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Title: UNCERTAINTY QUANTIFICATION FOR HOMELAND SECURITY APPLICATIONS

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Uncertainty Quantification for Homeland Security Applications (U)

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Given a set of simulated gamma-ray leakage measurements and the unknown object model that best fit these measurements, standard tools of uncertainty quantification in data-fitting were applied to develop an estimate of the uncertainty of the dimensions in the model based on the statistical uncertainty of the measurements. At least two issues were discovered that need further exploration. One is that in standard data analysis, there are usually many more data points than there are model parameters to be fit, so that calculating the inverse of the Hessian (or curvature) matrix to obtain the covariance matrix is straightforward; in Homeland Security applications, however, there are more unknowns than data points, and it is not obvious how the correct covariance matrix should be obtained if the Hessian matrix is singular. Thus, in most problems of interest, it is still unclear how to relate the uncertainty in measurements to the uncertainty in model dimensions. A related issue is how the uncertainty in model dimensions should be used to obtain the uncertainty in other model quantities, such as material masses. The standard procedure is to use the variances and covariances of the dimensions in the simple error propagation formula; an alternative is to randomly sample the model dimensions from Gaussian distributions whose widths are related to the uncertainty in the dimensions, compute the associated masses, and then fit the mass distributions to Gaussians whose widths are related to the uncertainty in the masses. Both of these procedures require knowledge of the covariance matrix for the model dimensions.

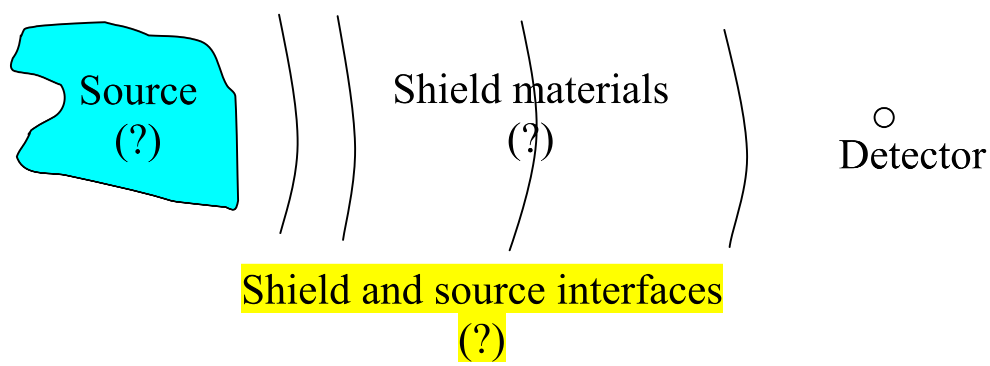
Thus, a program to extend the standard methods of uncertainty quantification to develop an estimate of the covariance matrix in the case of a singular Hessian matrix would be of interest for Homeland Security applications.

• Consider a border portal monitor (radiation detector) that "sees" a radioactive object. We want to use the data from the monitor to tell us how much radioactivity there is, with uncertainties.

We will start with an easier problem:

• Consider a radioactive object emitting γ rays of discrete energies that are well resolved using high-purity germanium (HPGe) detectors

• We want to use γ leakage measurements to tell us what the system is



• Notation:

M_o^g = measured leakage for γ line g ($g = 1,\ldots,G$)

σ_o^g = statistical uncertainty of M_o^g

M^g = calculated leakage for γ line g ($g = 1,\ldots,G$) for some *model*

model = a description of the system (materials, masses, interface locations, etc.), NOT a description of the γ transport process

• We assume that there is a single number (the γ leakage) associated with a single energy line

- We consider only the transport of photons of discrete energies and assume that any scattered photons lose energy and are removed. The angular flux of photons at the discrete energy denoted by index *g* is given by

$$\hat{\mathbf{\Omega}} \cdot \vec{\nabla} \psi^g(r, \hat{\mathbf{\Omega}}) + \Sigma_t^g(r) \psi^g(r, \hat{\mathbf{\Omega}}) = q^g(r)$$

for $g = 1, \ldots, G$. (This equation represents the *forward problem*.)

- The adjoint equation is

$$-\hat{\mathbf{\Omega}} \cdot \vec{\nabla} \psi^{*g}(r, \hat{\mathbf{\Omega}}) + \Sigma_t^g(r) \psi^{*g}(r, \hat{\mathbf{\Omega}}) = q^{*g}(r) \quad ,$$

where the source is actually the detector response function.

- These equations can be rendered in operator notation as

$$L^g \psi^g = q^g$$

and

$$L^{*g} \psi^{*g} = q^{*g} \quad .$$

- Suppose the scalar flux for each energy line *g* is measured at a detector. The quantity of interest is

$$M^g = \int dV \int d\hat{\mathbf{\Omega}} \Sigma_d^g(r) \psi^g(r, \hat{\mathbf{\Omega}}) \quad ,$$

where the detector response function $\Sigma_d^g(r)$ is zero outside the detector volume.

- Introducing the inner product notation $\langle \cdot \rangle$ to mean an integral over all phase space (volume and angle), the quantity of interest is

$$M^g = \left\langle \Sigma_d^g \psi^g \right\rangle \quad .$$

A weight function or detector efficiency can be built into $\Sigma_d^g(r)$.

- Jeffrey A. Favorite, "Using the Schwinger Variational Functional for the Solution of Inverse Transport Problems," *Nucl. Sci. Eng.*, **146**, to appear (January 2004).

  + The Schwinger method is iterative (i.e. implicit) but based on algebraic manipulations of the transport equation (i.e. explicit)

  + The method updates the unknown interface locations using

$$\underline{\underline{R}}\underline{\Delta r} = \frac{M^g - M_o^g}{M_o^g} \quad ,$$

where $\underline{\Delta r}$ is an $N \times 1$ vector and $\underline{\underline{R}}$ is a $G \times N$ matrix.

- Search schemes: Variational perturbation theory (Favorite) and a geometry-based scheme due to Diane Vaughan and Kevin Buescher (X-8)

- A derivative-based scheme [J. A. Favorite and R. Sanchez, "An Inverse Method for Radiation Transport," submitted to the 10th Int. Conf. Radiation Shielding/Radiation Protection and Shielding 2004, Funchal, Portugal, May 9–14 (2004)]

  + It can be shown that

$$\frac{\partial M^g}{\partial r_n} = \Delta q_n^g \int d\hat{\mathbf{\Omega}}\, \psi^{*g}(r_n) - \Delta\Sigma_{t,n}^g \int d\hat{\mathbf{\Omega}}\, \psi^{*g}(r_n)\psi^g(r_n) \quad ,$$

where Δq_n^g and $\Delta\Sigma_{t,n}^g$ are the source and cross section differences across interface r_n

  + If, for each line, $\varepsilon^g \equiv \frac{1}{2}\left(\frac{M^g - M_o^g}{\sigma_o^g}\right)^2$, then

$$\frac{\partial \varepsilon^g}{\partial r_n} = \frac{\left(M^g - M_o^g\right)}{\left(\sigma_o^g\right)^2}\frac{\partial M^g}{\partial r_n}$$

  + No numerical differentiation is required

Chi-squared and the covariance matrix

- χ^2:

$$\chi^2 = \sum_{g=1}^{G} \left(\frac{M^g - M_o^g}{\sigma_o^g} \right)^2$$

- χ^2 gradient vector:

$$\frac{\partial \chi^2}{\partial r_n} = 2 \sum_{g=1}^{G} \frac{M^g - M_o^g}{\left(\sigma_o^g\right)^2} \frac{\partial M^g}{\partial r_n}$$

- Hessian (curvature) matrix of χ^2:

$$\frac{\partial^2 \chi^2}{\partial r_n \partial r_m} = 2 \sum_{g=1}^{G} \left[\cancel{\frac{M^g - M_o^g}{\left(\sigma_o^g\right)^2} \frac{\partial^2 M^g}{\partial r_n \partial r_m}} + \frac{1}{\left(\sigma_o^g\right)^2} \frac{\partial M^g}{\partial r_m} \frac{\partial M^g}{\partial r_n} \right]$$

$$\approx 2 \sum_{g=1}^{G} \frac{1}{\left(\sigma_o^g\right)^2} \frac{\partial M^g}{\partial r_m} \frac{\partial M^g}{\partial r_n}$$

- Define the α matrix to be ½ the Hessian matrix of χ^2 (Press *et al*. call this the curvature in Chap. 15):

$$\left[\alpha_{nm}\right] = \sum_{g=1}^{G} \frac{1}{\left(\sigma_o^g\right)^2} \frac{\partial M^g}{\partial r_m} \frac{\partial M^g}{\partial r_n}$$

- The covariance matrix of uncertainties in the estimated values of the interface locations is the inverse of α (the curvature?):

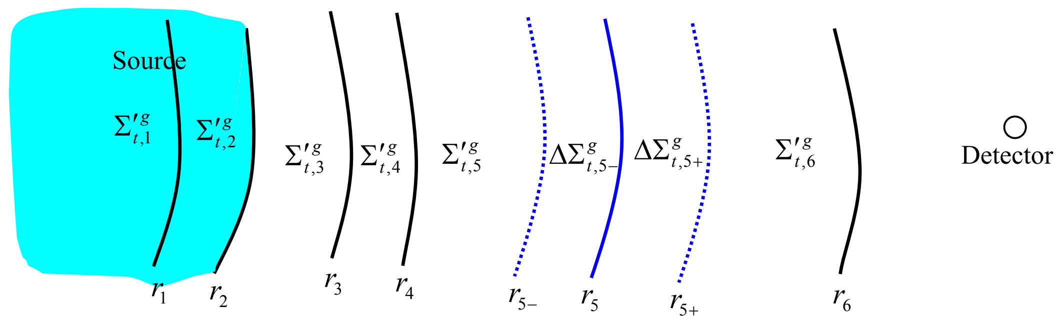
$$\underline{\underline{C}} = \underline{\underline{\alpha}}^{-1}$$

$$= \begin{bmatrix} \sigma_{r_1}^2 & \cdots & \sigma_{r_1 r_N}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{r_N r_1}^2 & \cdots & \sigma_{r_N}^2 \end{bmatrix}$$

- What if the Hessian is singular?

Relating uncertainty in interface locations to uncertainty in mass (1)

- Consider, for convenience, a spherically symmetric system



- What's the uncertainty in the mass of region *n*?

$$m_n = \frac{4\pi}{3}\rho_n\left(r_n^3 - r_{n-1}^3\right)$$

- Standard formula for propagation of errors:

$$\sigma_{m_n}^2 = \left(\frac{\partial m_n}{\partial r_n}\right)^2 \sigma_{r_n}^2 + \left(\frac{\partial m_n}{\partial r_{n-1}}\right)^2 \sigma_{r_{n-1}}^2 + 2\frac{\partial m_n}{\partial r_n}\frac{\partial m_n}{\partial r_{n-1}}\sigma_{r_n r_{n-1}}^2$$

$$= \left(4\pi\rho_n r_n^2\right)^2 \sigma_{r_n}^2 + \left(-4\pi\rho_n r_{n-1}^2\right)^2 \sigma_{r_{n-1}}^2 + 2\left(4\pi\rho_n r_n^2\right)\left(-4\pi\rho_n r_{n-1}^2\right)\sigma_{r_n r_{n-1}}^2$$

$$= \left(4\pi\rho_n\right)^2 \left(r_n^4\sigma_{r_n}^2 + r_{n-1}^4\sigma_{r_{n-1}}^2 - 2r_n^2 r_{n-1}^2\sigma_{r_n r_{n-1}}^2\right)$$

- Use the covariance matrix to randomly sample interface locations r_n and r_{n-1} from Gaussian distributions with the proper widths

- Use these to compute masses

- The masses should be distributed in a Gaussian whose width is σ_{m_n}

- What is the proper distribution for the interface locations?

$$\underline{\Delta r} = \underline{\underline{C}}^{\frac{1}{2}} \underline{\xi} \quad ,$$

where $\underline{\xi}$ represents N independent random numbers drawn from a Gaussian distribution with mean 0 and half-width 1

- What is the square root of the covariance matrix? Use singular value decomposition (SVD) on the Hessian:

$$\underline{\underline{\alpha}} = \underline{\underline{U}}\,\underline{\underline{W}}\,\underline{\underline{V}}^T \quad ,$$

where $\underline{\underline{W}} = \begin{bmatrix} w_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & w_N \end{bmatrix}$ is the diagonal matrix of singular values. Now

$$\underline{\underline{C}} = \underline{\underline{\alpha}}^{-1} = \underline{\underline{V}}\left[\operatorname{diag}\ 1/w_n\right]\underline{\underline{U}}^T$$

and

$$\underline{\underline{C}}^{\frac{1}{2}} = \underline{\underline{V}}\left[\operatorname{diag}\ 1/\sqrt{w_n}\right]\underline{\underline{U}}^T$$

- If $\underline{\underline{\alpha}}$ is *not* singular then $\underline{\underline{U}} = \underline{\underline{V}}$; if $\underline{\underline{\alpha}}$ is singular then $\underline{\underline{U}} \neq \underline{\underline{V}}$

- Use the covariance matrix to randomly sample interface locations r_n and r_{n-1} from Gaussian distributions with the proper widths

- Use these to compute leakage, M^g

- The leakages should be distributed in a Gaussian whose width is σ_o^g

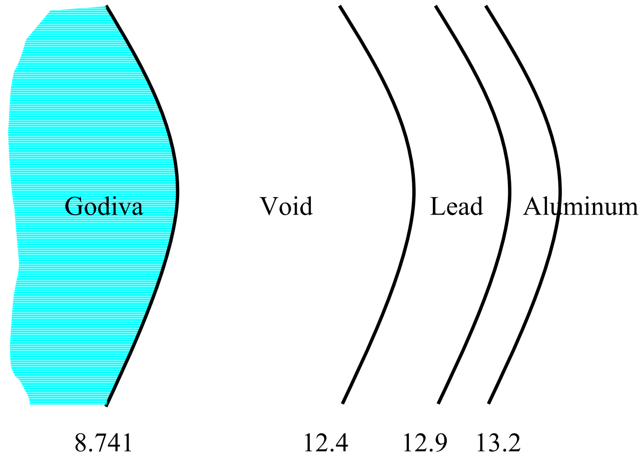
OR

- Use the standard formula for propagation of errors:

$$\left(\sigma^g\right)^2 = \sum_n \left(\frac{\partial M^g}{\partial r_n}\right)^2 \sigma_{r_n}^2 + 2\sum_{m>n}\sum_n \frac{\partial M^g}{\partial r_n}\frac{\partial M^g}{\partial r_m}\sigma_{r_n r_m}^2$$

- σ^g should equal σ_o^g

- Godiva (HEU) model:
- Spherical
- There are four uranium γ lines, but only three can escape this model



- γ leakage from a Monte Carlo calculation:

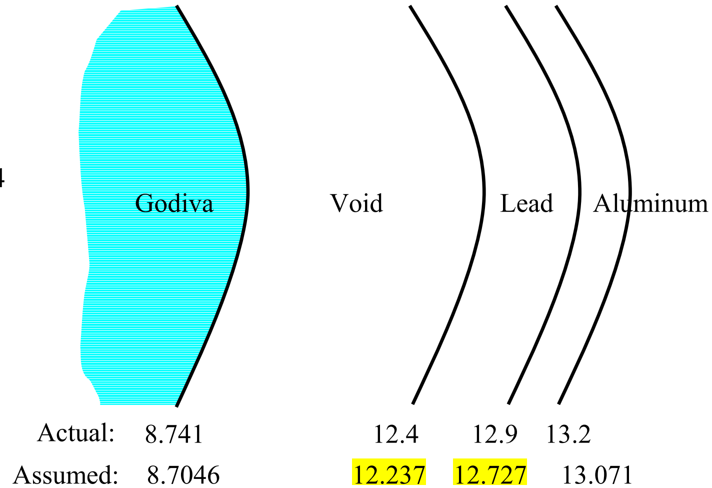
Energy (keV)	γ leakage (s^{-1}) and 1σ uncertainty
144	Not observed
186	$5.28 \times 10^3 \pm 40.82\%$
766	$2.50 \times 10^3 \pm 0.41\%$
1001	$1.01 \times 10^4 \pm 0.33\%$

- A one-dimensional deterministic S_N code, PARTISN, was used in the optimization process
  - + S_{32}
  - + No scattering
  - + Discrete-energy total cross sections from the Monte Carlo library
- The optimization details are interesting but not important here; assume that I've found the minimum χ^2 for each case

Estimating σ^g for the line leakages

Test problem 1: Two shield unknowns

- Godiva model:



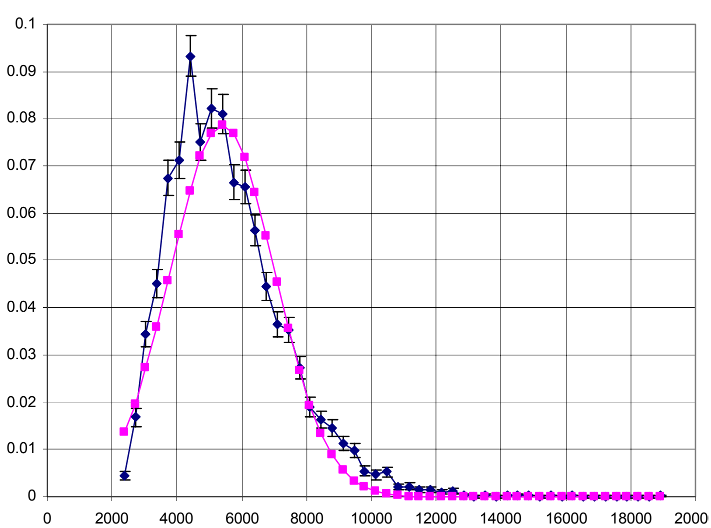
- The assumed r_1 and r_4 were not correct; this made little difference

- Standard deviation in line leakages (expressed as relative errors):

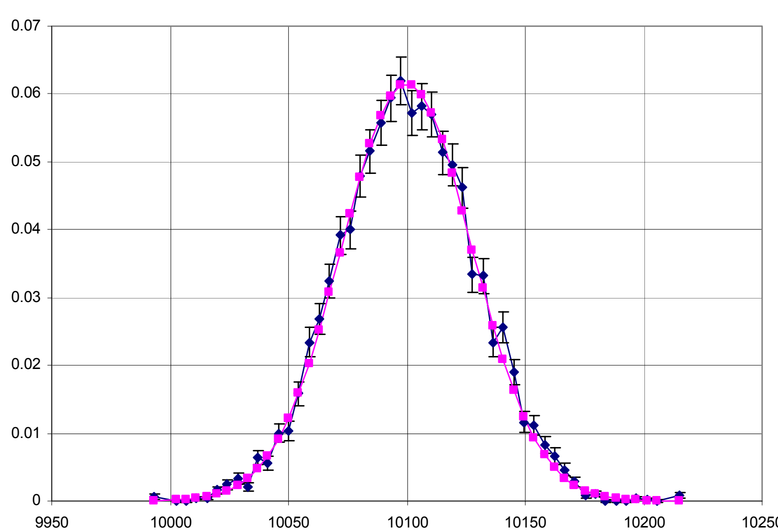
Line (keV)	σ_o^g	σ^g from error prop.	σ^g from Gauss. fit
186	0.408	0.316	0.299
766	0.0041	0.0034	0.0032
1001	0.0033	0.0028	0.0027

σ^g from error propagation and Gaussian fit are similar but smaller than σ_o^g.

- 186-keV line fit

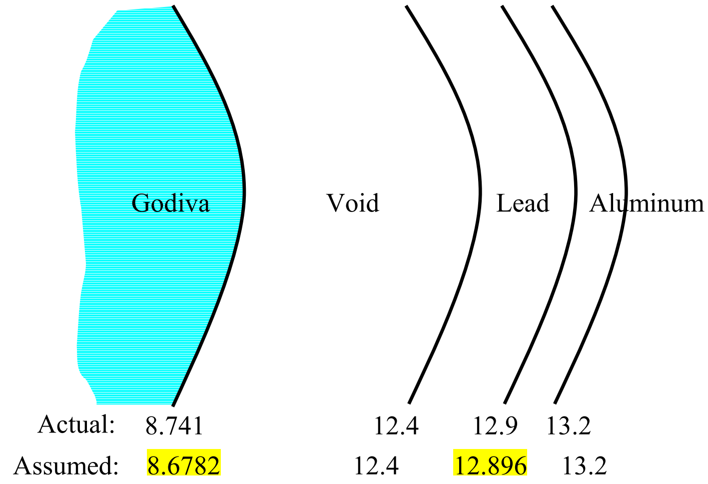


1001-keV line fit



Test problem 2: One shield, one source unknown

- Godiva model:

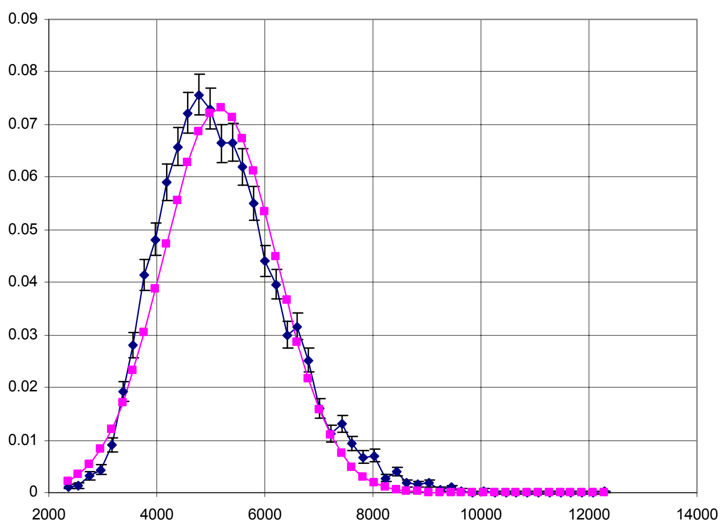


- Standard deviation in line leakages (expressed as relative errors):

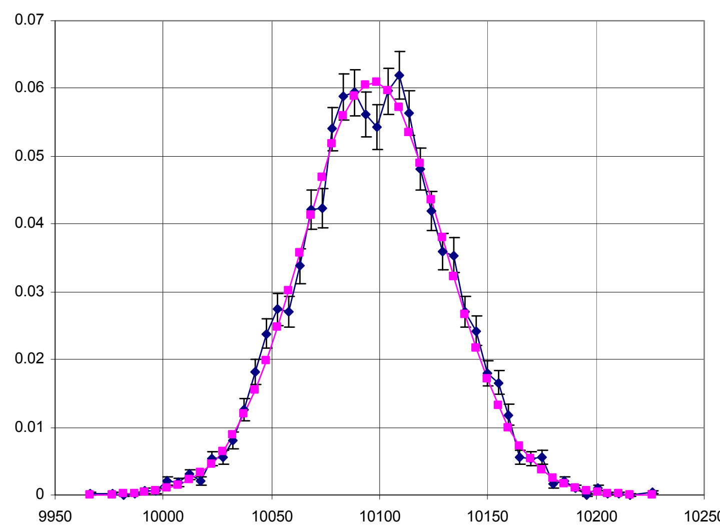
Line (keV)	σ_o^g	σ^g from error prop.	σ^g from Gauss. fit
186	0.408	0.218	0.204
766	0.0041	0.0037	0.0033
1001	0.0033	0.0031	0.0033

σ^g from error propagation and Gaussian fit are similar but smaller than σ_o^g.

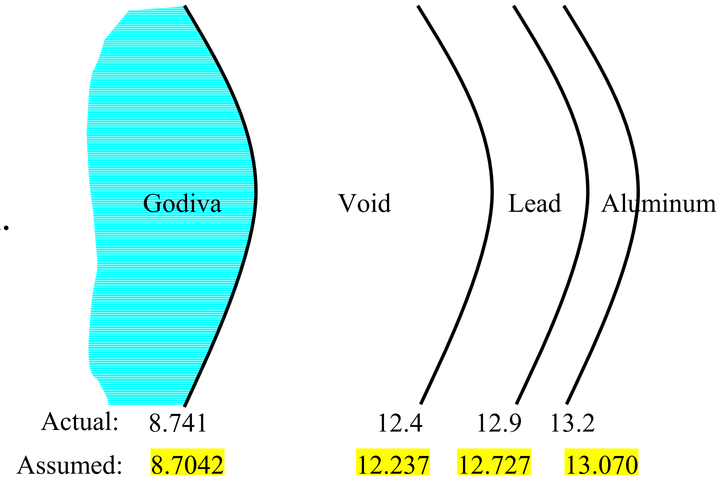
- 186-keV line fit



1001-keV line fit



- Godiva model:



- Note: The Hessian is singular for this problem.

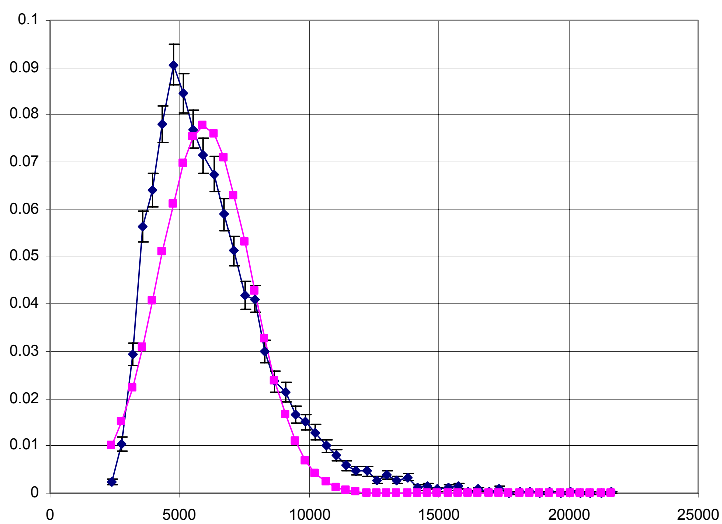
- Nevertheless, …

- Standard deviation in line leakages (expressed as relative errors):

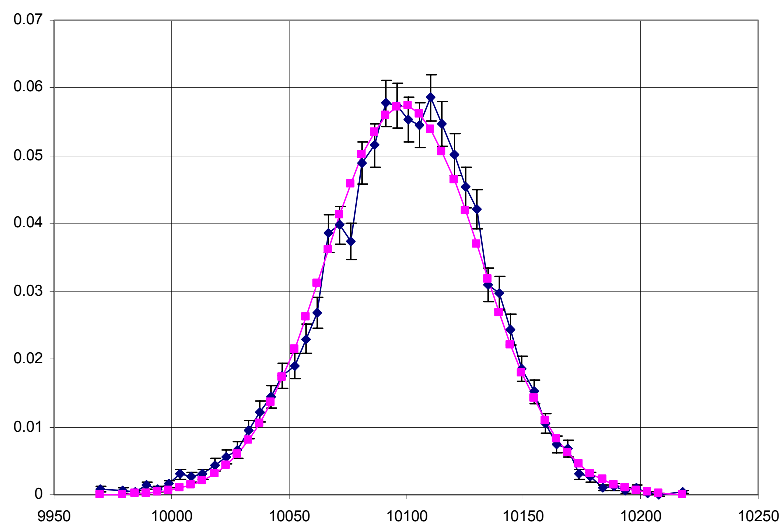
Line (keV)	σ_o^g	σ^g from error prop.	σ^g from Gauss. fit
186	0.408	0.408	0.296
766	0.0041	0.0041	0.0036
1001	0.0033	0.0033	0.0033

σ^g from error propagation is correct! σ^g from Gaussian fit is smaller than σ_o^g.

- 186-keV line fit

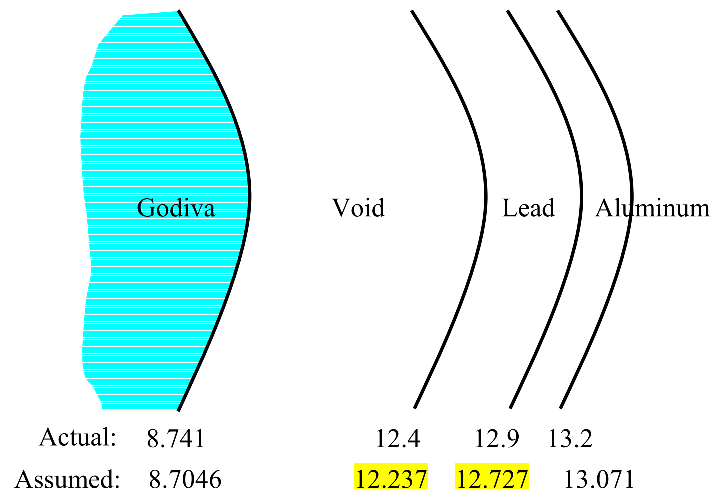


1001-keV line fit



Estimating σ_m for material masses

- Godiva model:



- Mass and standard deviation (from the error propagation formula):

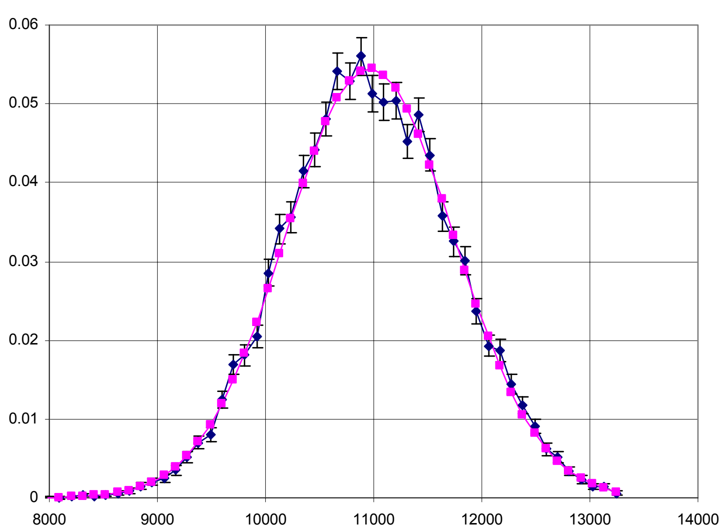
Shell	Mass (kg)	σ_m (kg)
Lead	10.950	0.797
Al	1.941	0.693

- Mass and standard deviation (from Gaussian fit):

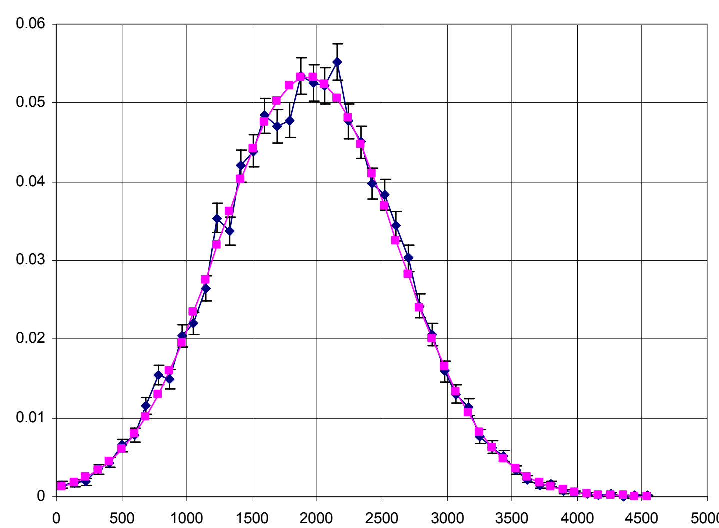
Shell	Mass (kg)	σ_m (kg)
Lead	10.963	0.783
Al	1.931	0.683

- Error propagation formula and Gaussian fit yield similar results.

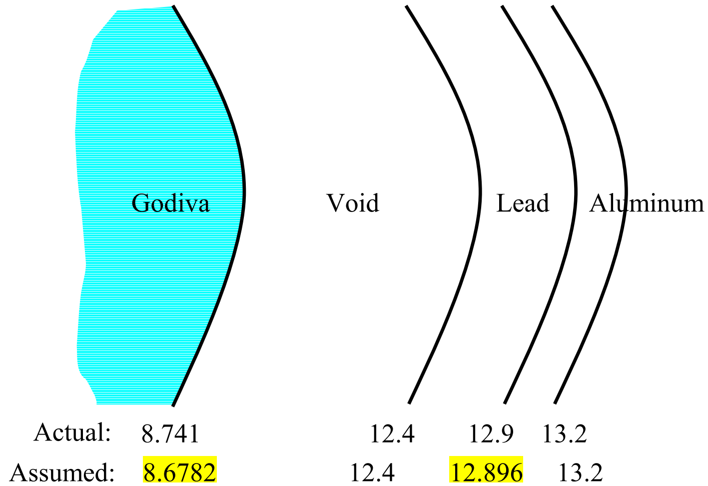
- Lead shell fit



Aluminum shell fit



- Godiva model:



- Mass and standard deviation (from the error propagation formula):

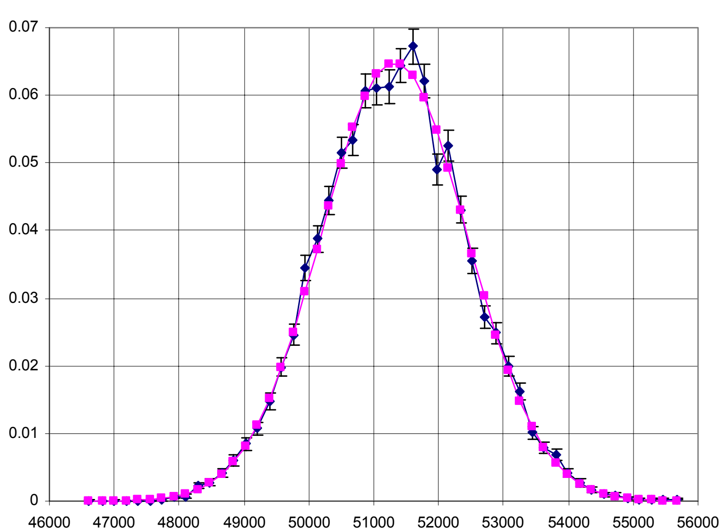
Shell	Mass (kg)	σ_m (kg)
Godiva	51.303	1.132
Lead	11.358	0.388
Al	1.759	0.092

- Mass and standard deviation (from Gaussian fit):

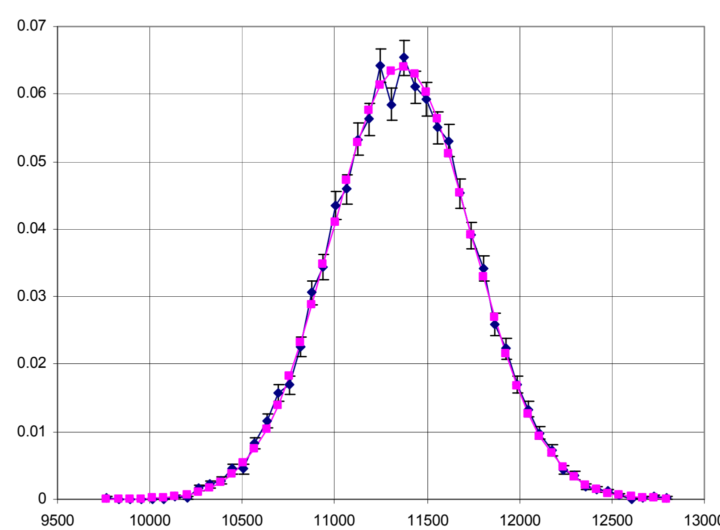
Shell	Mass (kg)	σ_m (kg)
Godiva	51.316	1.125
Lead	11.361	0.382
Al	1.758	0.091

- Error propagation formula and Gaussian fit yield similar results.

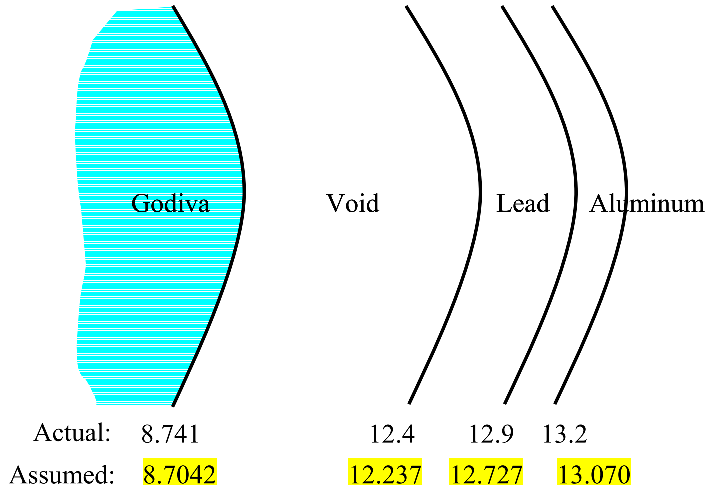
- Godiva fit



Lead shell fit



- Godiva model:



- Note: The Hessian is singular for this problem.

- Mass and standard deviation (from the error propagation formula):

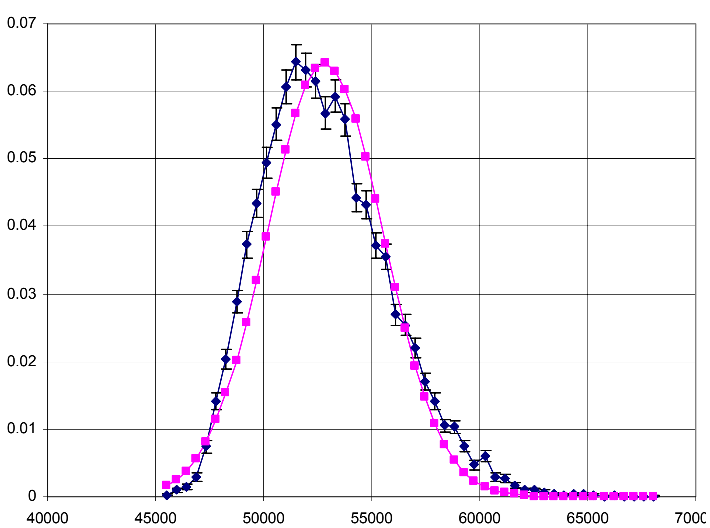
Shell	Mass (kg)	σ_m (kg)
Godiva	51.765	3.543
Lead	10.951	1.043
Al	1.936	2.004

- Mass and standard deviation (from Gaussian fit):

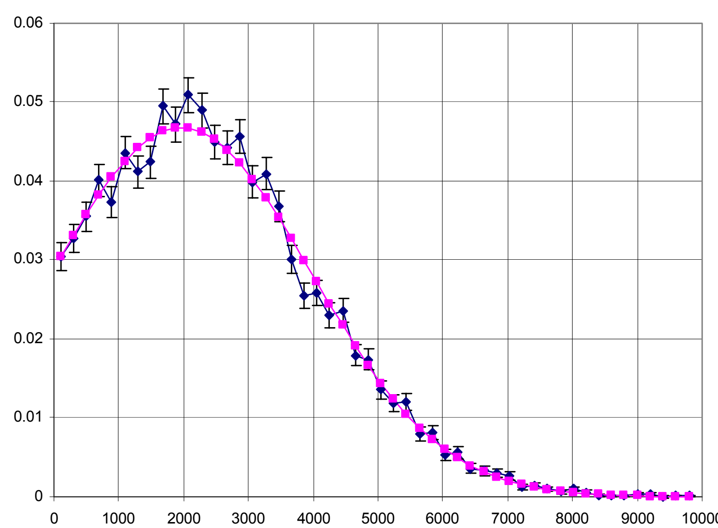
Shell	Mass (kg)	σ_m (kg)
Godiva	52.839	2.698
Lead	10.637	0.782
Al	1.966	2.007

- Which σ_m is correct? (Recall that err. prop. gave correct σ^g for lines.)

- Godiva fit

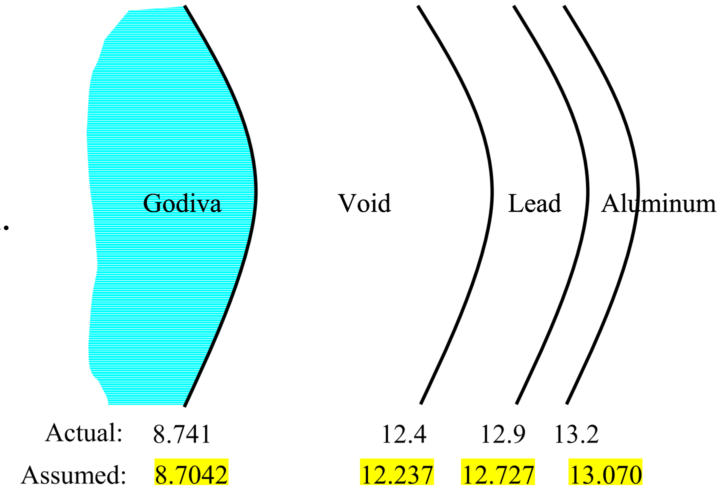


Aluminum shell fit



Test problem 3: All four radii unknown (2)

- Godiva model:



- Note: The Hessian is singular for this problem.

- Mass and standard deviation (from the error propagation formula):

Shell	Mass (kg)	σ_m (kg)
Godiva	51.765	3.543
Lead	10.951	1.043
Al	1.936	2.004

- Gaussian fit:

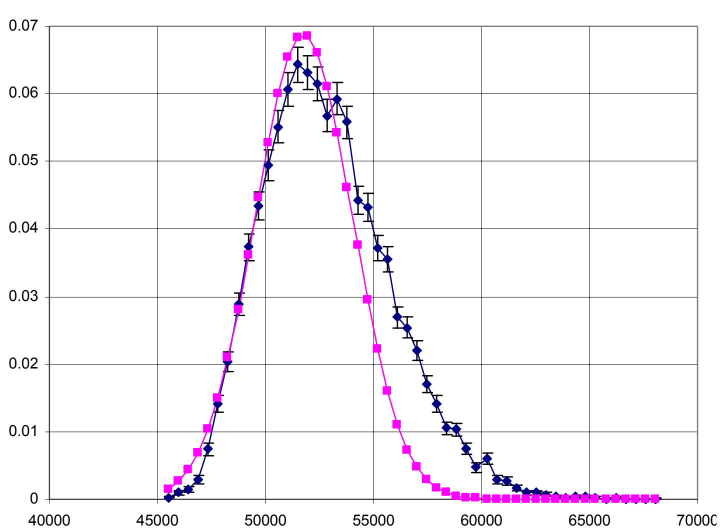
Shell	Mass (kg)	σ_m (kg)
Godiva	52.839	2.698
Lead	10.637	0.782
Al	1.966	2.007

Gaussian fit with mean fixed:

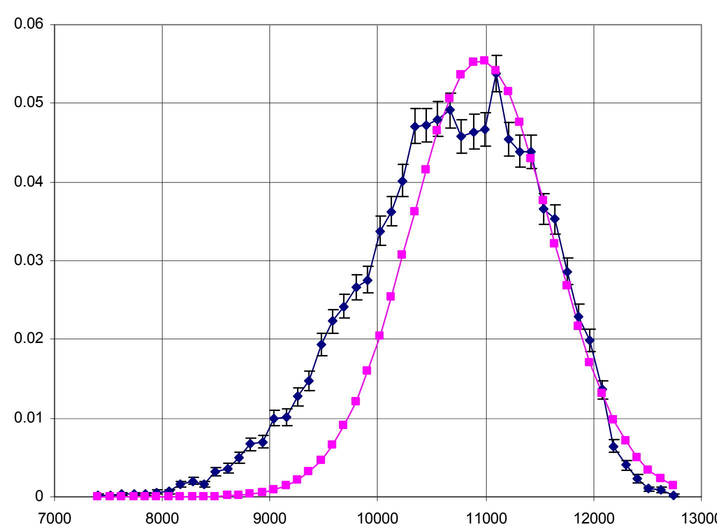
Shell	Mass (kg)	σ_m (kg)
Godiva	51.765	2.264
Lead	10.951	0.662
Al	1.936	2.022

- The fit should be two-sided.

- Godiva fit



Lead shell fit



- We have just begun to apply standard methods of uncertainty quantification to problems of concern to Homeland Security

- The work presented here was performed on a very small budget in order to understand the standard methods

- Numerical tests were run on a problem of interest, but this problem is much easier than the general portal monitor problem

- Areas in need of further research have been identified

  + For σ_m (statistical uncertainty in estimated mass), which is correct: the error propagation formula or Gaussian sampling of the unknown radii?

  + Why is σ^g (statistical uncertainty in line leakage estimated using covariance matrix of unknown radii) accurately calculated from the error propagation formula when the Hessian is singular, but not when the Hessian is not singular?

  + Why is σ^g *not* accurately calculated from Gaussian sampling of the unknown radii?

  + What are the implications of using SVD to invert a singular Hessian?

- Can these methods be applied to the more general portal monitor problem? (What does it mean to minimize χ^2 in such problems?)