

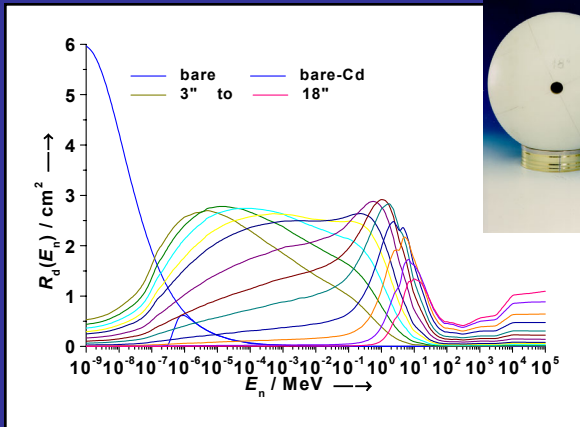
Unfolding techniques for neutron spectrometry

Marcel Reginatto
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Contents of the talk

- Bonner sphere spectrometry
- How “strong” is the data?
- How should we formulate the problem?
- Maximum entropy unfolding
- Bayesian parameter estimation
- Some concluding remarks

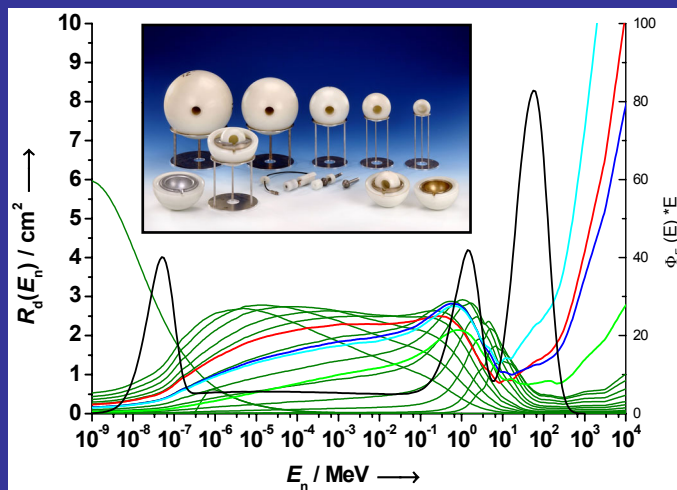
Bonner sphere spectrometer



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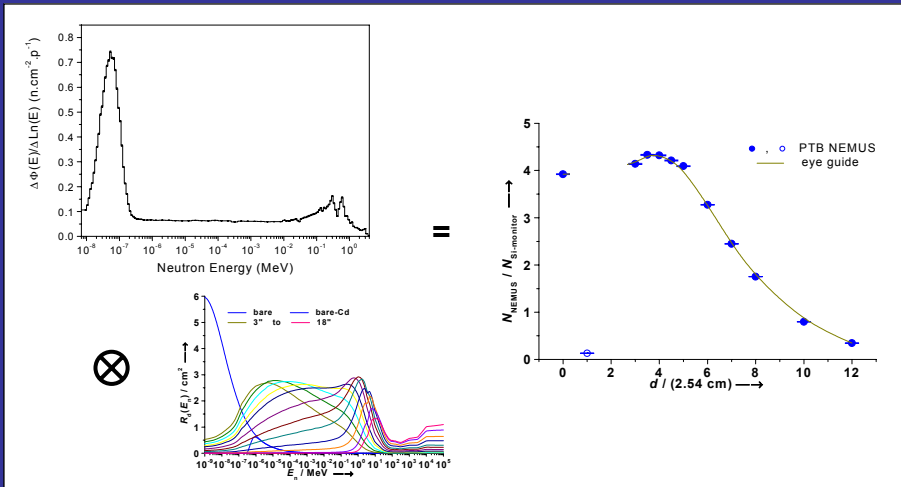
Extended range Bonner sphere spectrometer



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Bonner sphere measurements



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Different mathematical spaces!

Space of all possible spectra

$$\{ \Phi(E) \}$$

Space of measurements

$$\{ R_k(E) \}$$

$$\{ N_k, \sigma_k \}$$

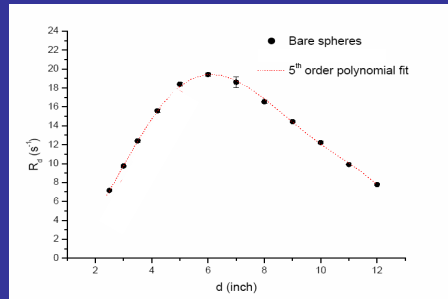


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Number of good data points (I)

Look at a plot of measured data versus sphere diameter



Number of "good" data points

~ number of points needed to define the smooth fit



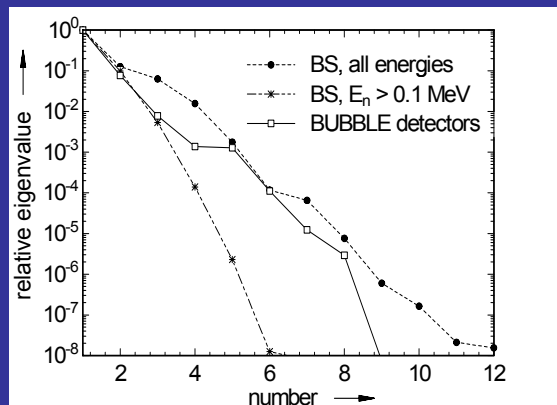
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Number of good data points (II)

Do a singular value decomposition (SVD) of the response matrix

Look at the number of "large" eigenvalues (say, within 1% of the largest eigenvalue)



M. Matzke, Radiat. Prot. Dosim. 107, 155-174, 2003



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The golden rule

“Lost information can never be retrieved; it can only be replaced by hypotheses”

D. Taubin, in “probabilities, data reduction and error analysis in the physical sciences”

Where can we get our hypotheses from?

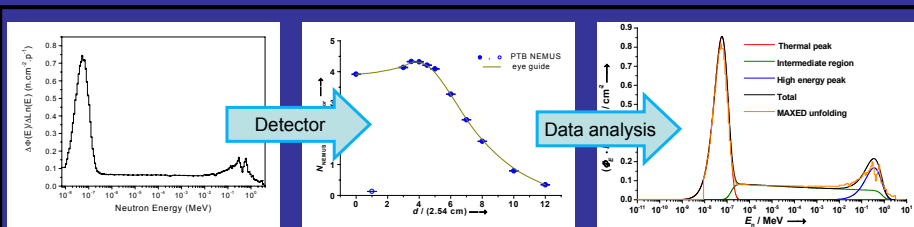
- Specific features of the experiment
- Physical principles that apply to the particles being measured
- General principles from probability theory and information theory



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Another view of a measurement



measurement:

spectrum *detector* measurement *data analysis* spectrum

communication system (Shannon, 1948):

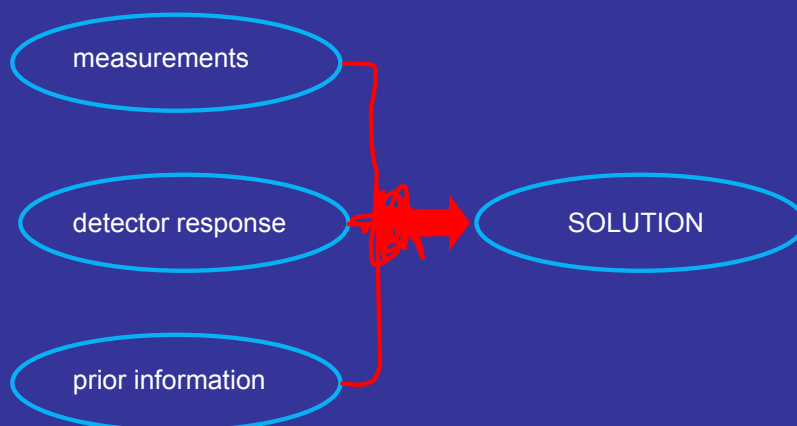
message *transmitter* (noisy) signal *receiver* message



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A recipe for unfolding



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Why is this problem difficult?

Some mathematical difficulties: non-uniqueness, stability of solutions, incorporation of prior information, computational problems, etc.

Problems are mostly *conceptual* in nature, not mathematical: unfolding is a problem of inference – it has to be formulated correctly!

Many different approaches are possible: the choice of unfolding method must be determined by the particular question that one wants to answer



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Many (too many!) unfolding methods

“Direct inversion”

- Matrix inversion
- Fourier transform methods
- Derivative methods

Regularization

- Linear regularization (Phillips-, Twomey-, Tikhonov-, Miller-, ...)

Iterative methods

- SAND-II (GRAVEL)
- Gold (BON)
- Doroshenko (SPUNIT)

Least-squares

- Linear least-squares

Maximum entropy

Parameter estimation

- Expansion in basis functions
- Bayesian methods

“Stochastic” methods

- Monte Carlo methods
- Genetic algorithms
- Neural networks



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Maximum entropy principle (MaxEnt)

Start with your best estimate of the spectrum, $\Phi^{DEF}(E)$

From all the spectra that fit the data, choose as solution spectrum $\Phi(E)$ the one that is “closest” to $\Phi^{DEF}(E)$

“Closest” means: the spectrum $\Phi(E)$ that maximizes the relative entropy,

$$S = - \int \left\{ \Phi(E) \ln \left(\frac{\Phi(E)}{\Phi^{DEF}(E)} \right) + \Phi^{DEF}(E) - \Phi(E) \right\} dE$$



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Relative entropy

The relative entropy is a fundamental concept in information theory and probability theory

It also known (to within a plus or minus sign) as Cross-entropy, Entropy, Entropy distance, Direct divergence, Expected weight of evidence, Kullback-Leibler distance, Kullback number, Discrimination information, Renyi's principle...



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Why use maximum entropy?

According to E. T. Jaynes:

Because it makes sense: of all the spectra that fit the data, you choose the one that is closest to your initial estimate

According to Shore and Johnson:

Because it is the only general method of inference that does not lead to inconsistencies



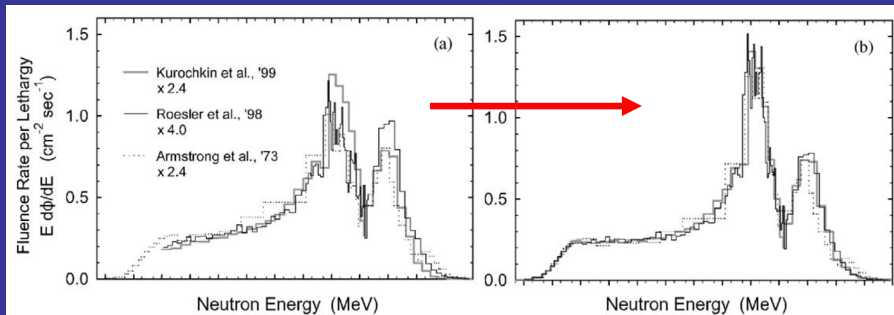
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Example of MaxEnt unfolding

Initial estimates

MAXED unfoldings



Goldhagen et al., Nuclear Instruments and Methods A 476, 42-51 (2002)



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Some properties of MaxEnt solutions

The solution spectrum can be written in closed form:

$$\Phi_i = \Phi_i^{DEF} \exp\left\{-\sum_k \lambda_k R_{ki}\right\}$$

→ standard sensitivity analysis, uncertainty propagation

Prior information is taken seriously!

For small adjustments, $\Phi(E)$ is linear in the responses:

$$\Phi_i = \Phi_i^{DEF} \exp\left\{-\sum_k \lambda_k R_{ki}\right\} \approx \Phi_i^{DEF} \left[1 - \sum_k \lambda_k R_{ki}\right]$$



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Bayesian parameter estimation

Thermal region:

- Magnitude

Intermediate region:

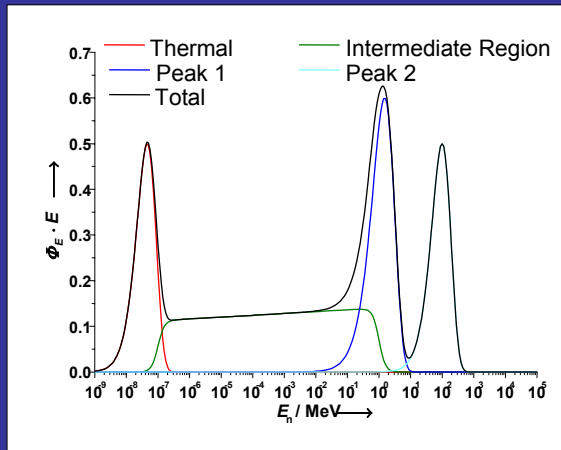
- Slope
- Magnitude

Peak 1

- Energy of the peak
- Magnitude
- Form / Width

Peak 2

- Energy of the peak
- Magnitude
- Form / Width



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What is a Bayesian approach?

An application of the rules of probability theory

The approach is conceptually clear

It is usually easier to set up a problem and solve it

Flexible approach

All uncertainties are described by probability distributions

All calculations are done in the space of parameters, not in the space of data

Bayesian and “orthodox” methods calculate different things



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We need only a few basic rules...

1. The sum rule:

$$P(A|I) + P(\bar{A}|I) = 1$$

2. The product rule:

$$P(A, B|I) = P(A|B, I)P(B|I)$$

3. Marginalization:

$$P(A|I) = \int dB P(A, B|I)$$

4. **Bayes' theorem:**

$$P(\text{hypothesis} | \text{data}, I) \\ \propto P(\text{data} | \text{hypothesis}, I) P(\text{hypothesis} | I)$$



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Software for Bayesian parameter estimation

WinBUGS: From MRC Biostatistics Unit in Cambridge and the Department of Epidemiology and Public Health of Imperial College at St Mary's, London.

Software for the Bayesian analysis of complex statistical models using Markov chain Monte Carlo (MCMC) methods (BUGS = Bayesian inference Using Gibbs Sampling)

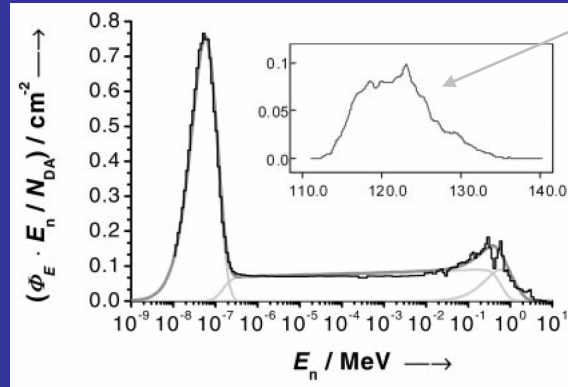
- Nice features:
 - Just download it from the internet
 - Excellent documentation with many examples
 - Programming language is fairly easy to learn



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Example of Bayesian parameter estimation



Posterior probability of the ambient dose equivalent

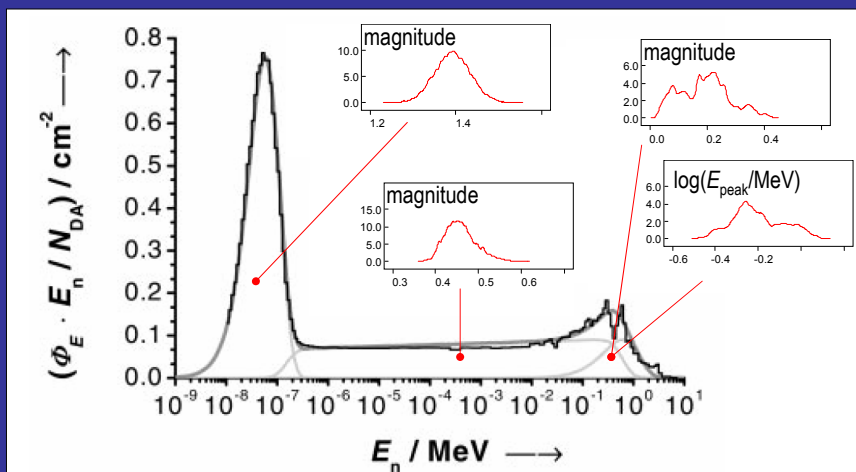
M. Reginatto, Radiat. Prot. Dosim. 121, 64-69, 2006



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Posterior probabilities of some parameters



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Some advantages of a Bayesian approach

The rules are clear and consistent (i.e., probability theory), and setting up problems is conceptually simple

Analysis leads to posterior probabilities for the parameters

- Uncertainties (also for derived quantities) are estimated directly from the posterior probabilities
- “Nuisance parameters” are easy to handle
- Calculations are done in parameter space, not in data space



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Summary: analysis of Bonner sphere data

We are dealing with a highly undetermined system:

Typically ~10 spheres only...

...but spectrum from thermal to a few tens or hundreds of MeV

We need to introduce prior information to restrict to physically meaningful solutions:

- Choose an initial estimate of spectrum (from Monte Carlo simulations, using physical principles, etc.)
 - Analyze the data using maximum entropy unfolding
- or
- Introduce a parametrized spectrum that is reasonably good
 - Analyze the data using Bayesian parameter estimation



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Thank you for your attention!



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