Improved (iterative) Bayesian unfolding

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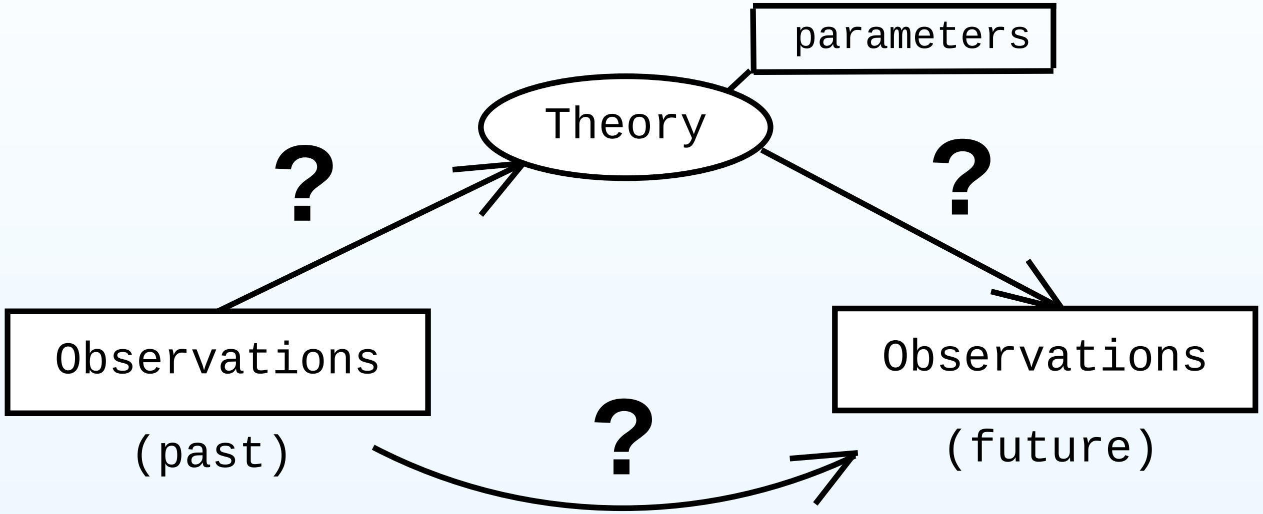
Outline

- 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
- 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)

    $\Rightarrow$ integrals over the weighted possibilities $\rightarrow$ MC
- Some examples on toy models

Learning from experience and source of uncertainty



Uncertainty:

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

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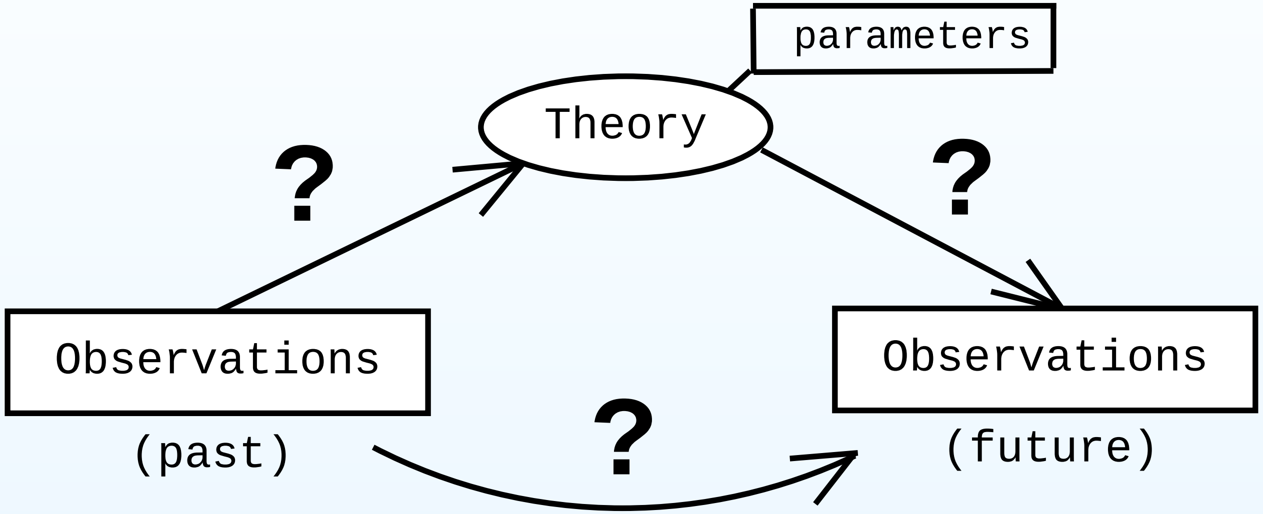


Uncertainty:

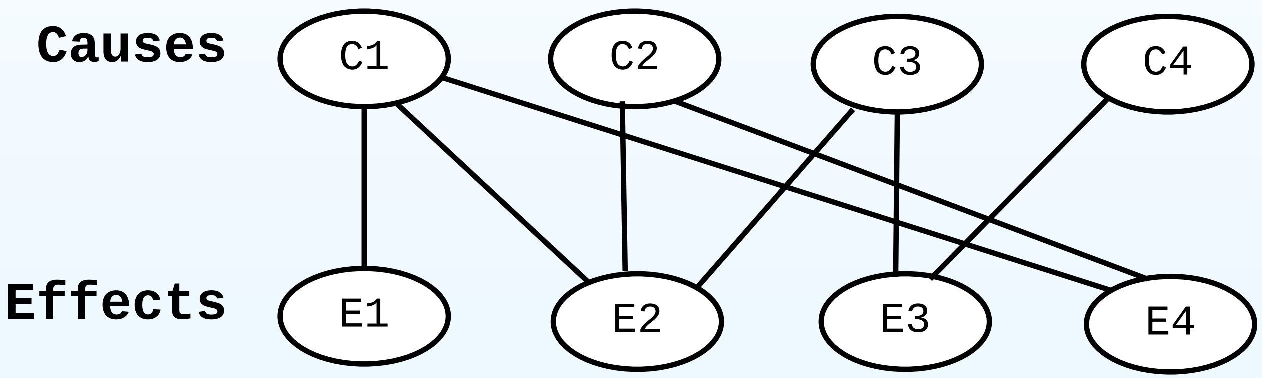
Theory	— ? ⟶		Future observations
Past observations	— ? ⟶		Theory
Theory	— ? ⟶		Future observations

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

CAUSE $\Longleftrightarrow$ EFFECT

Causes → 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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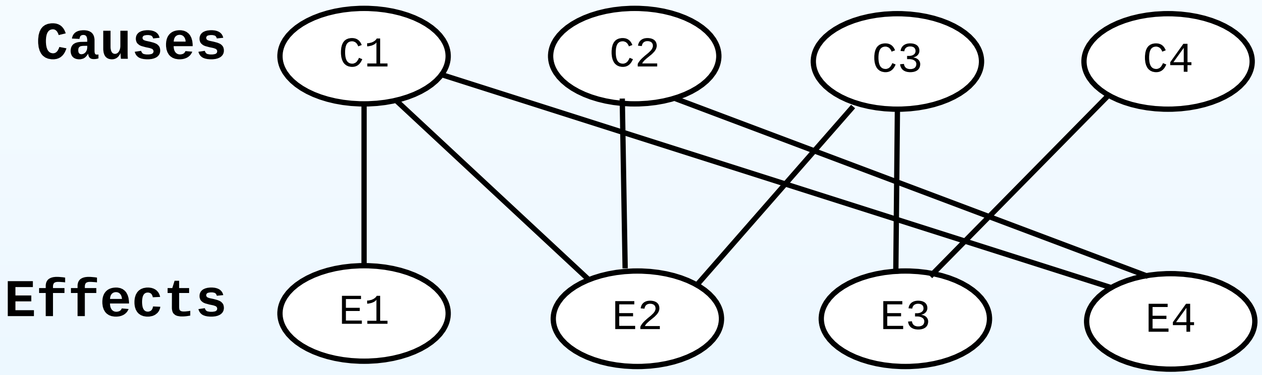

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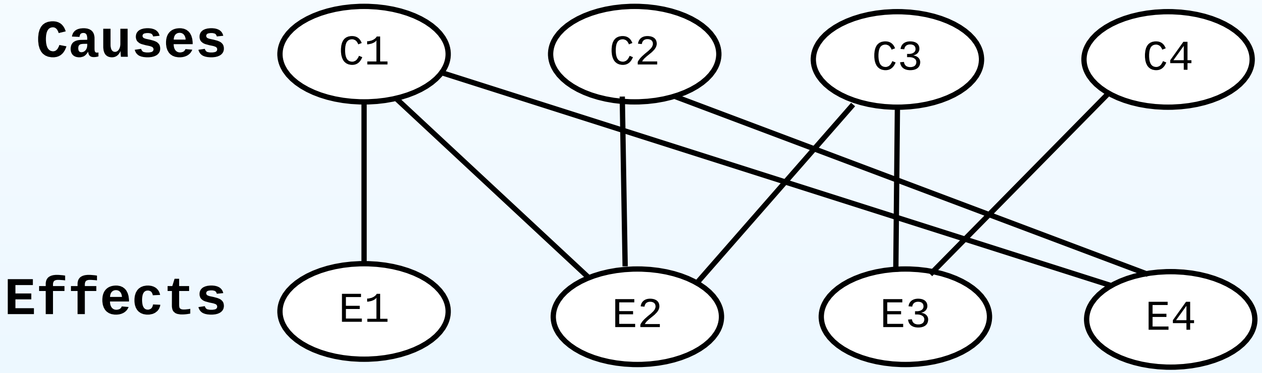

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$$\mathbf{E_2} \Rightarrow \{C_1,\, C_2,\, C_3\}?$$

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*)

Uncertainty and probability

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

- $P(-10 < \epsilon'/\epsilon \times 10^4 < 50) >> P(\epsilon'/\epsilon \times 10^4 > 100)$
- $P(170 \le m_{top}/\text{GeV} \le 180) \approx 70\%$
- $P(M_H < 200\,\text{GeV}) > P(M_H > 200\,\text{GeV})$

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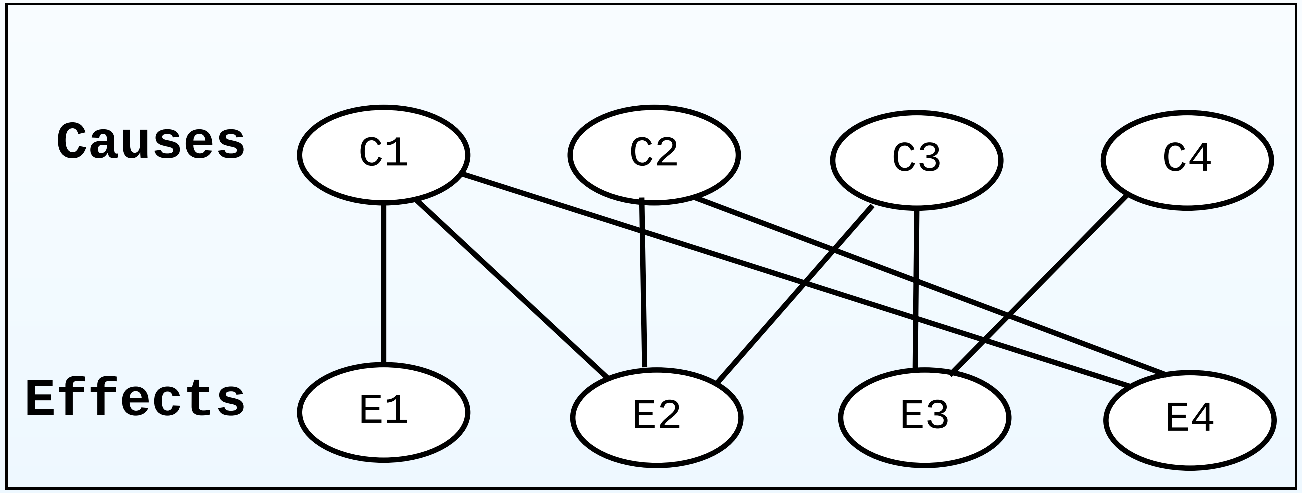
I stick to common sense (and physicists common sense) and assume that probabilities of causes, probabilities of of hypotheses, probabilities of the numerical values of physics quantities, etc. are sensible concepts that match the mind categories of human beings
(see D. Hume, C. Darwin + modern researches)

From causes to effects and back

Our original problem:



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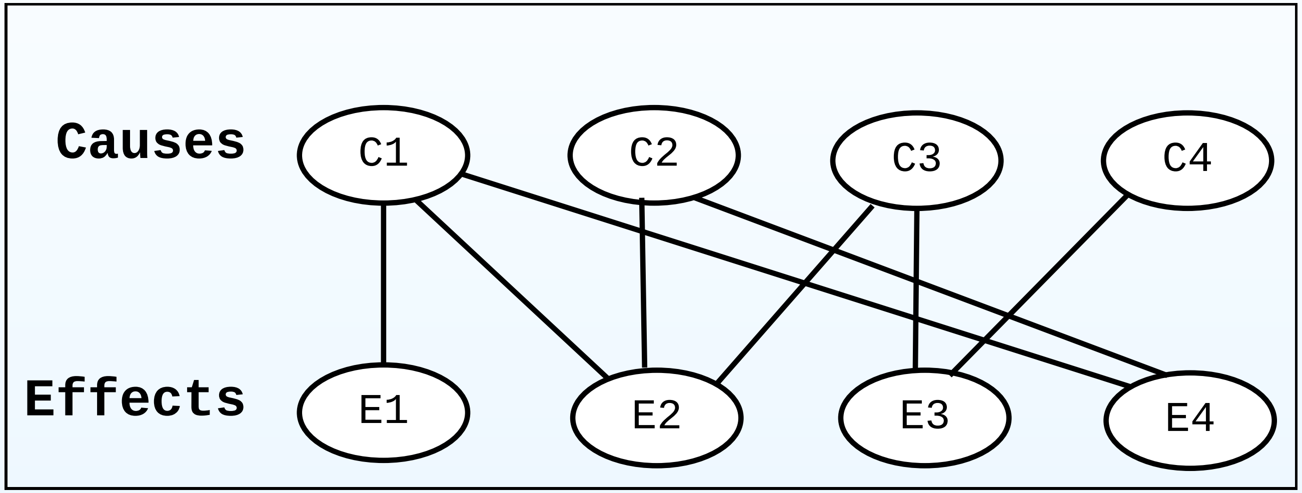

Our conditional view of probabilistic causation

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

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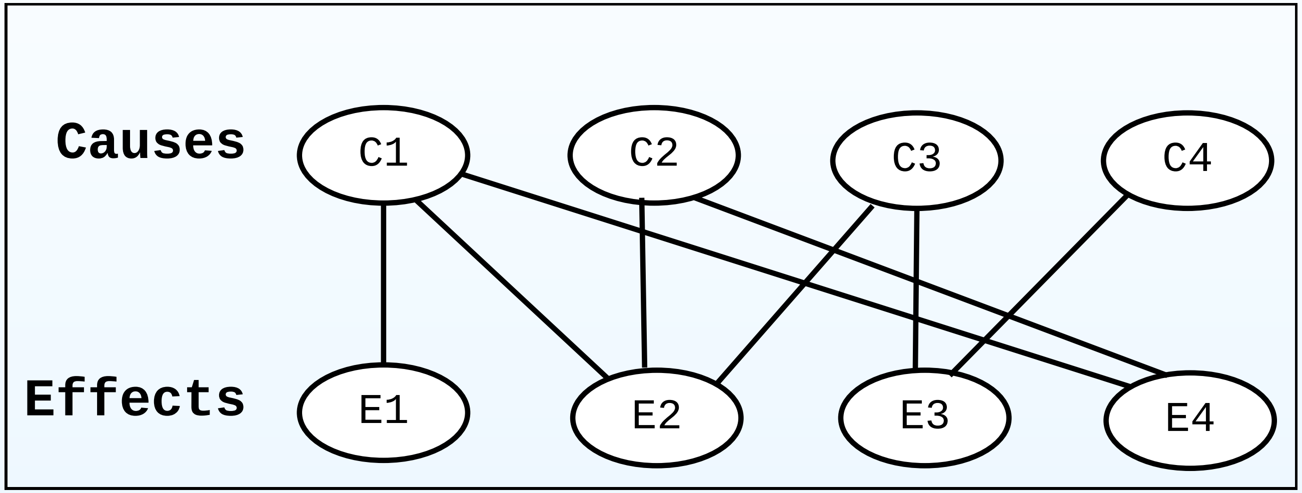

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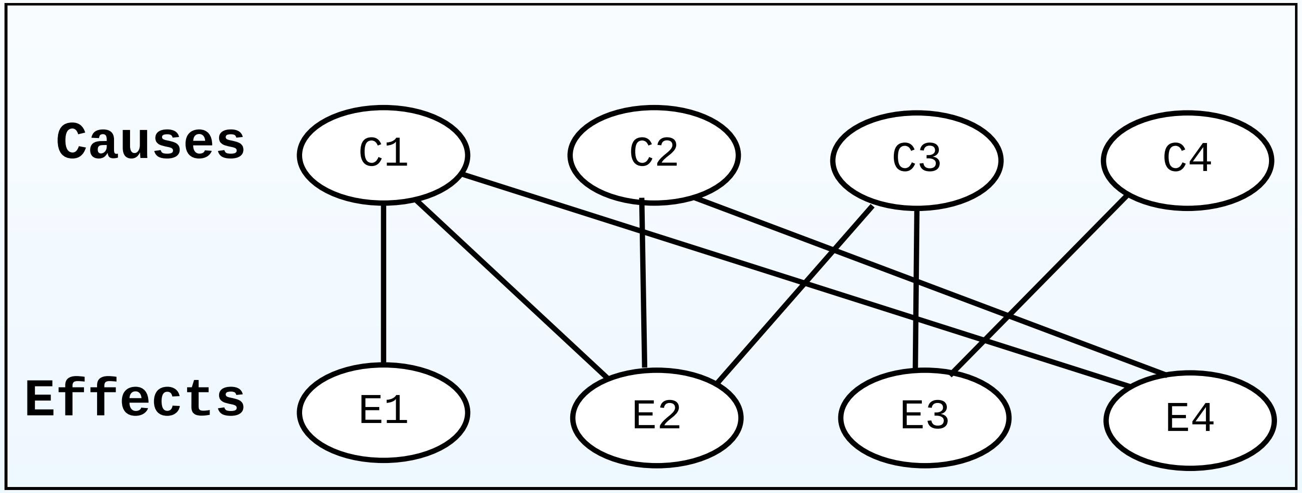

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The fourth basic rule of probability:

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

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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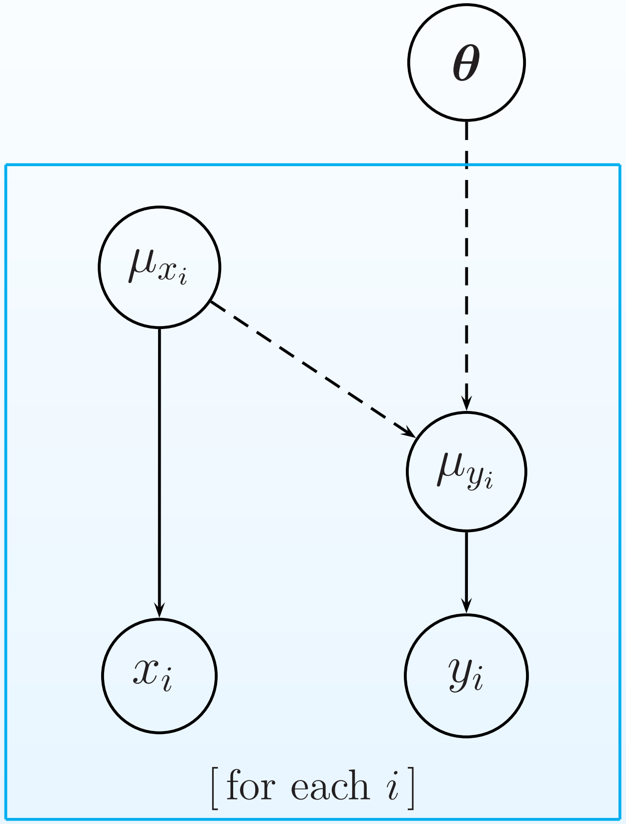
$\Rightarrow$ Bayes theorem

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

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

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BUT sometimes we wish to interpret the data as little as possible

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$\Rightarrow$ Unfolding (deconvolution)

Why unfolding?

Te idea is to provide somethimg similar to an experimental spectrum, with a minimal interpretation by the experimentalist, a part from correcting from distortions due to physics and detector effects (including background).

(The alternative would be to give a parametrized description of the true spectrum – a fit)

Smearing matrix $\longrightarrow$ unfolding matrix

Invert smearing matrix?

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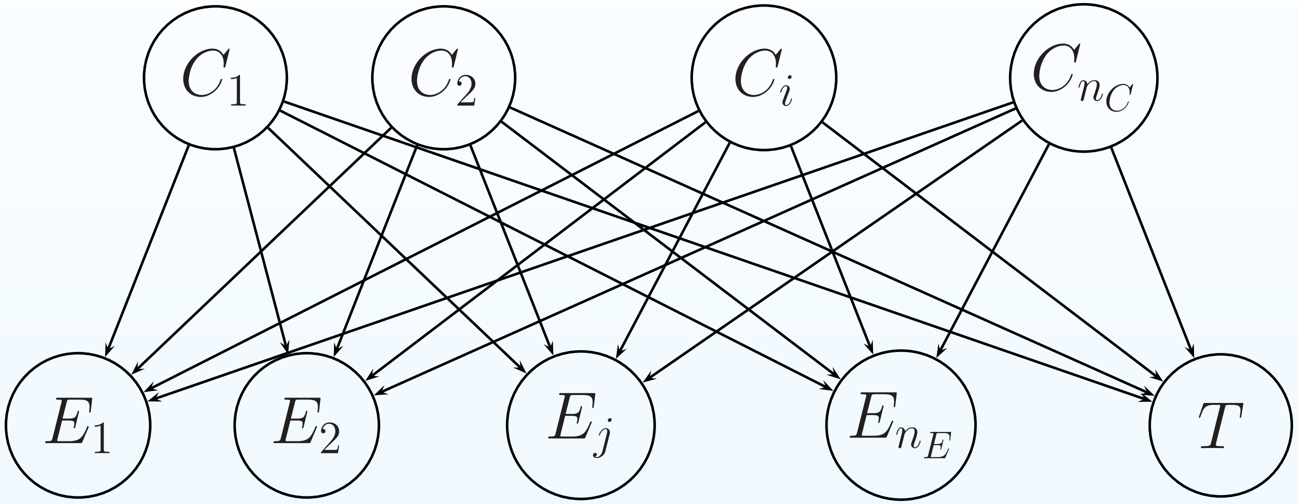
Indeed, matrix inversion is recognized to producing ‘crazy spectra’ and even negative values (unless such large numbers in bins such fluctuations around expectations are negligeable)

Discretized unfolding



(T: ‘trash’)

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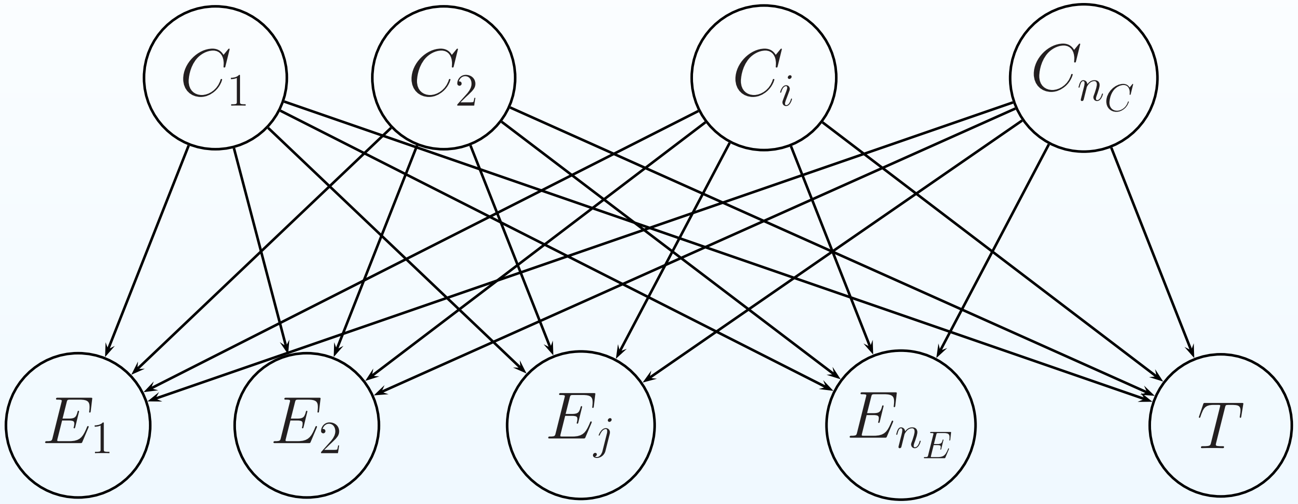

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$\boldsymbol{x}_C$ **:** *true spectrum* (nr of events in cause bins)

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

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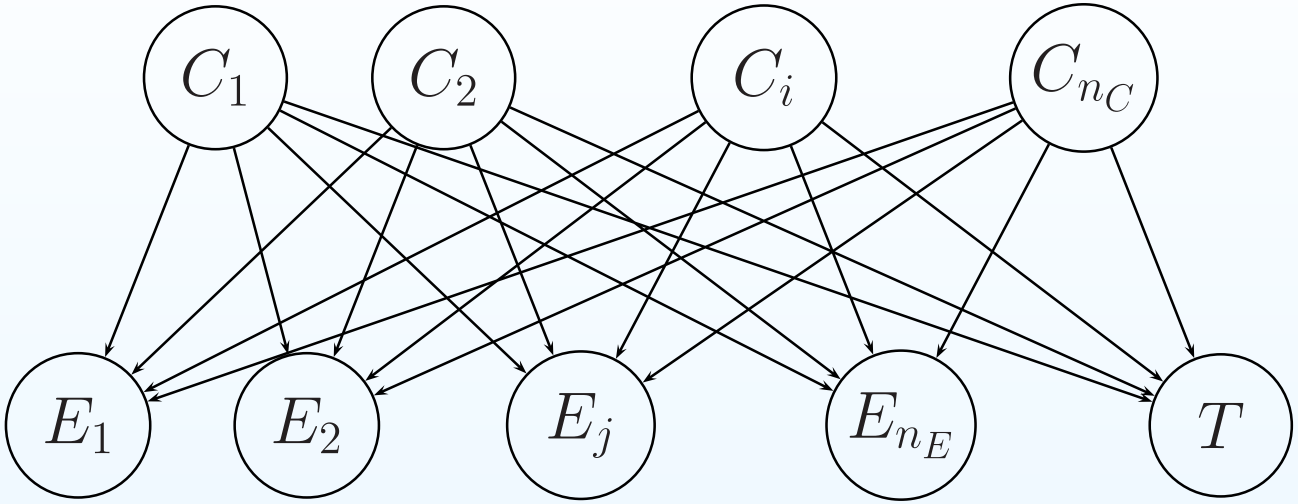

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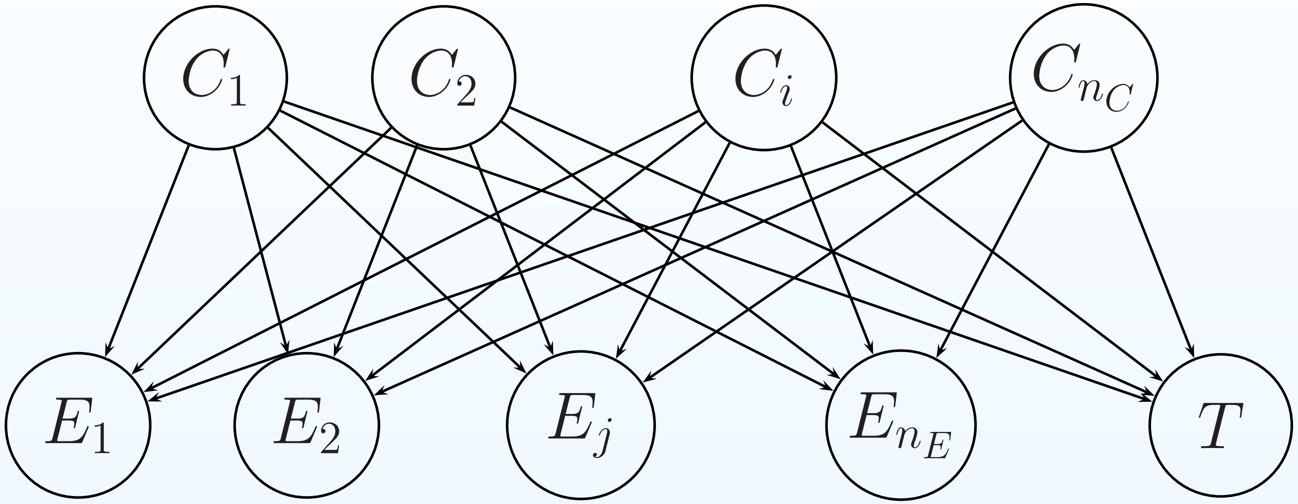
Our aim:

- **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, with $\lambda_{ji} \equiv P(E_j \,|\, C_i,\, I)$.

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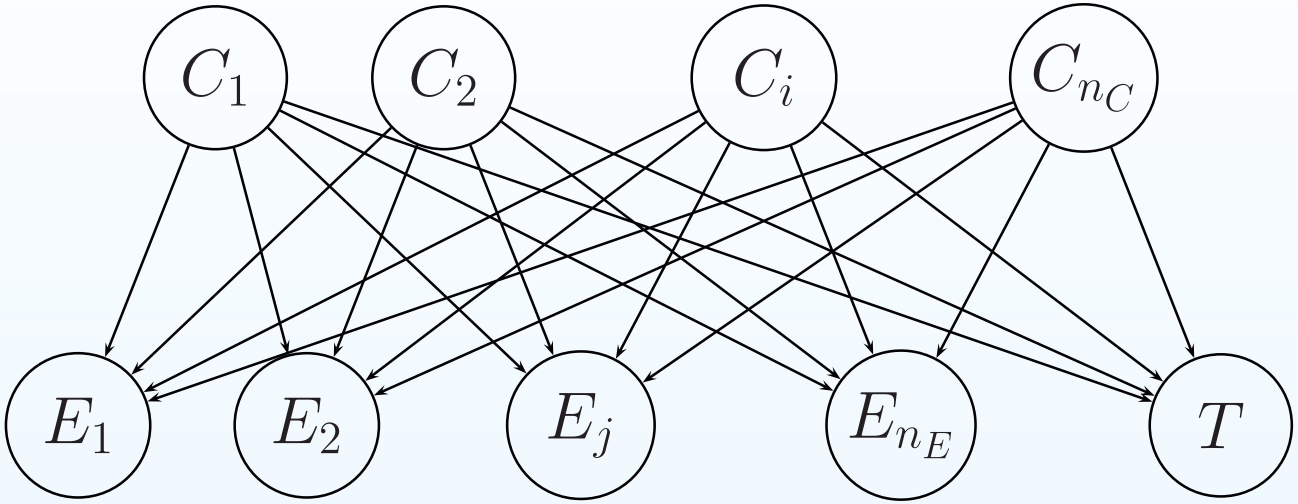

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$$\Rightarrow f(\Lambda \,|\, I)$$

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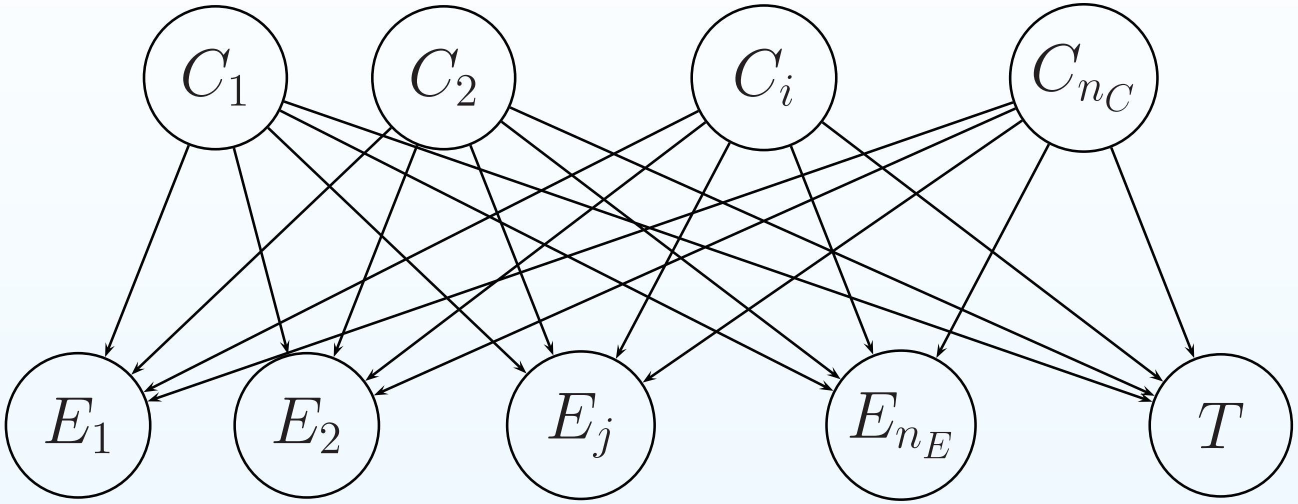

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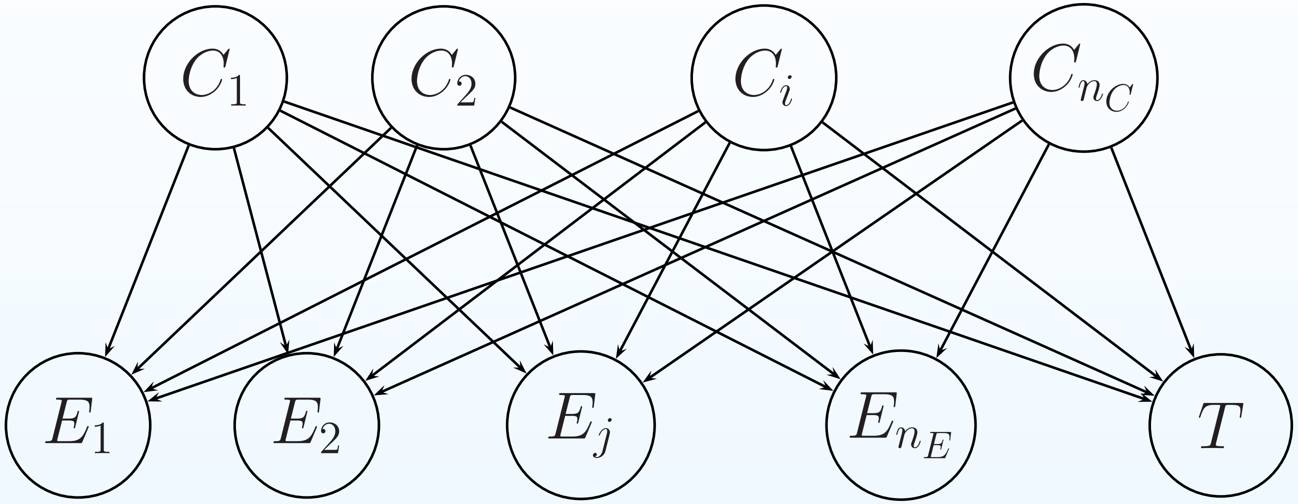
- for each possible Λ we have a pdf of spectra:
  $\rightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, \Lambda, I)$

Discretized unfolding



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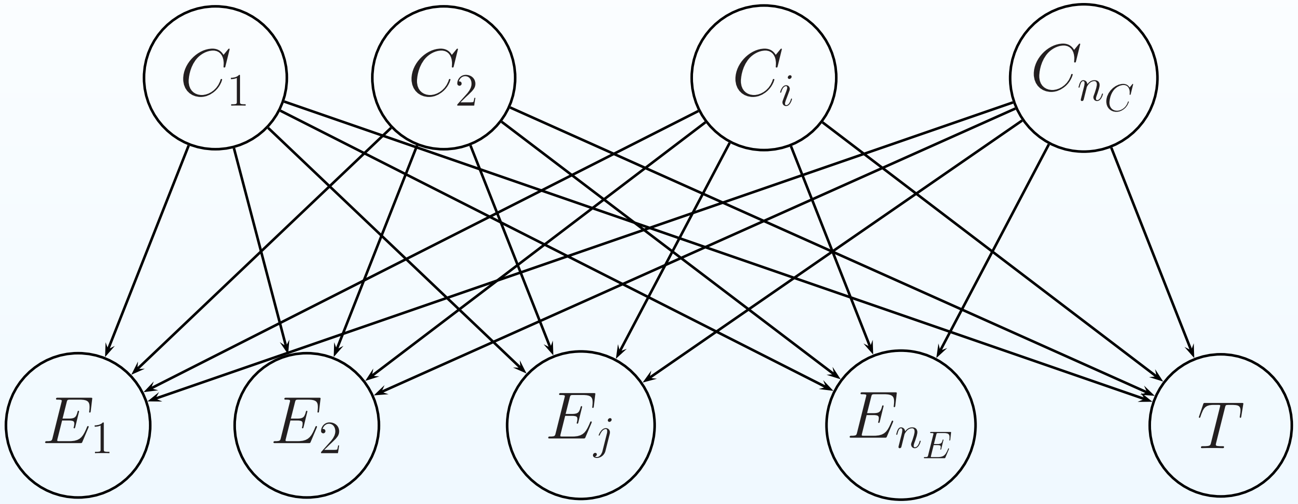
- for each possible Λ we have a pdf of spectra:
  $\longrightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, \Lambda, I)$
  $\Rightarrow P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, I) = \int P(\boldsymbol{x}_C \,|\, \boldsymbol{x}_E, \Lambda,\, I)\, f(\Lambda \,|\, I)\, \mathrm{d}\Lambda$ [by MC!]

Discretized unfolding



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- 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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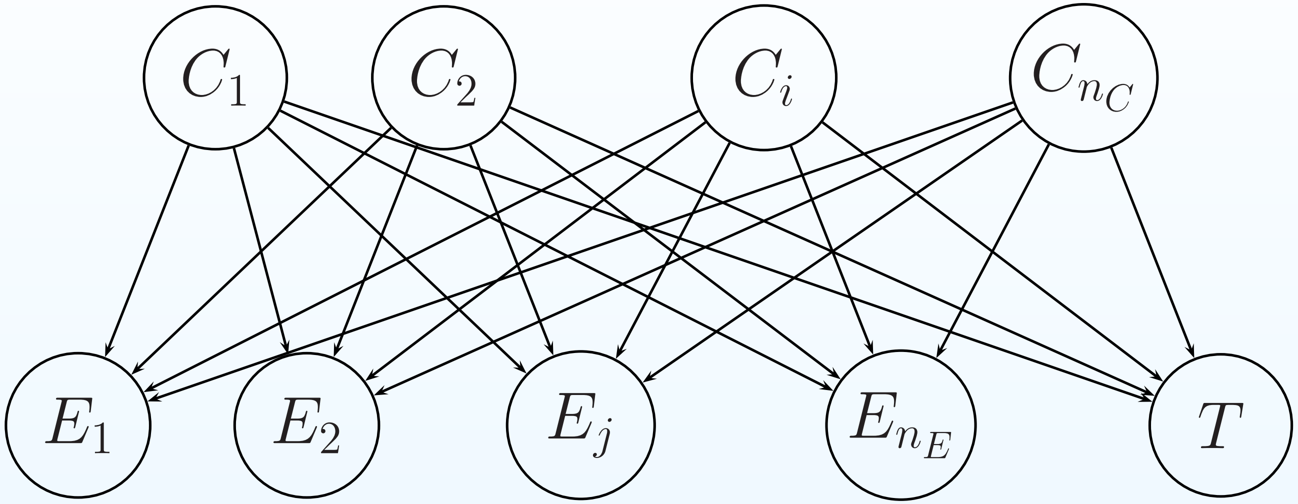

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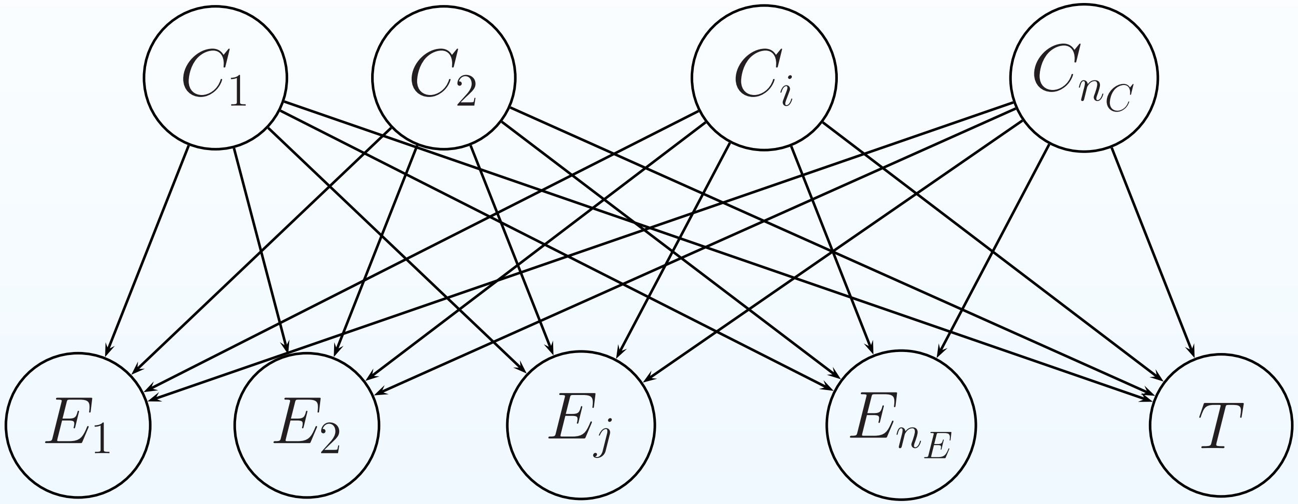
- Indifference w.r.t. all possible spectra

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

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



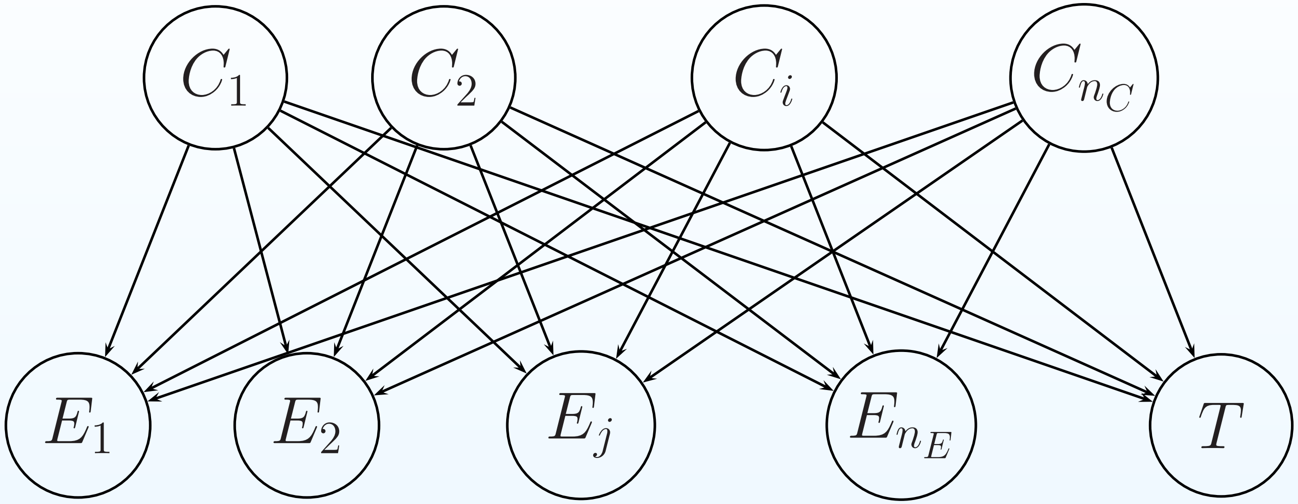
Given a certain number of events in a cause-bin $x(C_i)$, the number of events in the effect-bins, included the 'trash' one, is described by a multinomial distribution:

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

with

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

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



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

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

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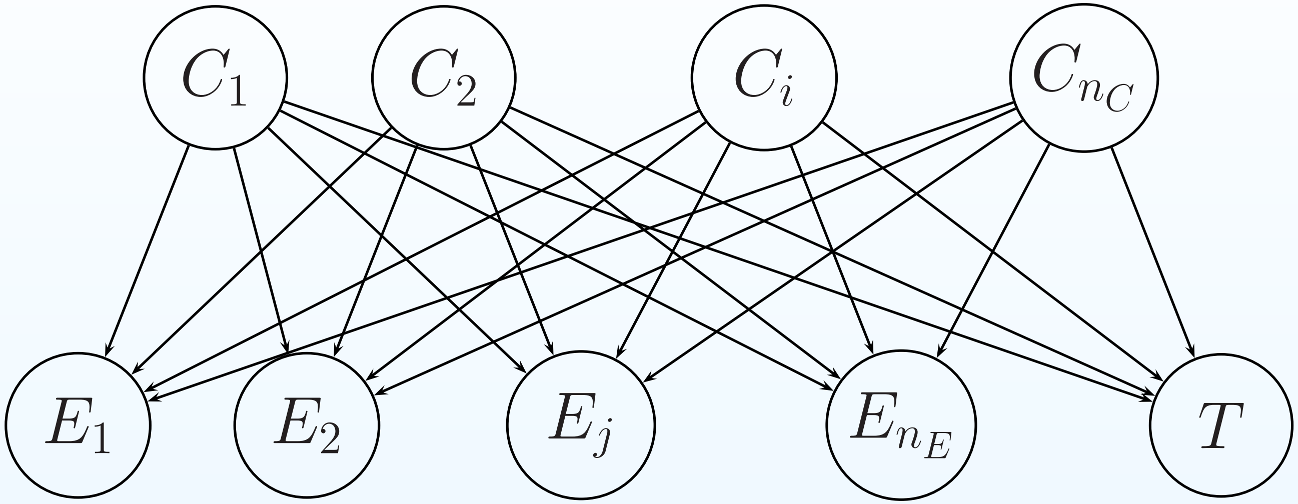

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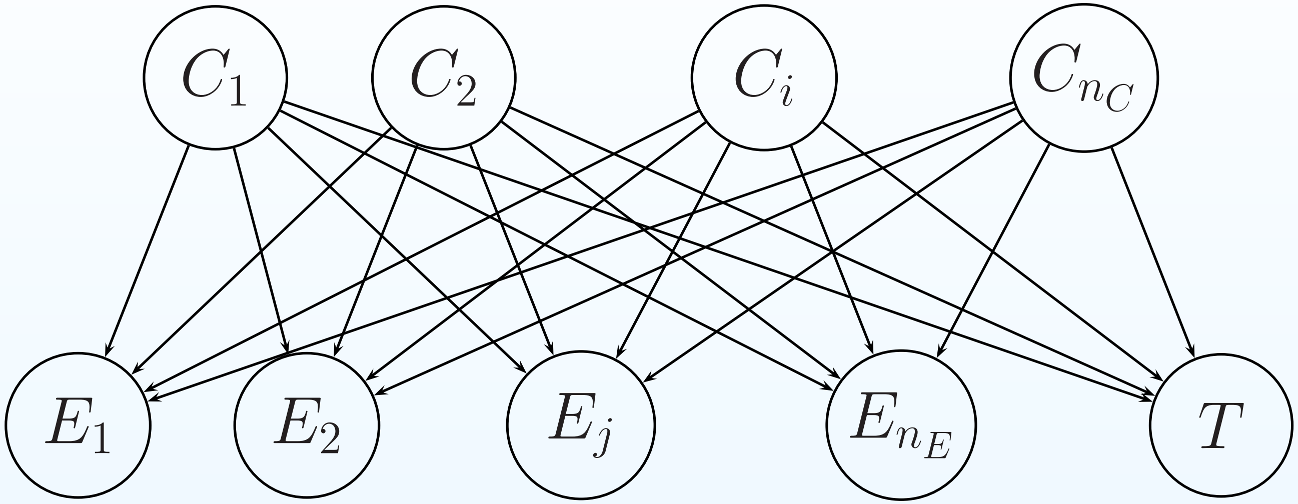

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$\Rightarrow$ STUCK!

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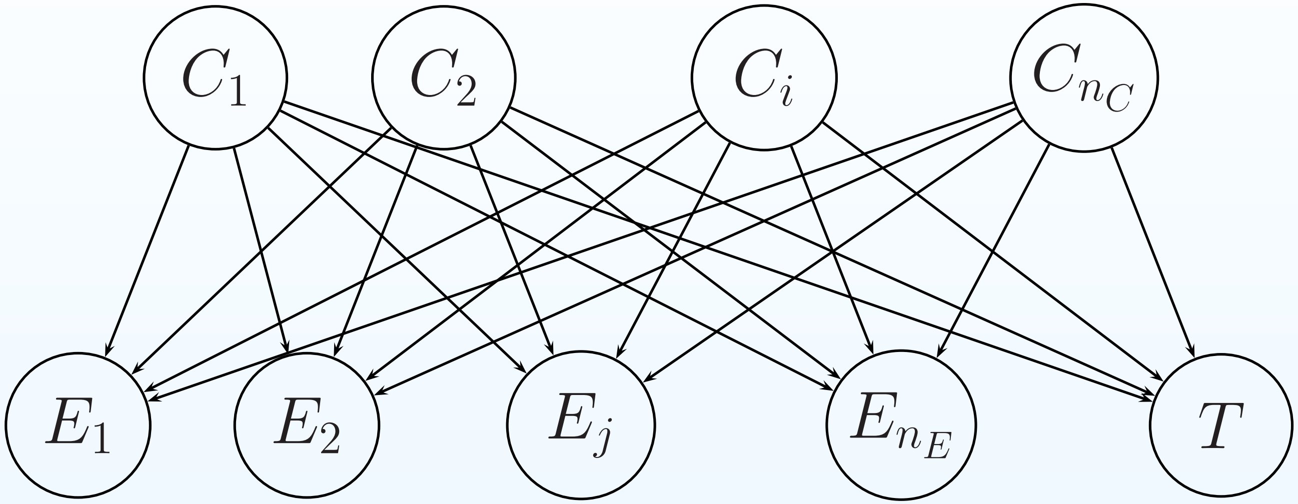

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$\Rightarrow$ STUCK!

$\Rightarrow$ Change strategy

The rescue trick

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

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

we restart from

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

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Consequences:

1. the sharing of observed events among the cause bins needs to be performed 'by hand';

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1. the sharing of observed events among the cause bins needs to be performed 'by hand';
2. a uniform prior $P(C_i \,|\, I) = k$ does not mean indifference over all possible spectra.

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

   ⇒ VERY STRONG prior that biases the result!

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

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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. [$\ast$] Assignement of events to cause bins:

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

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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:

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

(The Dirichlet is the prior conjugate of the Multinomial)

Improvements

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

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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4. $x(E_j) \rightarrow \mu_j$: 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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4. $x(E_j) \to \mu_j$:

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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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we are using a particular (flat) spectrum as prior

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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

($\Rightarrow$ unfolding Vs parametric inference)

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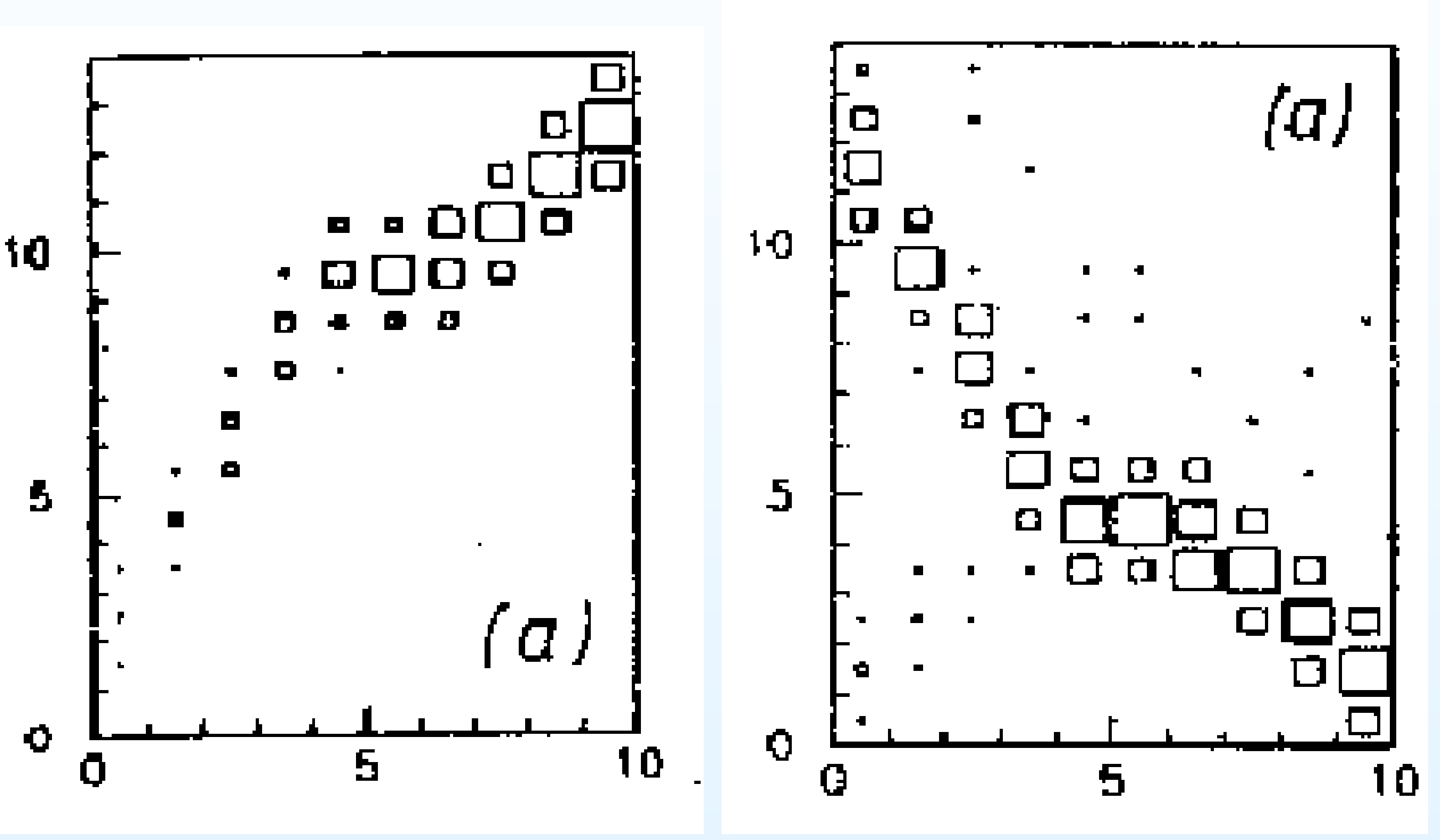
  $\Rightarrow$ Good compromize and good results

  $\Rightarrow$ Very 'Bayesian'

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

Examples

smearing matrix (from 1995 NIM paper)



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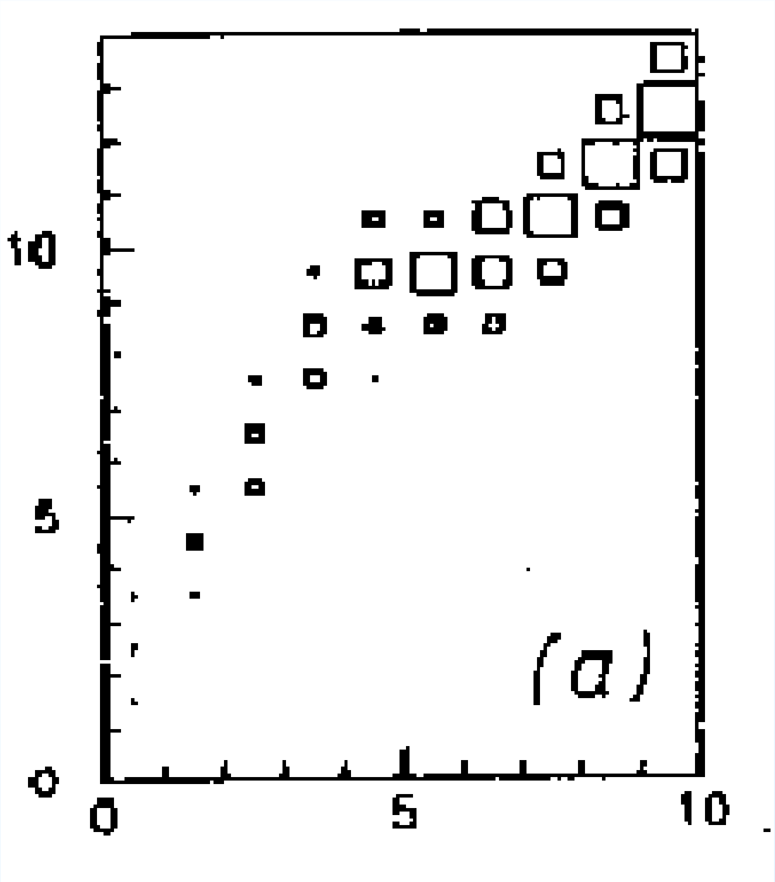

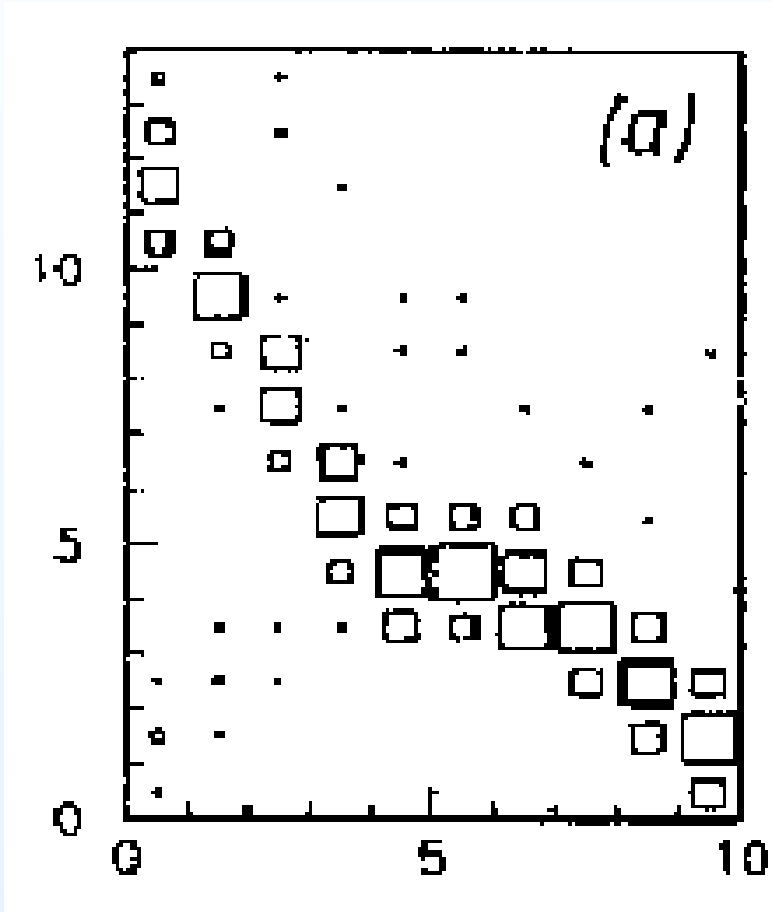

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$\Rightarrow$ watch DEMO

Conclusions

- left to users
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$\longrightarrow$ Some notes follow $\Longrightarrow$

Notes added

1. “iterative” put within parentheses in title
   (motivated by Zech’ classification of methods)
   (a) the spirit of the method is Bayesian
   (b) the iteration issue is secondary

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2. An interesting book:
   (thanks to Blobel)
   - J. Kaipio and E. Somersalo
     Statistical and Computational Inverse Problems
     Springer, 2004

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2. An interesting book:
3. Uncertainty due the possible choice among several smearing models, Λ_1, Λ_2, etc.
   (triggered by Marisa Sandhoff's talk)
   - the $\boldsymbol{\theta}_i$ sampling can be done at random form either matrix,
     with weights depending on our beliefs in the different unfolding models
     (obviously not yet implemented in the R code, and I am not sure I will do it, but it can be implemented in C/C++ versions)

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   “...it gives the best results (in terms of its ability to reproduce the true distribution) if one make a realistic guess about the distribution that the true values follow...
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$\Rightarrow$ just a honest statement: what is wrong with it?

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Buon divertimento!