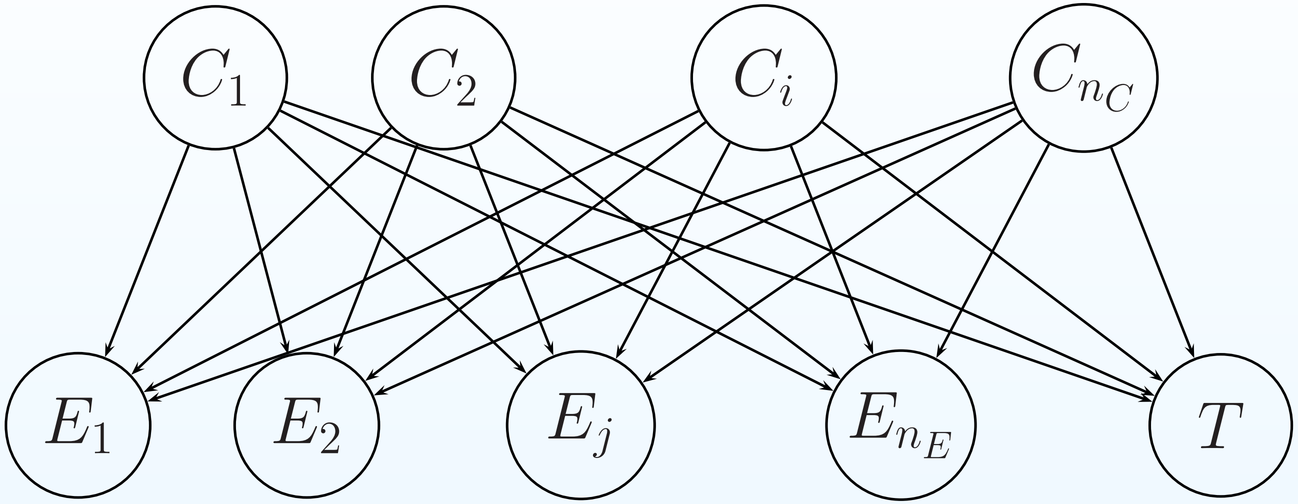
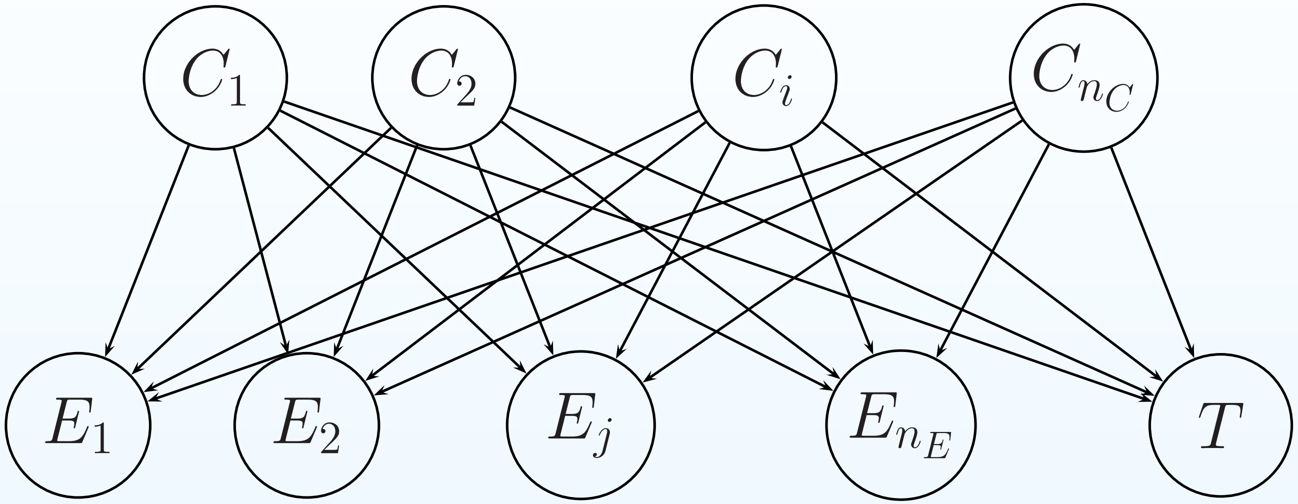
[Anyway, one might set up a procedure for a specific problem, test it with simulations and apply it to real data (the frequentistic way – if ther is *the way*...)]

Discretized unfolding



(T: ‘trash’)

Discretized unfolding



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$\boldsymbol{x}_C$: *true spectrum* (nr of events in cause bins)

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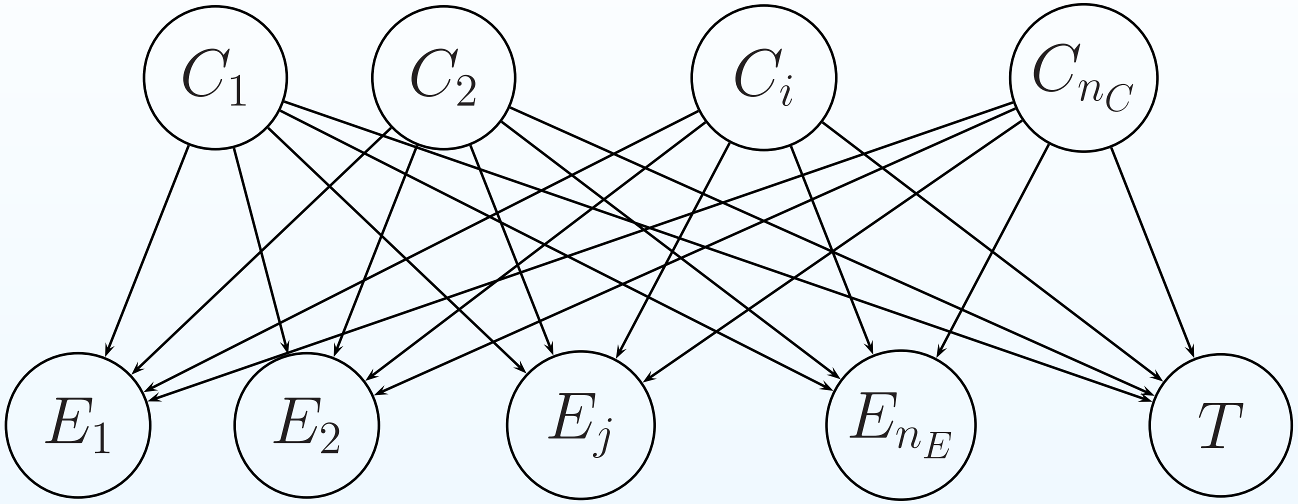

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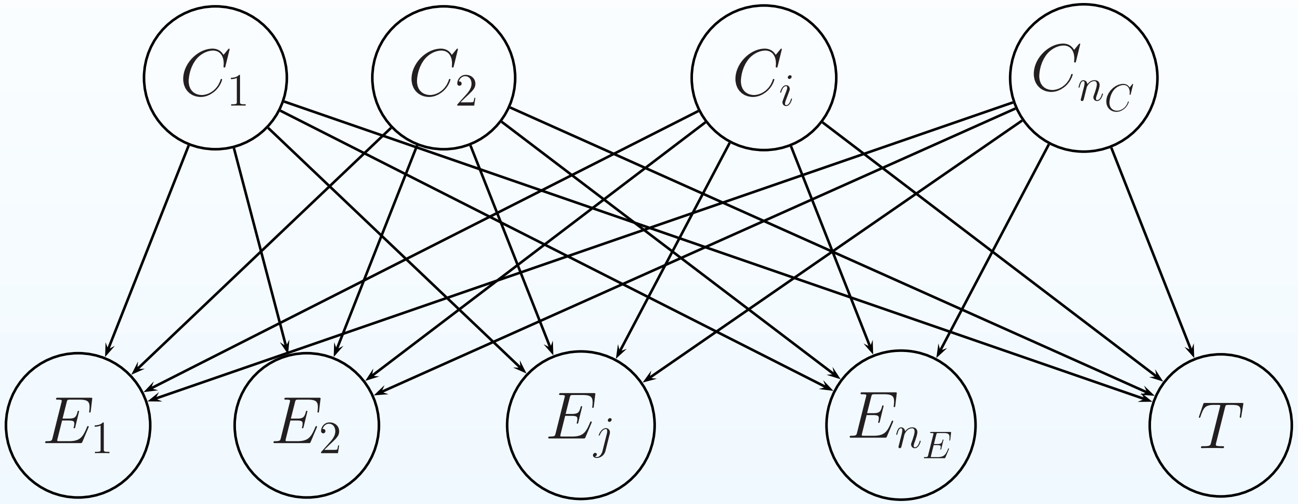
$\boldsymbol{x}_C$: *true spectrum* (nr of events in cause bins)

$\boldsymbol{x}_E$: *observed spectrum* (nr of events in effect bins)

Our aim:

- **not** to find *the* true spectrum
- but, more modestly, rank in beliefs all possible spectra that might have caused the observed one:
  $\Rightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, I)$

Discretized unfolding



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- $P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, I)$ depends on the knowledge of *smearing matrix* Λ,
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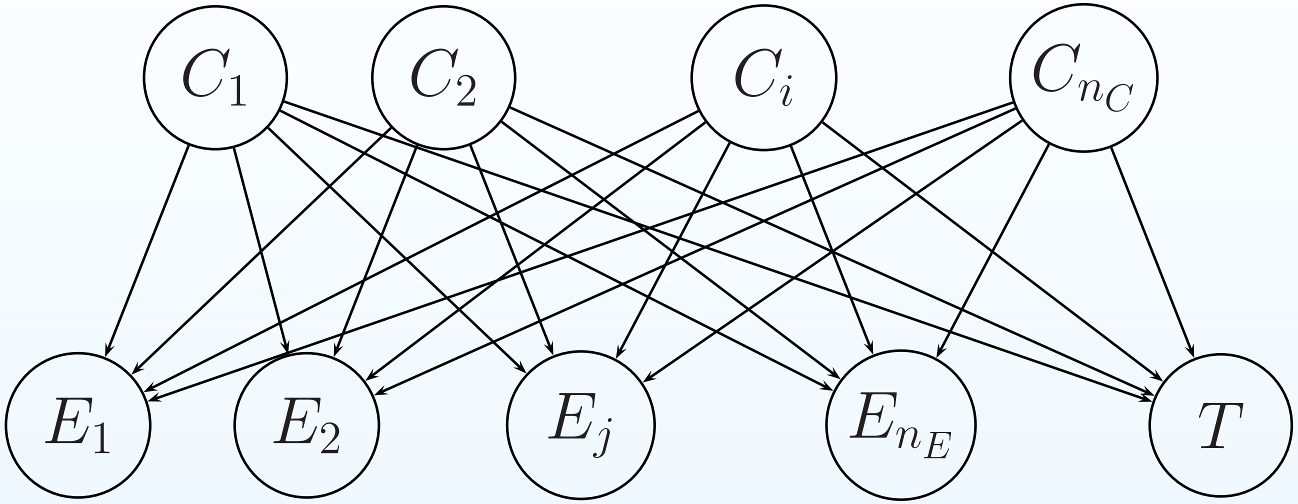

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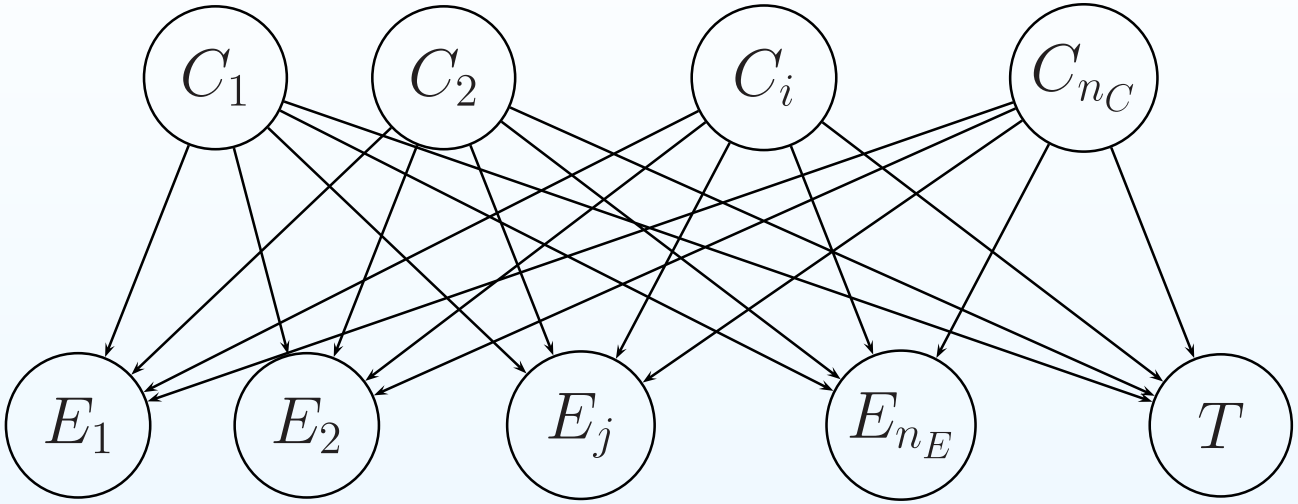

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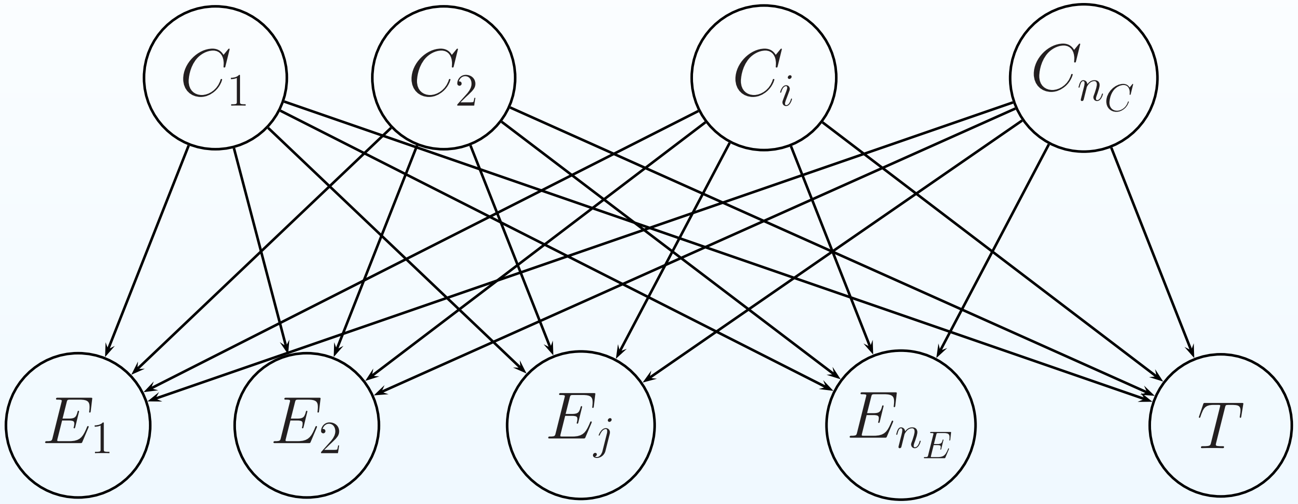

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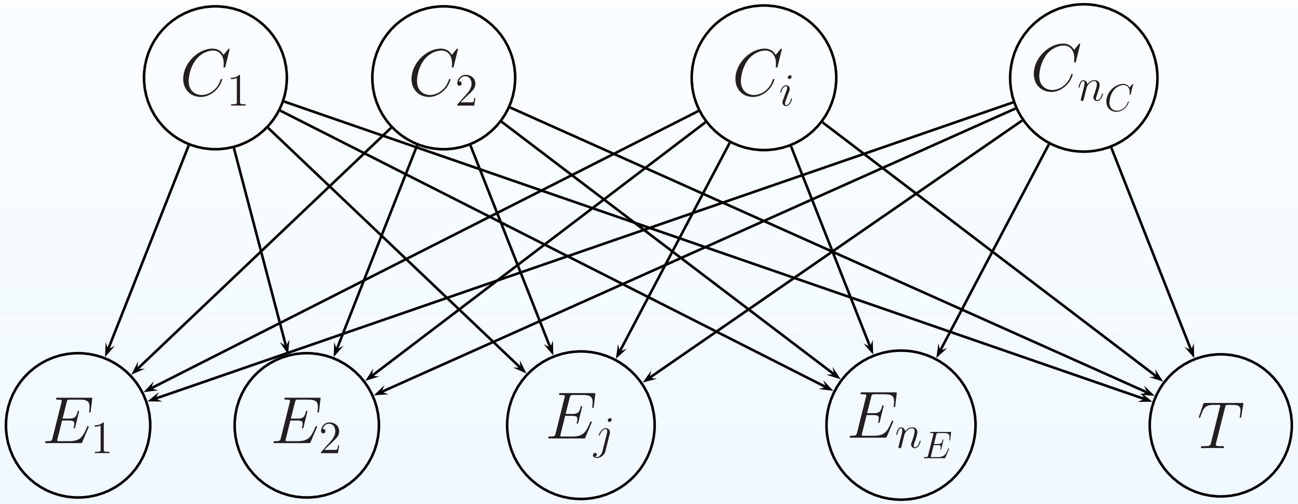
  $\rightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, \Lambda, I)$
  $\Rightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, I) = \int P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, \Lambda,\, I)\, f(\Lambda \,|\, I)\, \mathrm{d}\Lambda$ [by MC!]

Discretized unfolding



(T: ‘trash’)

- Bayes theorem:

$$P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E,\, \Lambda,\, I) \;\;\propto\;\; P(\boldsymbol{x}_E \,|\, \boldsymbol{x}_C,\, \Lambda,\, I) \cdot P(\boldsymbol{x}_C \,|\, I)\,.$$

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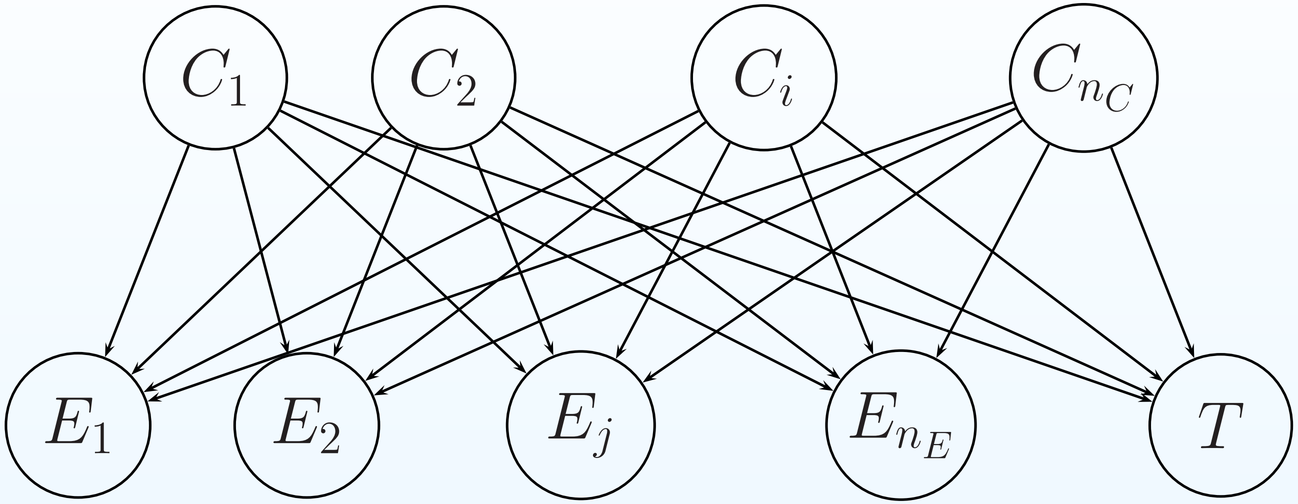

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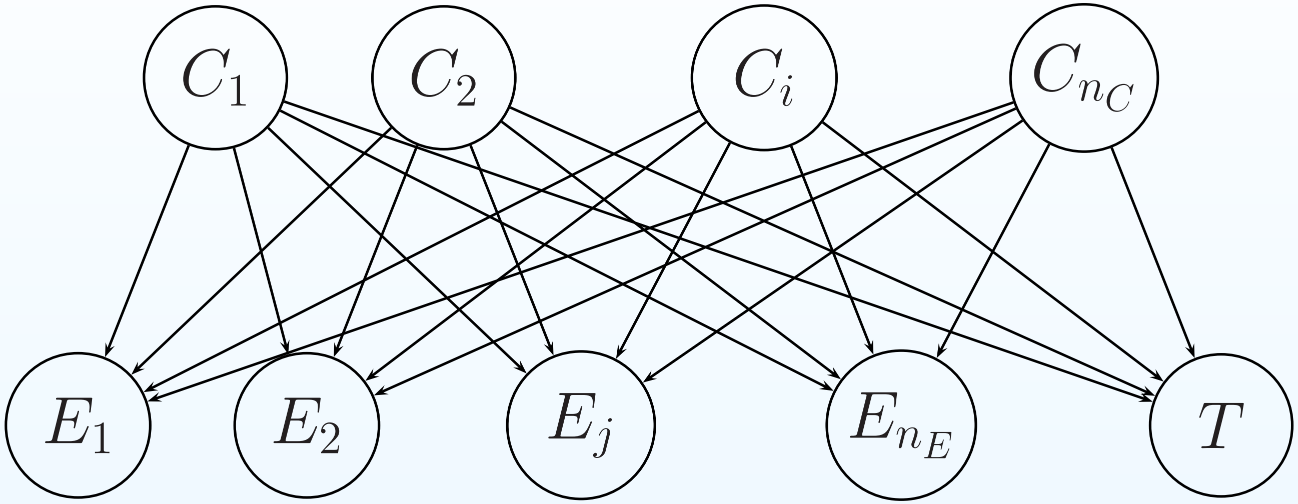
- Indifference w.r.t. all possible spectra

$$P(\boldsymbol{x}_C\,|\,\boldsymbol{x}_E,\,\Lambda,\,I) \;\propto\; P(\boldsymbol{x}_E\,|\,\boldsymbol{x}_C,\,\Lambda,\,I)$$

$P(\boldsymbol{x}_E \,|\, x_{C_i},\, \Lambda,\, I)$



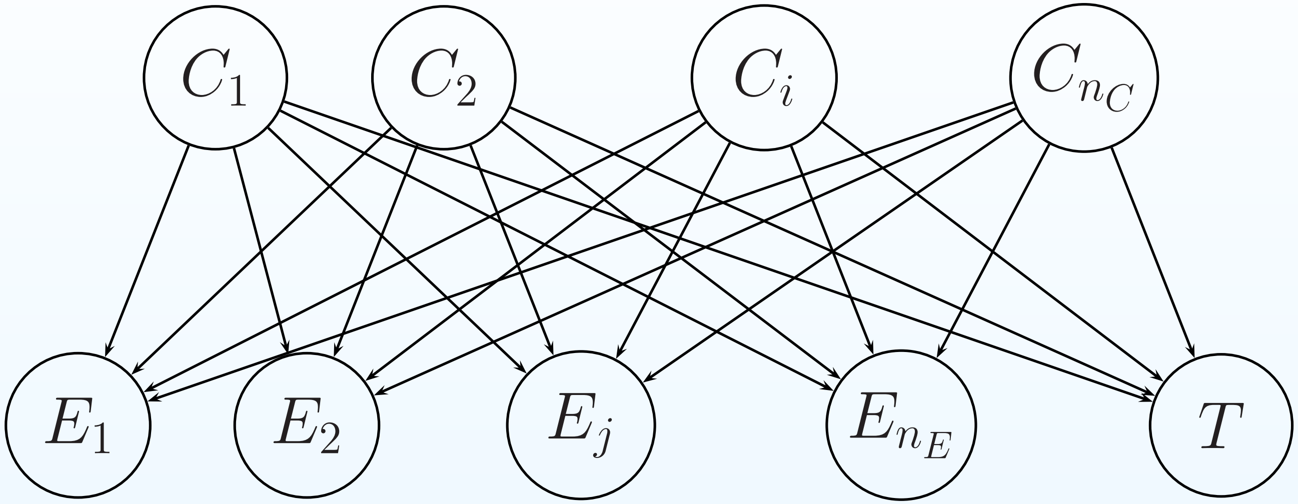
Given a certain number of events in a cause-bin $x(C_i)$, the number of events in the effect-bins, included the 'trash' one, is described by a multinomial distribution:

$$\boldsymbol{x}_E\big|_{x(C_i)} \;\sim\; \text{Mult}[x(C_i), \boldsymbol{\lambda}_i]\,,$$

with

$$\begin{aligned}\boldsymbol{\lambda}_i &= \{\lambda_{1,i},\, \lambda_{2,i},\, \ldots,\, \lambda_{n_E+1,i}\} \\ &= \{P(E_1 \,|\, C_i,\, I),\, P(E_2 \,|\, C_i,\, I), \ldots,\, P(E_{n_E+1,i} \,|\, C_i,\, I)\}\end{aligned}$$

$P(\boldsymbol{x}_E \,|\, \boldsymbol{x}_C,\, \Lambda,\, I)$



$\boldsymbol{x}_E|_{x(C_i)}$ multinomial random vector,

$\Rightarrow\ \boldsymbol{x}_E|_{\boldsymbol{x}(C)}$ sum of several multinomials.

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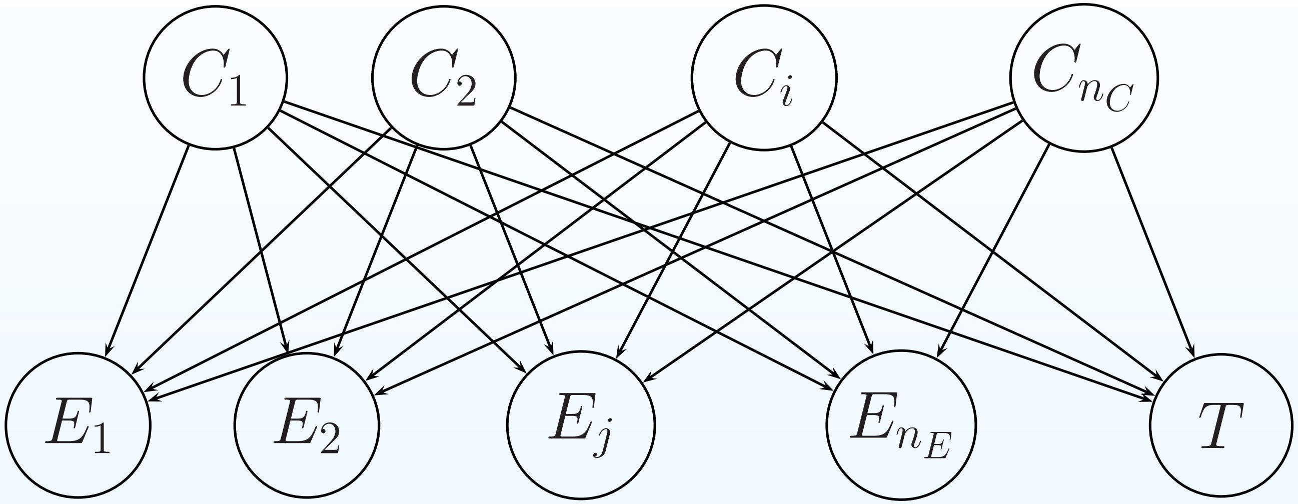

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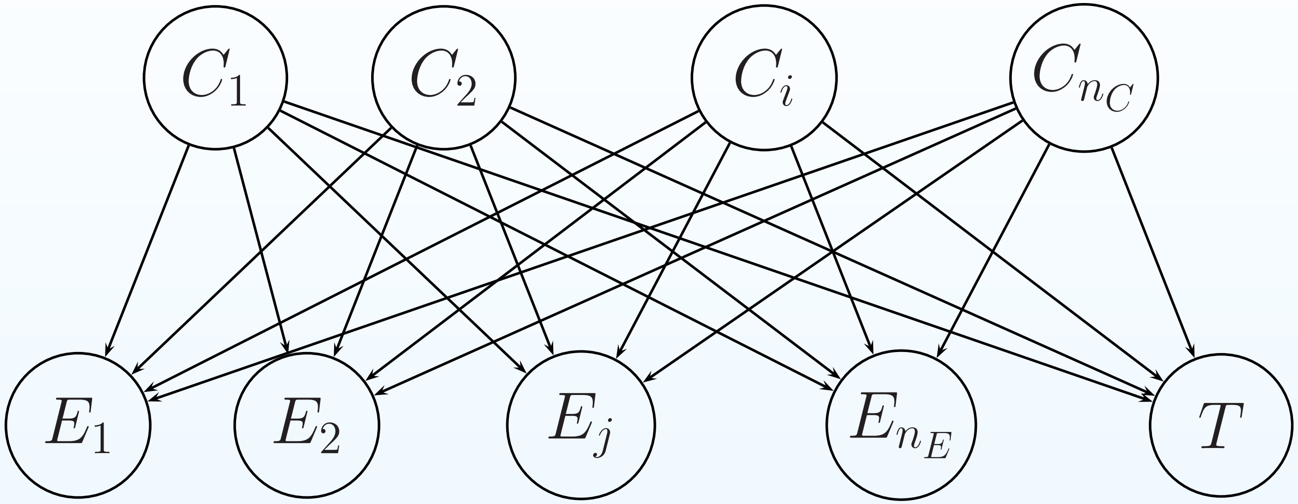

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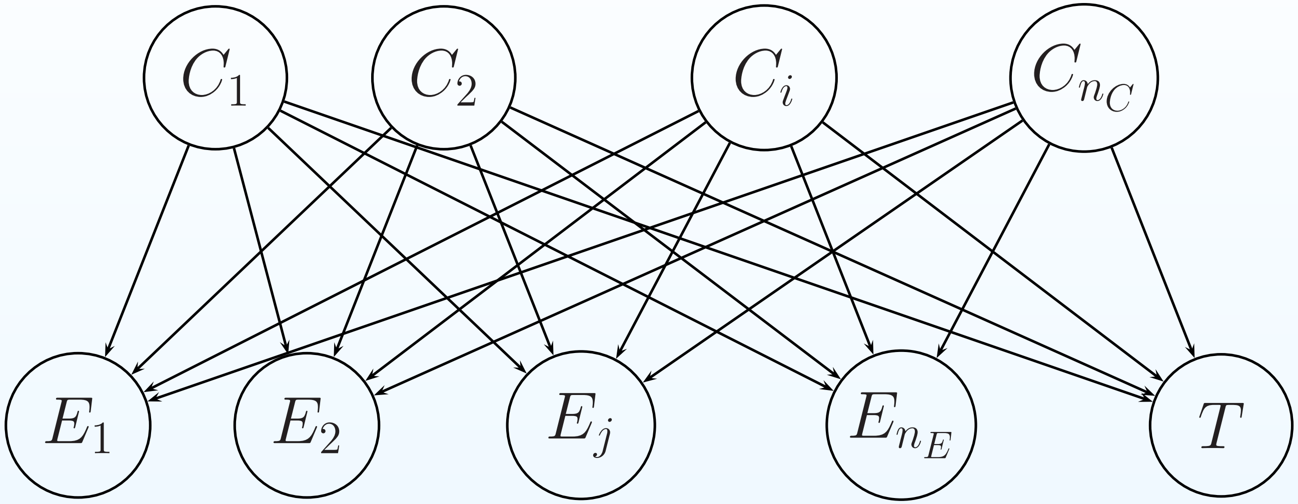

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no 'easy' expression for $P(\boldsymbol{x}_E \,|\, \boldsymbol{x}_C, \Lambda, I)$

$\Rightarrow$ STUCK!

$\Rightarrow$ Change strategy

The rescue trick

Instead of using the original probability inversion (applied directly) to spectra

$$P(\boldsymbol{x}_C\,|\,\boldsymbol{x}_E,\,\Lambda,\,I) \;\;\propto\;\; P(\boldsymbol{x}_E\,|\,\boldsymbol{x}_C,\,\Lambda,\,I)\cdot P(\boldsymbol{x}_C\,|\,I)\,,$$

we restart from

$$P(C_i\,|E_j,\,I) \;\;\propto\;\; P(E_j\,|\,C_i,\,I)\cdot P(C_i\,|\,I).$$

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Consequences:

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2. a uniform prior $P(C_i \,|\, I) = k$ does not mean indifference over all possible spectra.

   $\Rightarrow$ $P(C_i \,|\, I) = k$ is a well precise spectrum (in most cases far from the physical one)

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Old algorithm

1. [*] λ_{ij} estimated by MC simulation as

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or

$$\theta_{ij} = \frac{\lambda_{ji}\cdot P(C_i\,|\,I)}{\sum_i \lambda_{ji}\cdot P(C_i\,|\,I)}\,,$$

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3. [*] Assignement of events to cause bins:

$$\begin{aligned}
x(C_i)|_{x(E_j)} &\approx P(C_i\,|E_j,\,I)\cdot x(E_j)\\
x(C_i)|_{\boldsymbol{x}_E} &\approx \sum_{j=1}^{n_E} P(C_i\,|E_j,\,I)\cdot x(E_j)\\
x(C_i) &\approx \frac{1}{\epsilon_i}\,x(C_i)|_{\boldsymbol{x}_E}\,,
\end{aligned}$$

with $\epsilon_i = \sum_{j=1}^{n_E} P(E_j\,|\,C_i,\,I)$

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with $\epsilon_i = \sum_{j=1}^{n_E} P(E_j\,|\,C_i,\,I)$

4. [∗] Uncertainty by 'standard error propagation'

Improvements

1. $\boldsymbol{\lambda}_i$: having each element λ_{ji} the meaning of "p_j" of a Multinomial distribution, their distribution can easily (and conveniently and realistically) modelled by a Dirichlet:

$$\boldsymbol{\lambda}_i \quad \sim \quad \text{Dir}[\boldsymbol{\alpha}_{prior} + \boldsymbol{x}_E^{MC}\big|_{x(C_i)^{MC}}] ,$$

(The Dirichlet is the prior conjugate of the Multinomial)

Improvements

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$$\boldsymbol{\lambda}_i \;\sim\; \text{Dir}[\boldsymbol{\alpha}_{prior} + \boldsymbol{x}_E^{MC}\big|_{x(C_i)^{MC}}],$$

2. uncertainty on $\boldsymbol{\lambda}_i$:
taken into account by sampling $\Rightarrow$ equivalent to integration

$$\Rightarrow P(\boldsymbol{x}_C\,|\,\boldsymbol{x}_E, I) \;=\; \int P(\boldsymbol{x}_C\,|\,\boldsymbol{x}_E, \Lambda,\, I)\, f(\Lambda\,|\,I)\, \mathrm{d}\Lambda$$

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3. sharing $x_{E_j} \rightarrow \boldsymbol{x}_C$: done by a Multinomial:

$$\boldsymbol{x}_C\big|_{x(E_j)} \;\sim\; \text{Mult}[x(E_j),\, \boldsymbol{\theta}_j]\,,$$

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4. $x(E_j) \to \mu_j$: what needs to be shared is not the observed number $x(E_j)$, but rather the estimated true value μ_j: remember $x(E_j) \sim \text{Poisson}[\mu_j]$

$$\mu_j \sim \text{Gamma}[c_j + x(E_j), r_j + 1],$$

(Gamma is prior conjugate of Poisson)

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   BUT μ_i is real, while the the number of event parameter of a multinomial must be integer $\Rightarrow$ solved with interpolation

5. uncertainty on μ_i: taken into account by sampling

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- Empirical approach (with help of simulation):
  - 'True spectrum' recovered in a couple of steps
  - Then the solution starts to diverge towards a wildy oscillating spectrum (any unavoidable fluctuation is believed more and more. . .)
    $\Rightarrow$ find empirically an optimum

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  - intermediate smoothing $\Rightarrow$ we belief physics is 'smooth'
  - . . . but 'irregularities' of the data are not washed out

(⇒ unfolding Vs parametric inference)

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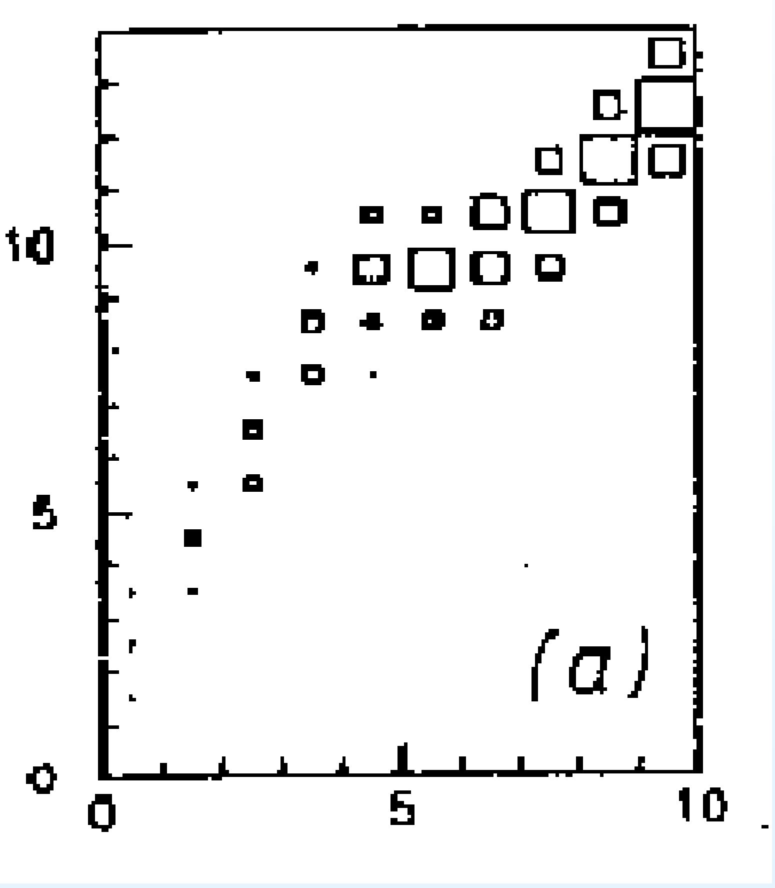
  $\Rightarrow$ Good compromize and good results

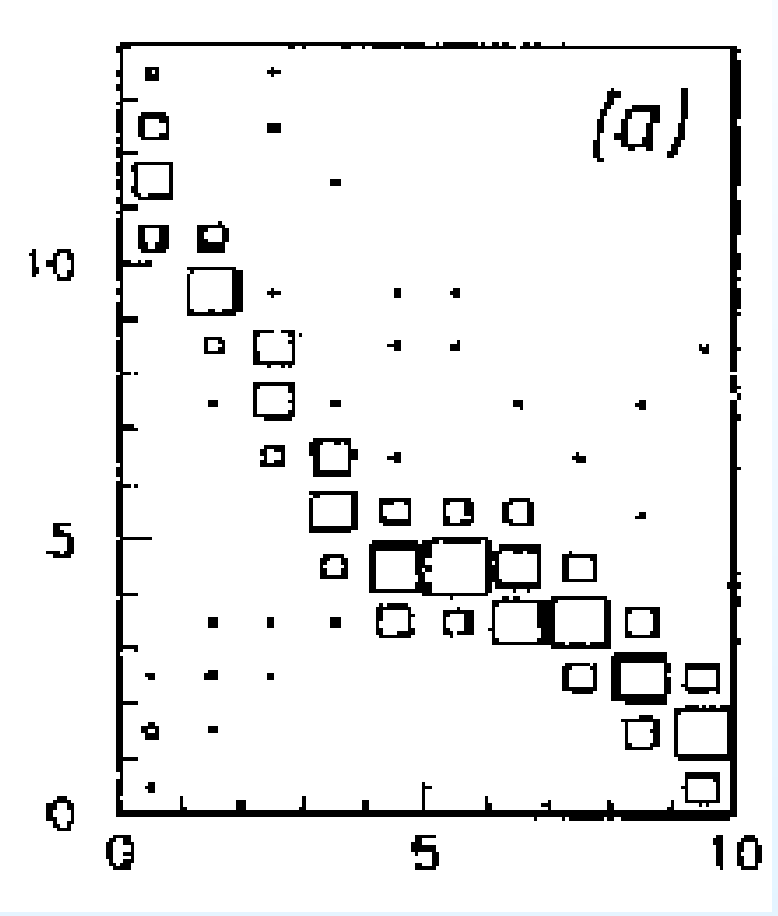
  $\Rightarrow$ Very 'Bayesian'

  $\Rightarrow$ No oscillations for $n_{steps} \to \infty$

Examples

smearing matrix (from 1995 NIM paper)





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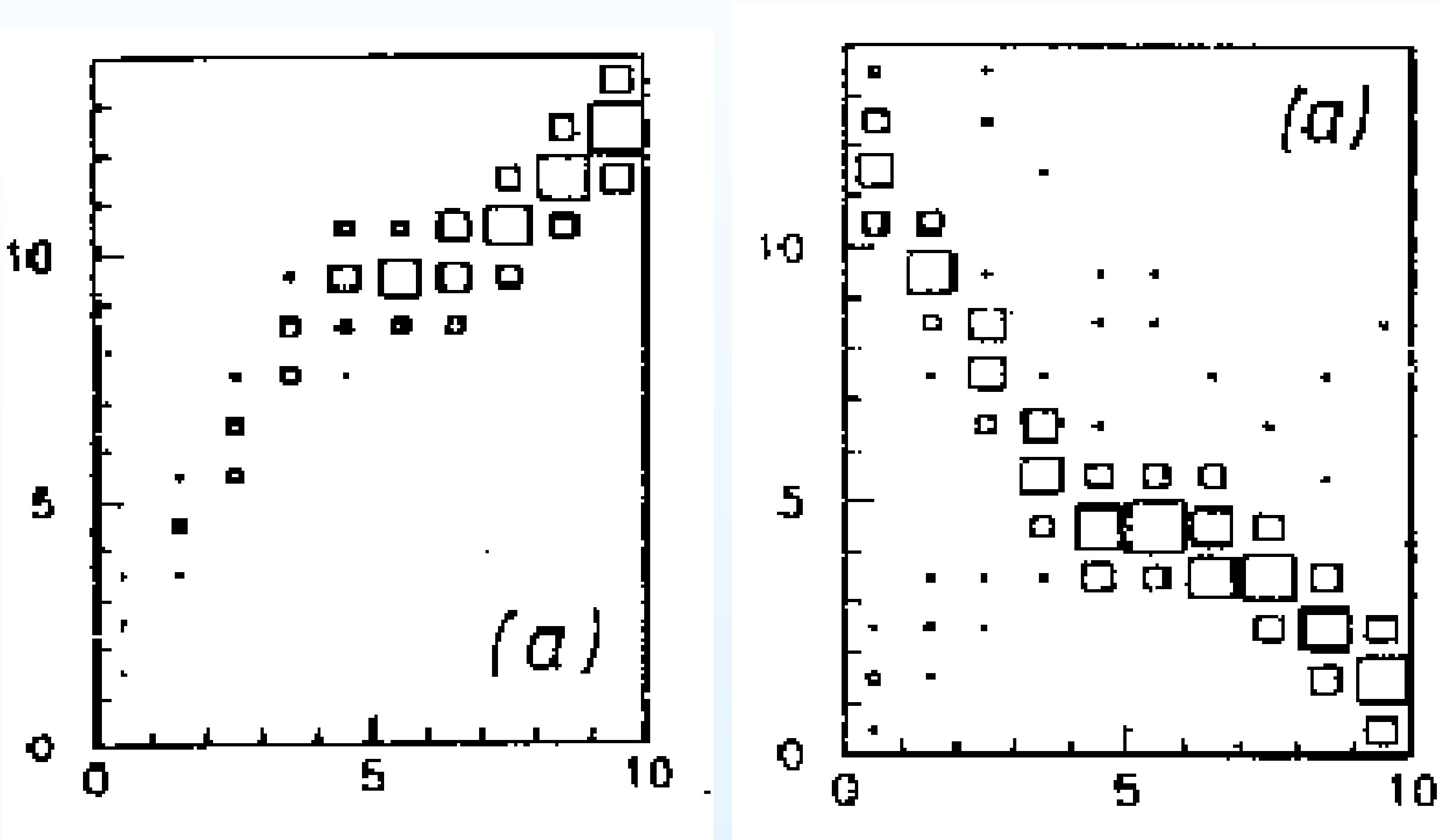

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$\Rightarrow$ watch DEMO

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- A probabilistic approach ('Bayesian') offers a consistent framework to handle consistently a large variaty of problem
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- **conclusions left to users**
  1. "non chiedere all'oste com'è il vino"...
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Extra references (including on yesterday comments) $\Longrightarrow$

References

['BR' stands for "GdA, Bayesian Reasoning in Data Analysis"]

- new unfolding: arXiv:1010.0632v1;
- for a multilevel introduction to probabilistic reasoning, including a short introduction to Bayesian networks: arXiv:1003.2086v2;
- ISO sources of uncertainties: BR, sec. 1.2;
- on uncertainties due to systematics: BR, secs. 6.8-6.10, 8.6-8.14, 12.2.2;
- 'asymmetric errors' and their potential dangers: physics/0403086;
- about the Gauss' derivation of the 'Gaussian': BR, 6.12; web site on "Fermi, Bayes and Gauss"
- box and ball 'game': AJP 67, issue 12 (1999) 1260-1268;

References

- upper/lower limits Vs sensitivity bounds: BR, secs. 13.16-13.18;
- fits from a Bayesian network perpective: physics/0511182;
- criticisms about 'tests': BR, 1.8;
- . . . but why "do they often work?": BR, 10.8;
- on the reason why 'standard' confidence intervals and confidence levels do not tell how much we are confident on something: BR, 1.7; arXiv:physics/0605140v2 (see also talk by A. Caldwell);
- on how to subtract the expected background in a probabilistics way: BR, 7.7.5;
- for a nice introduction to MCMC: C. Andrieu at al. "An introduction to MCMC for Machine Learning", downloadable pdf.