Bayesian analysis in nuclear physics

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Tutorials presented at LANSCE
Los Alamos Neutron Scattering Center
July 25 – August 1, 2005

Los Alamos
NATIONAL LABORATORY

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http://www.lanl.gov/home/kmh/

LA-UR-05-5680

Goals of tutorials

My aim is to

- present overview of Bayesian and probabilistic modeling
- cover basic Bayesian methodology relevant to nuclear physics, especially cross section evaluation
- point way to how to do it

- convince you that
  - Bayesian analysis is a reasonable approach to coping with measurement uncertainty

- Many thanks to my T-16 colleagues
  - Gerry Hale, Toshihiko Kawano, Patrick Talou

Outline – three tutorials

1. **Bayesian approach**
   - probability – quantifies our degree of uncertainty
   - Bayes law and prior probabilities
2. **Bayesian modeling**
   - Peelle's pertinent puzzle
   - Monte Carlo techniques; quasi-Monte Carlo
   - Bayesian update of cross sections using Jezebel criticality expt.
3. **Bayesian data analysis**
   - linear fits to data with Bayesian interpretation
   - uncertainty in experimental measurements; systematic errors
   - treatment of outliers, discrepant data
4. **Bayesian calculations**
   - Markov chain Monte Carlo technique
   - analysis of Rossi traces; alpha curve
   - background estimation in spectral data

Slides and bibliography

- These slides can be obtained by going to my public web page:
  http://public.lanl.gov/kmh/talks/
  - link to **tutorial slides**
  - short **bibliography** relevant to topics covered in tutorial
  - other presentations, which contain more detail about material presented here
- Noteworthy books:
  - D. Sivia, *Data Analysis: A Bayesian Tutorial* (1996); lucid pedagogical development of the Bayesian approach with an experimental physics slant
  - D. L. Smith, *Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology* (1991); lots of good advice relevant to cross-section evaluation
  - G. D'Agostini, *Bayesian Reasoning in Data Analysis: A Critical Review*, (World Scientific, New Jersey, 2003); Bayesian philosophy
  - A. Gelman et al., *Bayesian Data Analysis* (1995); statisticians' view
  - W. R. Gilks et al., *Markov Chain Monte Carlo in Practice* (1996); basic MCMC text

Tutorial 2
Bayesian modeling

Peelle's Pertinent Puzzle (1987)

Overview:

- Paradoxical result produced by strong correlations in uncertainties
- Probabilistic view of PPP
- Specific probabilistic model for PPP elucidates how correlations in uncertainties arise
- Plausible experimental situation consistent with PPP result
- Bayesian approach to coping with uncertainty in model
- With probabilistic modeling, you can go beyond simple linear, additive models
- PPP underlines the need to specify **how** uncertainties contribute to reported data

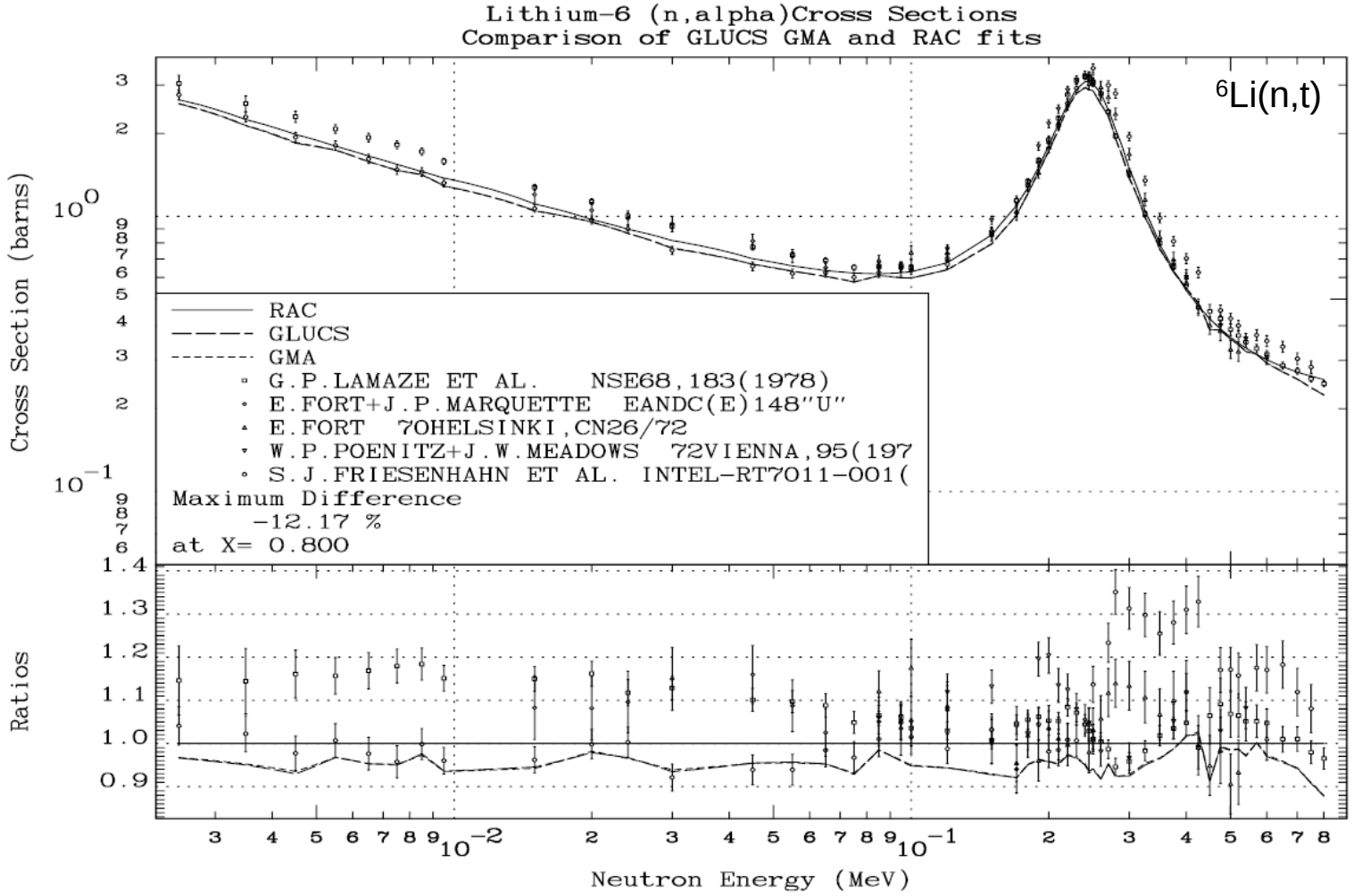
Peelle's pertinent puzzle

- Robert Peelle (ORNL) posed the PPP in 1987:
  Given two measurements of same quantity x:
  $m_1 = 1.5$; $m_2 = 1.0$,
  each with independent standard error of 10% ,
  and fully correlated standard error of 20% .
  Weighted average using least-squares is $x = 0.88 \pm 0.22$

- Peelle asks "under what conditions is this result reasonable?"
- By extension, if this not reasonable, what answer is appropriate?
- PPP is pertinent – its effect has been observed in nuclear data evaluation for decades
- Comment – PPP description of errors is ambiguous, which leads to numerous plausible interpretations

PPP in cross-section evaluation

- Although the PPP problem may seem academic, it has significant real-world consequences in cross-section evaluation
  - historically, fits to several data sets fall below lowest measurements



from Pronyaev, *INDC(NDS)*-438, p. 163 (2003)

note large data discrepancies

Standard solution to PPP

- The solution given in PPP is based on standard matrix equations for least-squares result:

  estimated value $\boldsymbol{x} = (\boldsymbol{G}^T\boldsymbol{C}^{-1}\boldsymbol{G})^{-1}\boldsymbol{G}^T\boldsymbol{C}^{-1}\boldsymbol{m}$

  covariance in estimate $\boldsymbol{V} = (\boldsymbol{G}^T\boldsymbol{C}^{-1}\boldsymbol{G})^{-1}$

  where the sensitivity matrix is $\boldsymbol{G} = [1.0 \;\; 1.0]$

  and the measurements are the vector $\boldsymbol{m} = [1.5 \;\; 1.0]^T$

  with covariance matrix $\boldsymbol{C} = \begin{pmatrix} 1.5^2 * (0.1^2 + 0.2^2) & 1.5 * 1.0 * 0.2^2 \\ 1.5 * 1.0 * 0.2^2 & 1.0^2 * (0.1^2 + 0.2^2) \end{pmatrix}$

- Result is $x = 0.88 \pm 0.22$
- This result is smaller than both measurements, which seems implausible

Probabilistic view of standard PPP solution

- Consider the probability density function (pdf) for the variables

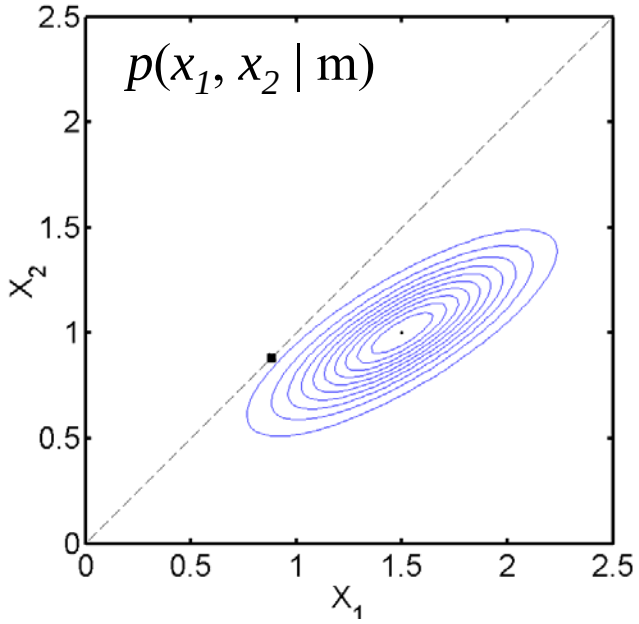
$$\boldsymbol{x} = [x_1 \;\; x_2]^T$$

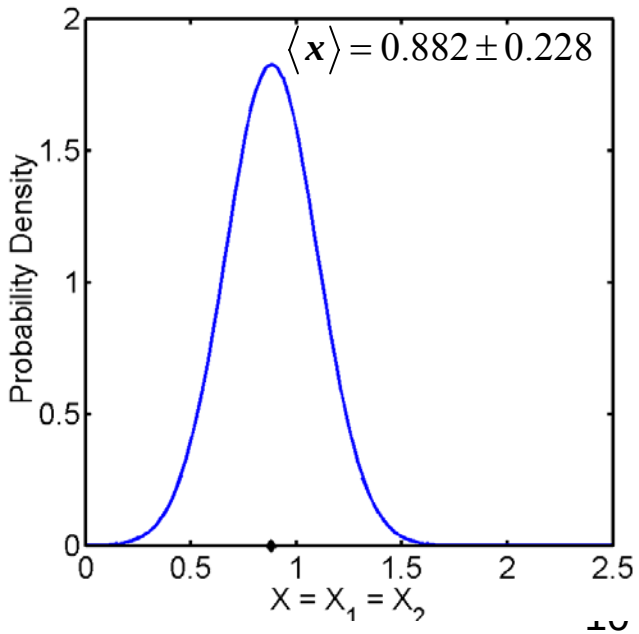
$$p(\boldsymbol{x} \mid \boldsymbol{m}) \propto \exp\left\{-\frac{1}{2}^T (\boldsymbol{x}-\boldsymbol{m})^T \boldsymbol{C}^{-1} (\boldsymbol{x}-\boldsymbol{m})\right\}$$

where measurements are $\boldsymbol{m} = [1.5 \;\; 1.0]^T$ and their covariance matrix is

$$\boldsymbol{C} = \begin{pmatrix} 1.5^2 * (0.1^2 + 0.2^2) & 1.5 * 1.0 * 0.2^2 \\ 1.5 * 1.0 * 0.2^2 & 1.0^2 * (0.1^2 + 0.2^2) \end{pmatrix}$$

- For $x = x_1 = x_2$ (diagonal of 2D pdf), $p(x|\boldsymbol{m})$ is normal distribution centered at 0.88





Probabilistic model for additive error

- Represent common uncertainty in measurements by systematic additive offset Δ: $x_1 = m_1 + \varepsilon_1 + \Delta; \quad x_2 = m_2 + \varepsilon_2 + \Delta$
  - where the ε_i represent the random fluctuations
- Bayes law gives joint pdf for x and Δ

$$p(x, \Delta \mid \boldsymbol{m}) = p(\boldsymbol{m} \mid x, \Delta)\, p(x)\, p(\Delta)$$

where priors $p(x)$ is uniform and $p(\Delta)$ assumed normal ($\sigma_\Delta = 0.2$)

- Writing $p(x, \Delta \mid \boldsymbol{m}) \propto \exp\{-\varphi\}$ and assuming normal distributions

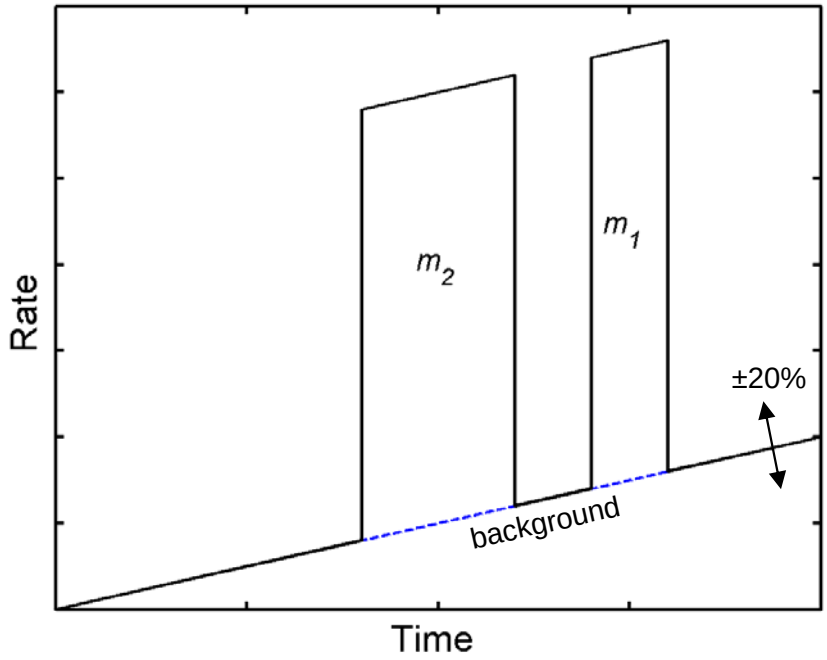
$$2\varphi = \frac{(x_1 - m_1 - \Delta)^2}{\sigma_1^2} + \frac{(x_2 - m_2 - \Delta)^2}{\sigma_2^2} + \frac{\Delta^2}{\sigma_\Delta^2}$$

where $\sigma_1 = 0.1 * m_1; \quad \sigma_2 = 0.1 * m_2; \quad \sigma_\Delta = 0.2$

- Pdf for x obtained by integration: $p(x \mid \boldsymbol{m}) = \int p(x, \Delta \mid \boldsymbol{m})\, \mathrm{d}\Delta$
- This model equivalent to $p(\boldsymbol{x} \mid \boldsymbol{m}) \propto \exp\left\{-\frac{1}{2}^{T} (\boldsymbol{x} - \boldsymbol{m})^T \boldsymbol{C}^{-1} (\boldsymbol{x} - \boldsymbol{m})\right\}$

Plausible experimental scenario

- Under what conditions is PPP result reasonable?
- Suppose that
  - measurements made in intervals shown
  - from experience with apparatus, we know background increases linearly in time
  - background subtraction for m_1 is 1.5 times larger than for m_2; leads to stated covariance matrix
- For this scenario, the additive model is appropriate, and the PPP solution, 0.88, is the correct answer



Probabilistic model for normalization error

- Represent common uncertainty in measurements by systematic error in normalization factor c: $cx = m_1 + \varepsilon_1; \quad cx = m_2 + \varepsilon_2$
  - where the ε_i represent the random fluctuations
- Following same development as before, where prior $p(c)$ assumed normal with expected value of 1 and $\sigma_c = 0.2$
- Writing $p(cx, c \mid \boldsymbol{m}) \propto \exp\{-\varphi\}$

$$2\varphi = \frac{(cx - m_1)^2}{\sigma_1^2} + \frac{(cx - m_2)^2}{\sigma_2^2} + \frac{(c-1)^2}{\sigma_c^2}$$

where $\sigma_1 = 0.1 * m_1; \quad \sigma_2 = 0.1 * m_2; \quad \sigma_c = 0.2$

- Divide $p(cx, c)$ by Jacobian $J = 1/c$ to get $p(x, c)$, which is a log-normal distribution
- $p(x)$ obtained by numerical integration: $p(x \mid \boldsymbol{m}) = \int p(x, c \mid \boldsymbol{m})\,\mathrm{d}c$
- This approach promoted by D. Smith (1991)

Probabilistic view of normalization error

- Consider the probability density function (pdf) for variables $\boldsymbol{x} = [x_1 \;\; x_2]^T$

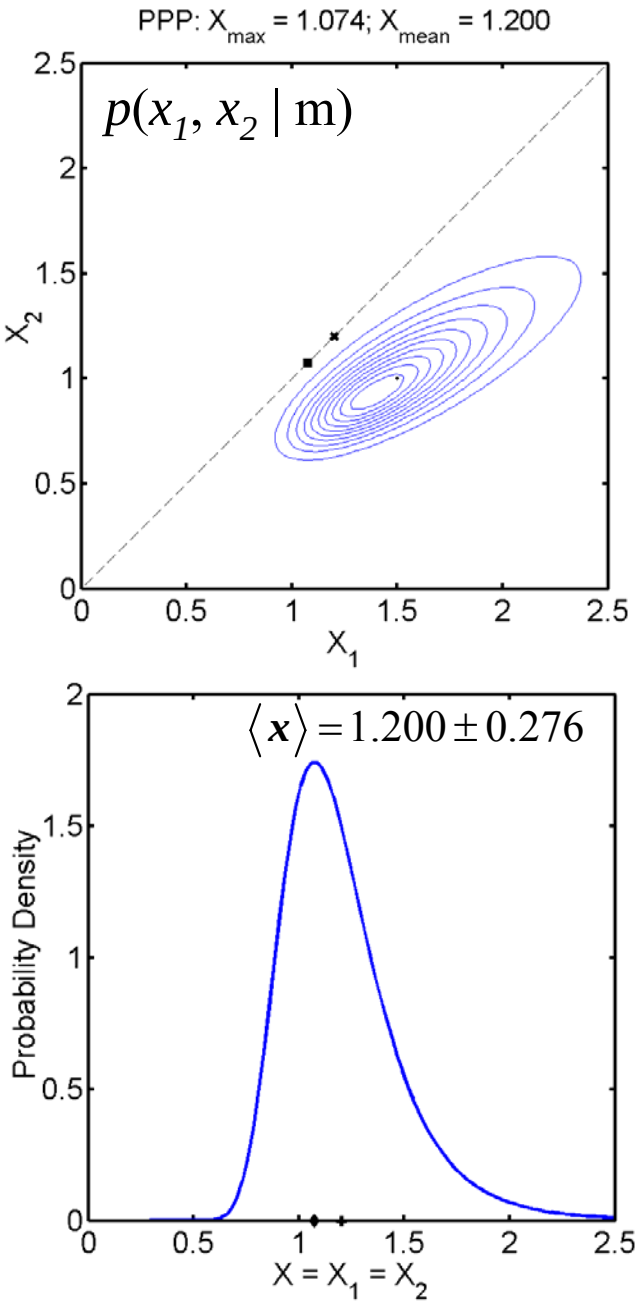
$$\chi^2 = \left(\frac{cx_1 - m_1}{m_1\rho_1}\right)^2 + \left(\frac{cx_2 - m_2}{m_2\rho_2}\right)^2 + \left(\frac{c-1}{\sigma_c}\right)^2;$$

$$\sigma_c = \rho_c;$$

where measurements are $\boldsymbol{m} = [1.5 \;\; 1.0]^T$

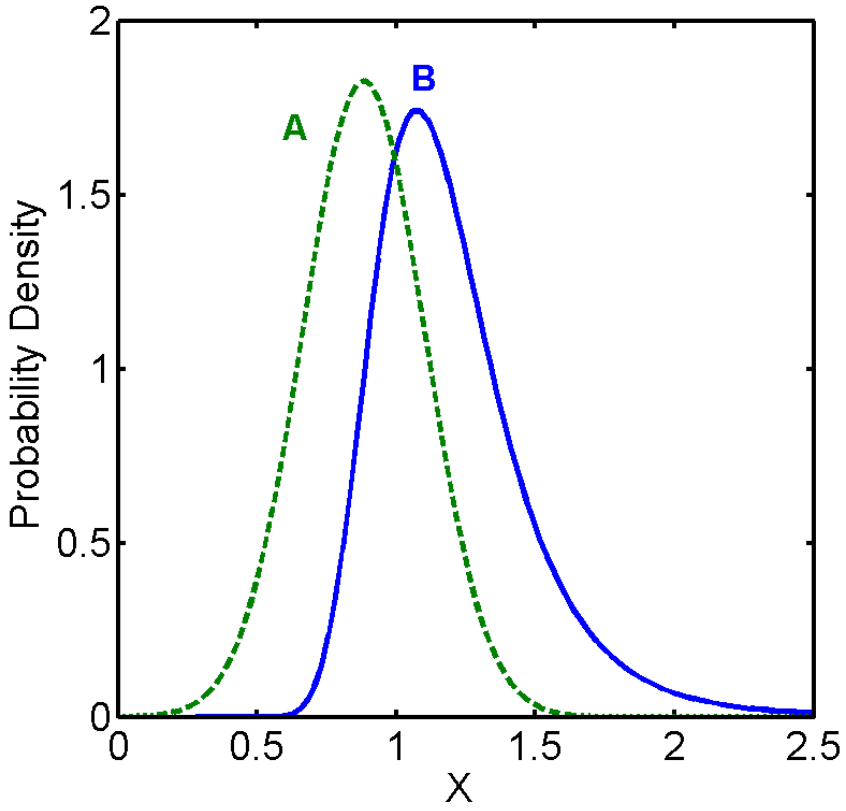
  - also, divide $p(cx, c)$ by Jacobian $J = 1/c$ to get $p(x, c)$,
  - for $x = x_1 = x_2$ (diagonal of 2D pdf), $p(x|\boldsymbol{m})$ is not a simple normal distribution
  - max at: $x_{max} = 1.074$
  - posterior mean and rmsd:

$$x = 1.200 \pm 0.276$$



Probabilistic model for normalization error

- Compare pdfs for two models for correlated effect:
  - A – additive offset
  - B – normalization factor
- Observe significant difference in two results
  - emphasizes need to know which kind of effect leads to correlation
- Probabilistic modeling is capable of handling a variety of known effects



But which model should we use?

- Ambiguity in specifying source of correlation leads to uncertainty about which model to use
- Bayesian approach can handle model uncertainty

$$p(x \mid \boldsymbol{m}) = \int p(x, M \mid \boldsymbol{m})\,\mathrm{d}M$$

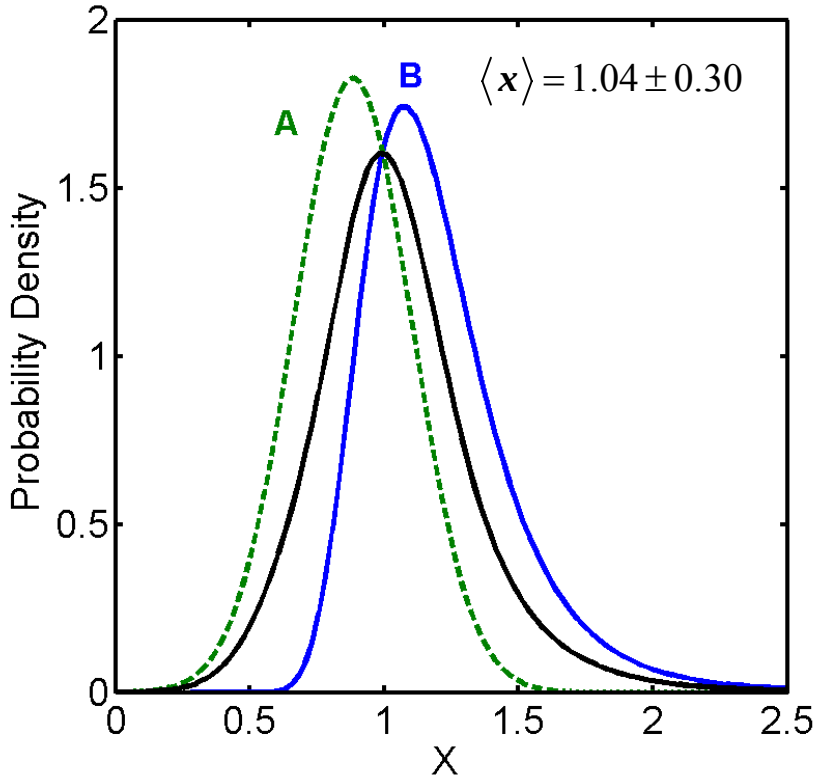
$$= \int p(x \mid \boldsymbol{m}, M)\, p(M)\,\mathrm{d}M$$

$$= \frac{1}{2} p(x \mid \boldsymbol{m}, M_1) + \frac{1}{2} p(x \mid \boldsymbol{m}, M_2)$$

  - for two equally likely models M_1 and M_2

- Answer is average **both** pdfs!!

$$x = 1.04 \pm 0.30$$



solid black line is average of A and B

An alternative approach

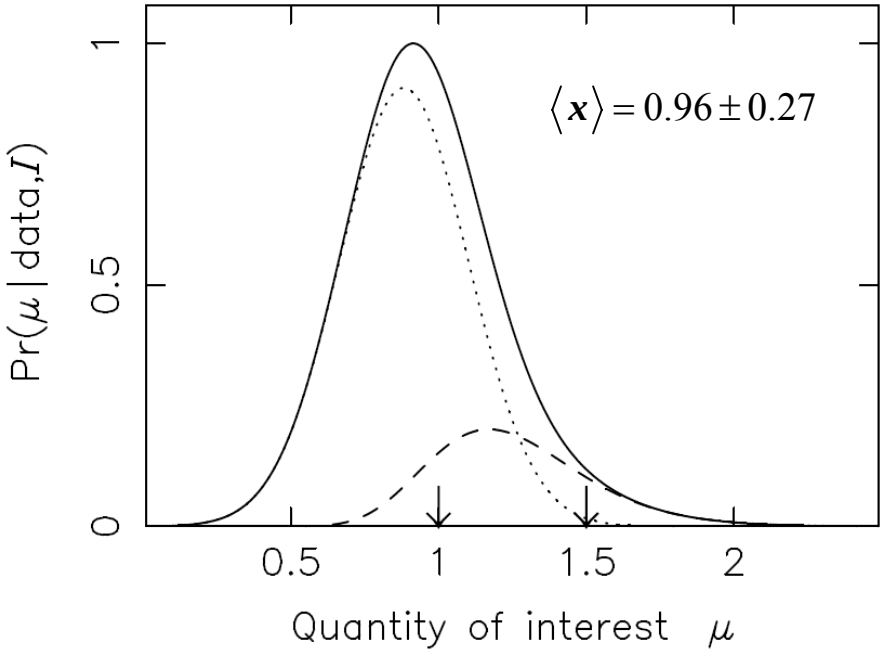
- Devinder Sivia offers an variation on this approach
- Use data to help decide which model to use

$$p(x \mid \boldsymbol{m}) = \sum_i p(x, M_i \mid \boldsymbol{m})$$

$$= \sum_i p(x \mid \boldsymbol{m}, M_i)\, p(M_i \mid \boldsymbol{m})$$

$$= w_1\, p(x \mid \boldsymbol{m}, M_1) + w_2\, p(x \mid \boldsymbol{m}, M_2)$$

  - where w_i is proportional to the evidence integral for $p(M_i \mid \boldsymbol{m})$
- Answer is: $x = 0.96 \pm 0.27$
- Comment: relative weights depend heavily on resp. priors; perhaps not a good situation



solid black line is weighted average of other two distributions

from D. Sivia, *Proc. AMCTM Conf.*, (World Scientific, 2005)

Conclusions

- PPP result is consistent with plausible experimental scenario
  - in which correlated (systematic) error contributes additively to result
- Ambiguous statement of the PPP leads to other interpretations
  - some of which yield more plausible answers
- Analysts need better information to analyze data without guessing

- Probabilistic modeling can cope with various known uncertainty effects

Conclusions

- **Experimenters – please provide measurement details**
- Some of the details needed:
  - specify standard errors as precisely as possible, indicating where uncertainties in their assessment lie
  - specify components in uncertainties and whether they are
    - independent, or correlated, e.g., systematic errors
    - given relative to measured quantities or inferred values
    - additive (background subtraction) or multiplicative (normalization)
- **Correlation matrix by itself is not enough**
- Another issue in PPP is inconsistency between two measurements: one can cope with this discrepancy by introducing notion that the true errors may differ from quoted errors, i.e., treatment of outliers

Monte Carlo techniques

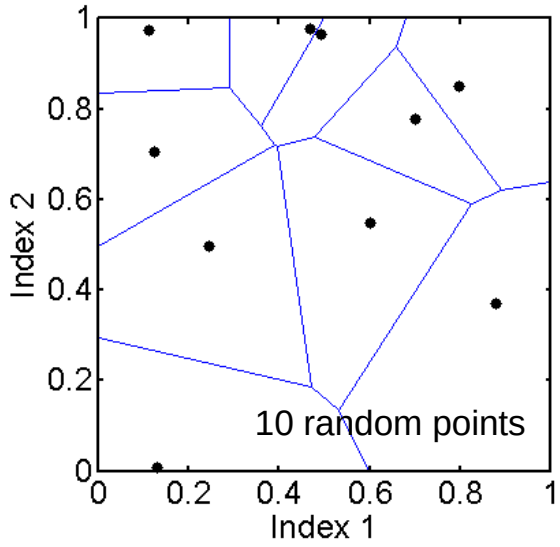
Monte Carlo – represent pdf by a set of point samples

- Typically use MC to draw samples from posterior for parameters, which are fed into model to get prediction; **predictive distribution**
- Visualization of pdf, uncertainty
- Numerical calculations
  - estimation of mean, standard deviation, correlations
  - integration, marginalization
- Quasi-Monte Carlo – select points with more uniform distribution
  - provide more accurate estimates for fixed number of samples
  - often deterministic point sets
- Markov chain Monte Carlo
  - draw random samples for numerically-defined pdf
  - facilitates inference through numerical calculations

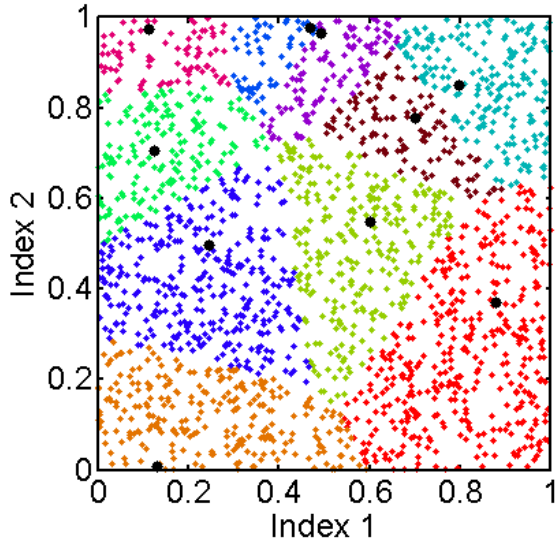
Voronoi analysis

- Voronoi diagram
  - partitions domain into polygons
  - points in *i*th Voronoi region are closest to *i*th generating point, $\boldsymbol{x}_i$
  - boundaries often obtained by geometrical construction
- Monte Carlo technique for Voronoi analysis
  - randomly throw large number of points $\boldsymbol{z}_k$ into region
  - compute distance of each $\boldsymbol{z}_k$ to all generating points $\{\boldsymbol{x}_i\}$
  - $\boldsymbol{z}_k$ belongs to Voronoi region of closest $\boldsymbol{x}_j$
  - can compute volume, first moment , radial moments, identify neighbors, …
- Readily extensible to high dimensions

Geometric construction



Monte Carlo



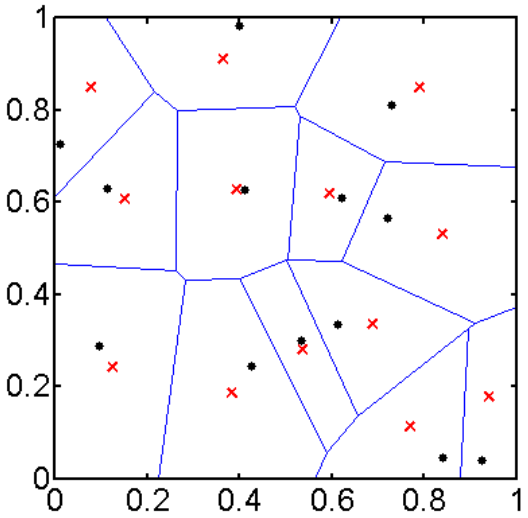
Centroidal Voronoi Tessellation

- Plot shows 13 random points (·) and the centroids of their Voronoi regions (×)
- A point set is called a Centroidal Voronoi Tessellation (CVT) when the generating points $\mathbf{z}^j$ coincide with the centroids their Voronoi regions; a CVT minimizes

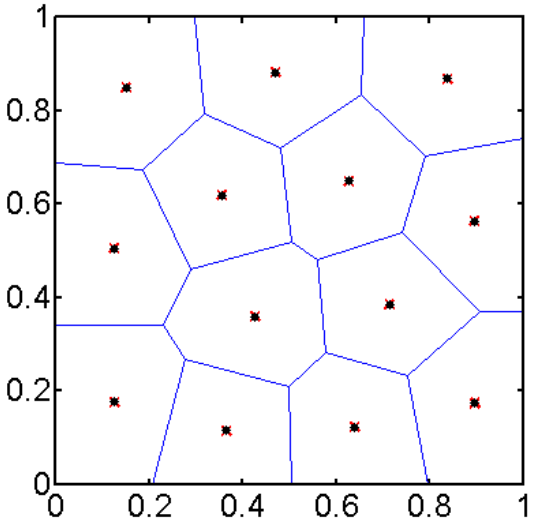
$$\sum_j \int_{V_j} \left|\mathbf{z}^j - \mathbf{x}\right|^2 d\mathbf{x}$$

- Algorithm (McQueen)
  - start with arbitrary set of generating points
  - perform Voronoi analysis using Monte Carlo
  - move each generating point to its Voronoi centroid
  - iterate lasts two steps until convergence
- Final CVT points are uniformly distributed

Start with random points

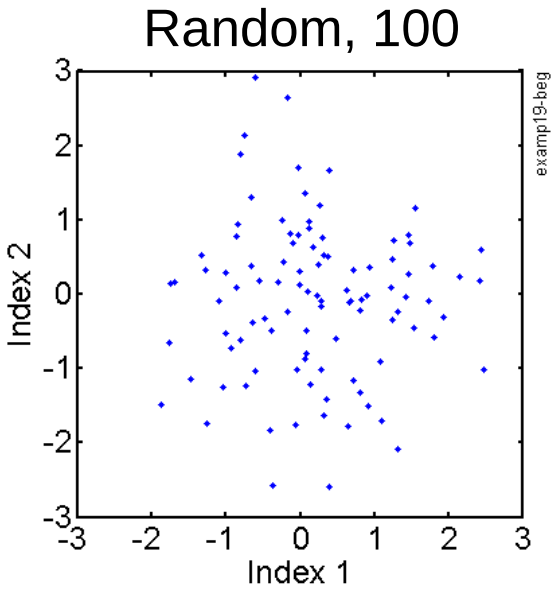


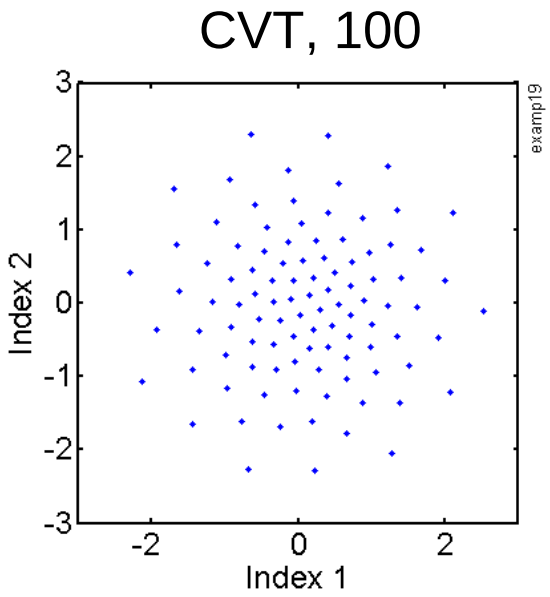
Final CVT point set



CVT for multi-variate normal distribution

- CVT algorithm works for an arbitrary density function, e.g., a normal distribution
- In above MC algorithm for Voronoi analysis, simply draw random numbers from desired distribution
- Plots show starting random point set and final CVT set
- Radii of points are rescaled to achieve desired average variance along axes
- CVT points appear uniformly distributed within constraint of adhering to unit-variance normal distribution
- This kind of distribution may have benefits for MC calculations and visualizations





Sampling from correlated normal distribution

- Want to draw samples from multi-variate normal distribution with known covariance $\mathbf{C}_\mathbf{x}$
- Important to include correlations among uncertainties, i.e., off-diagonal elements
- Algorithm:
  - perform eigenanalysis of covariance matrix of *d* dimensions

$$\mathbf{C}_\mathbf{x} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\mathrm{T}$$

    where $\mathbf{U}$ is orthogonal matrix of eigenvectors and
    $\boldsymbol{\Lambda}$ is the diagonal matrix of eigenvalues
  - draw *d* samples from uncorrelated unit-variance normal distr., ξ_i
  - scale this vector by $\lambda_i^{1/2}$
  - transform vector into parameter space using the eigenvector matrix
  - to summarize, fluctuations are given by: $\Delta\mathbf{x} = \mathbf{U}\boldsymbol{\Lambda}^{1/2}\boldsymbol{\xi}$

Sampling from correlated normal distribution

Proof of algorithm:

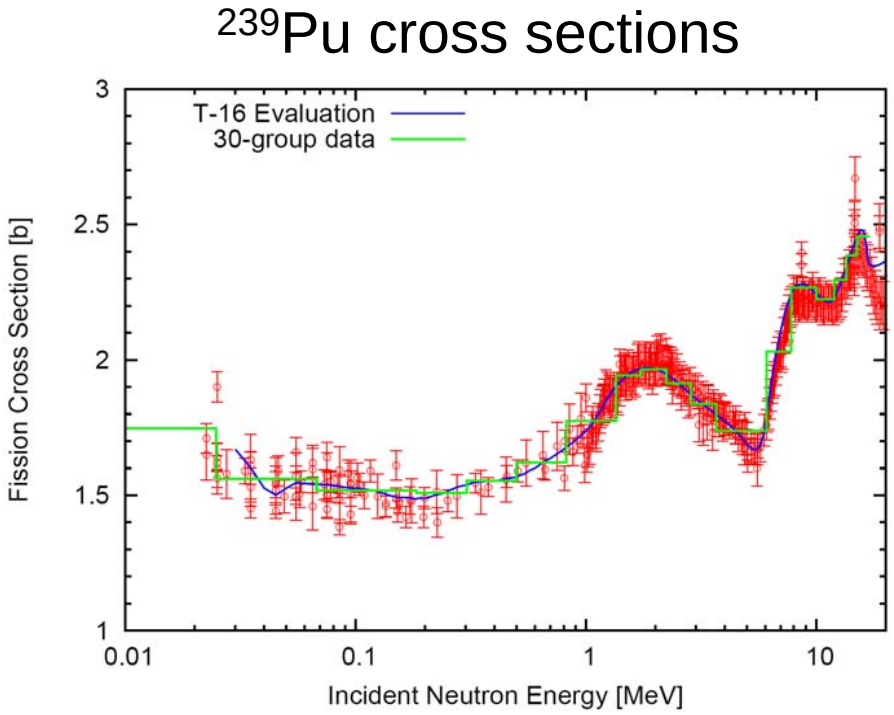
- Want to draw samples from multi-variate normal distribution with specified covariance $\mathbf{C}_\mathbf{x}$
- Algorithm:
  - fluctuations given by: $\Delta\mathbf{x} = \mathbf{U}\boldsymbol{\Lambda}^{1/2}\boldsymbol{\xi}$
    where ξ_i randomly drawn from uncorrelated normal pdf and
    $\mathbf{U}$ and $\boldsymbol{\Lambda}$ come from an eigenanalysis of $\mathbf{C}_\mathbf{x}$: $\mathbf{C}_\mathbf{x} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\mathrm{T}$
    where $\mathbf{U}$ is orthogonal matrix of eigenvectors and
    $\boldsymbol{\Lambda}$ is the diagonal matrix of eigenvalues
- Proof:
  - Covariance of an ensemble of $\mathbf{x}$ vectors is

$$\mathbf{C} = \left\langle \Delta\mathbf{x}\,\Delta\mathbf{x}^\mathrm{T} \right\rangle = \left\langle \mathbf{U}\boldsymbol{\Lambda}^{1/2}\boldsymbol{\xi}\boldsymbol{\xi}^\mathrm{T}\boldsymbol{\Lambda}^{1/2}\mathbf{U}^\mathrm{T} \right\rangle$$
$$= \mathbf{U}\boldsymbol{\Lambda}^{1/2}\left\langle \boldsymbol{\xi}\boldsymbol{\xi}^\mathrm{T} \right\rangle \boldsymbol{\Lambda}^{1/2}\mathbf{U}^\mathrm{T} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\mathrm{T} = \mathbf{C}_\mathbf{x}$$

  - thus, the fluctuations $\Delta\mathbf{x}$ have the desired covariance

Neutron cross sections

- Plot shows
  - measured fission cross sections for neutrons on ^{239}Pu; red data points
  - inferred cross sections; blue line
  - weighted average in 30 energy bins (groups); green histogram
- PARITSN code simulates neutron transport based on multigroup, discrete-ordinates method
  - uses 30 energy bins (groups)
  - calculates criticality for specified configuration of fissile-material
  - establish dependence of criticality experiment to cross sections



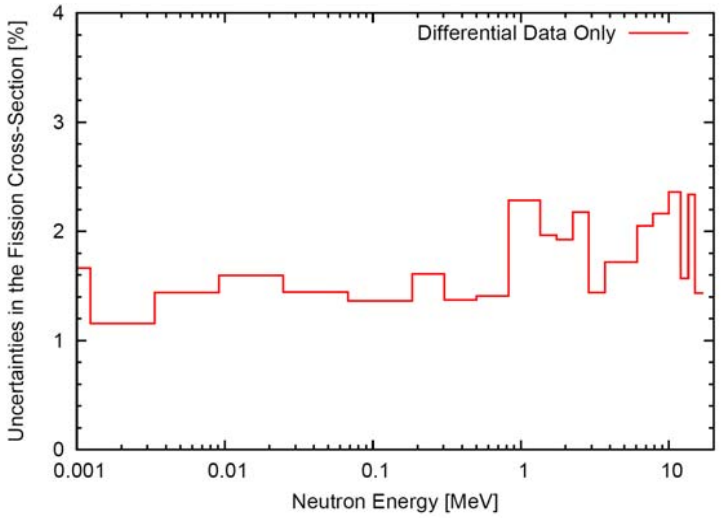
cross section evaluation, P. Young et al.

Neutron cross sections - uncertainties

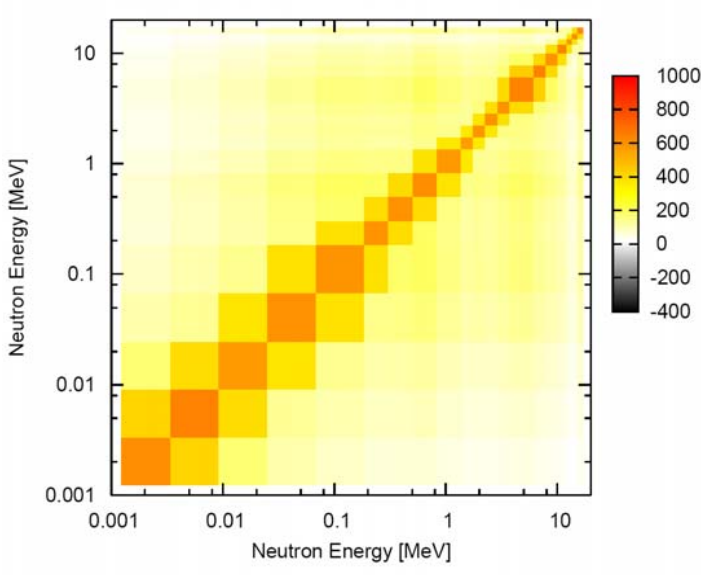
- Analysis of measured cross sections yields a set of evaluated cross sections

- Uncertainties in evaluated cross sections are ~ 1.4-2.4 %
- Covariance matrix important
- Strong positive correlations caused by normalization uncertainties in each experiment

standard error in cross sections



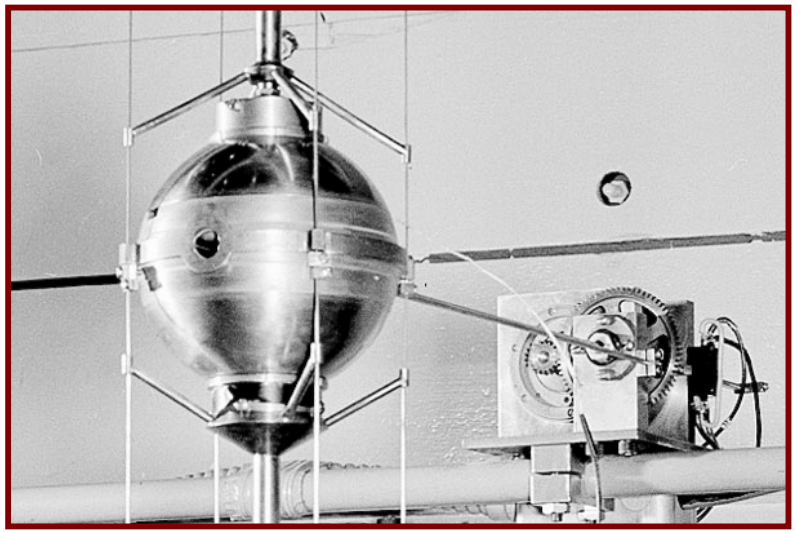
correlation matrix



JEZEBEL – criticality experiment

- JEZEBEL experiment (1950-60)
  - fissile material ^{239}Pu
  - measure neutron multiplication as function of separation of two hemispheres of material
  - summarize criticality with neutron multiplication factor, $k_{eff} = 0.9980 \pm 0.0019$
  - very accurate measurement

JEZEBEL set up

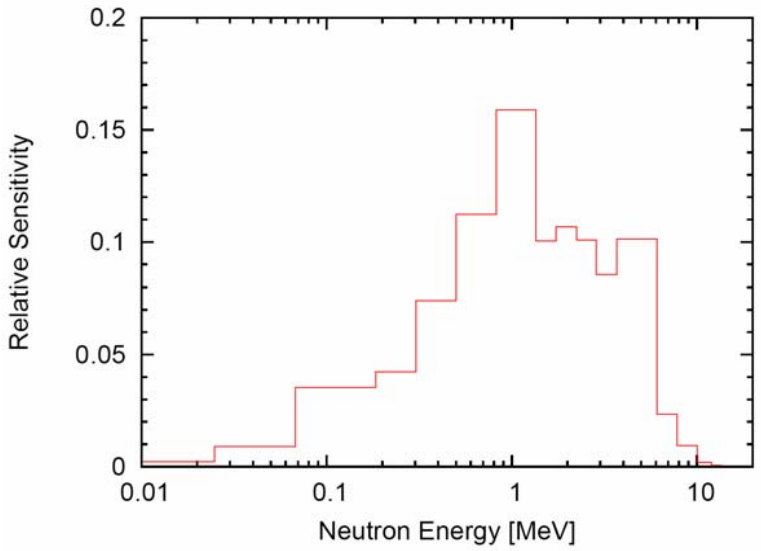


- Our goal – use highly accurate JEZEBEL measurement to improve our knowledge of ^{239}Pu cross sections

JEZEBEL – sensitivity analysis

- PARITSN code calculates k_{eff} on basis of neutron cross sections
- Sensitivity of k_{eff} to cross sections found by perturbing cross section in each energy bin by 1% and observing increase in k_{eff}
- Observe that 1% increase in all cross sections results in 1% increase in k_{eff} , as expected

k_{eff} sensitivity to cross sections



Bayesian update

- For data linearly related to the parameters, the Bayesian (aka Kalman) update for Gaussian distributions is

$$\mathbf{C}_1^{-1}\mathbf{x}_1 = \mathbf{C}_0^{-1}\mathbf{x}_0 + \mathbf{S}_\mathbf{y}^{\mathrm{T}}\mathbf{C}_\mathbf{y}^{-1}\mathbf{S}_\mathbf{y}(\mathbf{y}-\mathbf{y}_0)$$

$$\mathbf{C}_1^{-1} = \mathbf{C}_0^{-1} + \mathbf{S}_\mathbf{y}^{\mathrm{T}}\mathbf{C}_\mathbf{y}^{-1}\mathbf{S}_\mathbf{y}$$

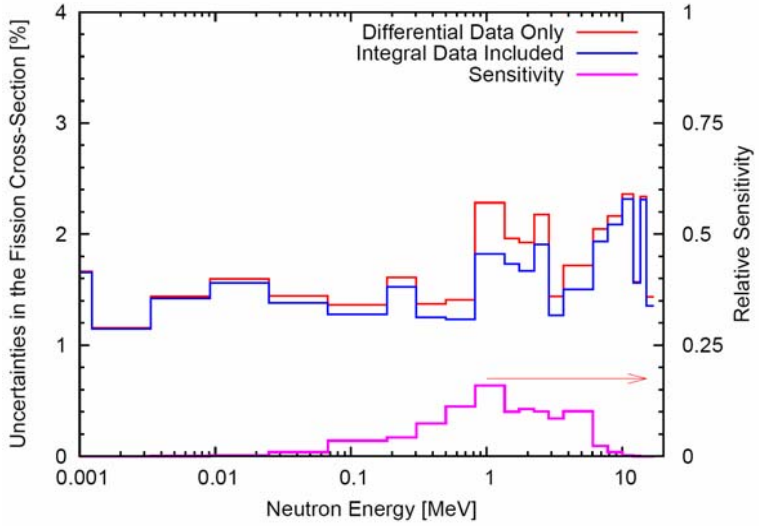
  - $\mathbf{x}_0$ and $\mathbf{x}_1$ are parameter vectors before and after update
  - $\mathbf{C}_0$ and $\mathbf{C}_1$ are their covariance matrices
  - $\mathbf{y}$ and $\mathbf{C}_\mathbf{y}$ are the measured data vector and its covariance
  - $\mathbf{y}_0$ is the value of $\mathbf{y}$ for $\mathbf{x}_0$
  - $\mathbf{S}_\mathbf{y}$ is the matrix of the sensitivity of $\mathbf{y}$ to $\mathbf{x}$; $\partial\mathbf{y}/\partial\mathbf{x}$

- For the JEZEBEL case, $\mathbf{y}$ is a scalar (k_{eff}), $\mathbf{C}_\mathbf{y}$ is a scalar (variance), and $\mathbf{S}_\mathbf{y}$ is a vector

Updated cross sections

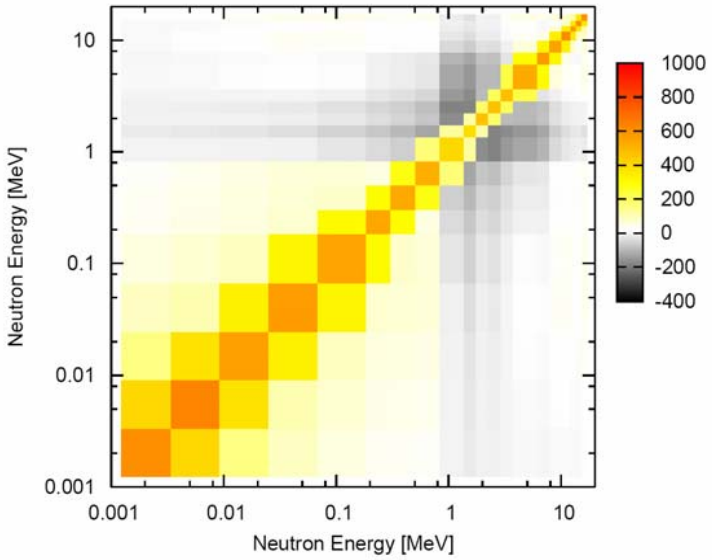
- Plot shows uncertainties in cross sections before and after using JEZEBEL measurement
- Modest reduction in uncertainties; follows energy dependence of sensitivity

standard error in cross sections



- Correlation matrix is significantly altered
- Strong negative correlations introduced by integral constraint of matching JEZEBEL's k_{eff}
  - reduction in uncertainties in future prediction depends on how closely its sensitivity matches JEZEBEL's

correlation matrix

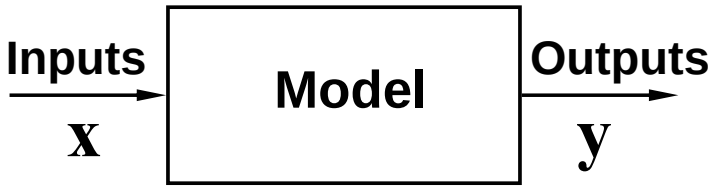


Linear-response model – output uncertainty

- Assume outputs of a model are linearly related to perturbations in the inputs,

$$\delta \boldsymbol{y} = \mathbf{S}_{\mathbf{y}}^{\mathrm{T}} \delta \mathbf{x}$$

  - where $\mathbf{S}_{\mathbf{y}}$ is sensitivity matrix $\partial \mathbf{y} / \partial \mathbf{x}$



- The covariance in the output $\mathbf{y}$ is

$$\mathbf{C}_{\mathbf{y}} = \mathbf{S}_{\mathbf{y}}^{\mathrm{T}} \mathbf{C}_{\mathbf{x}} \mathbf{S}_{\mathbf{y}}$$

  - when output *y* is a scalar, the covariance $\mathbf{C}_{\mathbf{y}}$ is a scalar (variance), and $\mathbf{S}_{\mathbf{y}}$ is a vector

- If linear model is sufficient and one knows $\mathbf{S}_{\mathbf{y}}$, then predictive distribution is easily characterized
- For complex simulations, $\mathbf{S}_{\mathbf{y}}$ is not usually known

Uncertainty in subsequent simulations

- Our goal is to use updated cross sections in new calculations
  - expect that integral constraint will reduce uncertainties
- Demonstrate usefulness of quasi-MC in form of CVT point sets by "predicting" k_{eff} measured in JEZEBEL
  - for this demo, assume linear model with known sensitivity vector
  - under this assumption, we can calculate exact answer and compare to MC-style sampling to obtain predictive distribution
- For a new physical scenario, we would not have sensitivity vector and would have to do full simulation calculation
  - thus, only a modest number of function evaluations can be done

Accuracy of predicted k_{eff} and its uncertainty

- Prediction based on liner model with know sensitivities
  - only 30 sample sets allowed for neutronics calc. because of time
  - check accuracy of predicted mean and standard deviation
- Conclude – CVT is more accurate than random sampling

Performance summary from 1000 runs, each with set of 30 sample vectors; 'rot' indicates single sample set randomly rotated to achieve each new one

	est. mean k_{eff}		est. std. dev. k_{eff}	
	avg.	rms dev.	avg.	rms dev.
random	0.99788	0.00037	0.00191	0.00028
random-rot	0.99824	0.00010	0.00218	0.00010
CVT-rot	0.99796	0.00001	0.00197	0.00002
exact-linear	0.99796	-	0.00195	-

Summary

In this tutorial:

- Peelles' pertinent puzzle
  - impact on cross-section evaluation
  - probabilistic modeling; additive and multiplicative systematic effects
  - experimenters need to provide more than correlation matrices
- Monte Carlo
  - generation of samples with specified covariance matrix
  - quasi-Monte Carlo – more uniformly spaced points than random
  - Centroidal Voronoi Tessellation (CVT) algorithm
- Bayesian updating of cross sections to include integral data
  - JEZEBEL criticality experiment
  - integral constraint results in negative correlations
  - CVT point set improves prediction accuracy