SAMMY Workshop Part 4.3b

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Part 4.3b, PUPs & IDCs

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Fitting: Bayes' method, cont.

- **Needed –**
  - **to include all uncertainties for all parameters**
  - **to treat covariance matrices quickly, efficiently, and accurately**
- **Solution –**
  - **use PUPs**
  - **use IDC**

See paper # 119 at ND2004: "Treatment of Data Uncertainties"

Fitting procedure, PUPs

- **Bayes' Equations for updating parameters *P* are**

$$P' - P = M'Y \qquad M' = \left(W + M^{-1}\right)^{-1}$$

$$Y = G^t V^{-1}(d - t) \qquad W = G^t V^{-1} G$$

$$V = v + g\, m\, g^t$$

- **where**
  - **Data can be raw or reduced**
  - **Covariance matrix for reduced data is calculated at the true values of the cross section**
    - **i.e., derivatives are calculated at true values**

"true" ➔ "theoretical"

Benefits of this definition of DCM:

- **Consistent and reasonable results are obtained**
  - **when fitting raw data**
  - **when fitting reduced data**

"results" = values and covariance matrix for varied parameters

- **"All" prior uncertainties are reflected in the final results**
  - **for varied parameters (as usual)**
  - **for unvaried parameters**
    - **experiment-related parameters**
    - **non-varied theory parameters also**

Implementation in SAMMY

- **Any parameter may be treated in this fashion**
  - **Designation: Propagated Uncertainty Parameter**
  - **Short-hand notation: PUP** **(Thanks to Royce Sayer for suggesting this name)**
- **How to use?**
  - **Simply flag with "3" rather than "1" or "0"**
  - **Provide uncertainties for PUPs in the same manner as for varied parameters**

Which parameters can be PUPs?

tr044	(tr009)	resonance parameters (res)
tr059	(tr093)	R-matrix radii (rad)
tr040	(tr011)	R-external (ext)
tr038	(tr007)	broadening etc (brd)
tr041	(tr012)	normalization and background (nbk)
tr097	(tr056)	background functions (bgf)
tr068	(tr021)	Oak Ridge resolution function (orr)
tr096	(tr054)	RPI resolution function (rpi)
tr062	(tr029)	nuclide abundance (iso)
tr066	(many)	miscellaneous parameters (msc)
tr055	(tr055)	paramagnetic cross section (pmc)

Not working yet:
- **detector efficiency (det)**
- **user-defined resolution function (udr)**

PUP test case

Related Un-PUP test case

How do we know the PUP theory and implementation are correct?

- **Use a variety of different methods, compare results**
- **Methods?**
  - **Vary the parameter**
  - **Use explicit data covariance matrix**
  - **Use as PUP with implicit data covariance matrix**
- **What is meant by "results" ?**
  - **Values for the (other) varied parameters**
  - **Associated covariance matrix**

Extensive tests have been made

All five methods give almost Identical results for the first iteration.

1. Treat as fitting parameter
2. If possible, treat as IDC (Implicit Data Covariance) parameter
   - For normalization & backgrounds, this option has been available for many years
3. Treat as user-supplied IDC
   - Derivatives were generated via a special SAMMY run
4. Treat with explicit data covariance
5. Treat as PUP parameter

almost identical results

Identical results

Identical for first iteration

Conclusions: this works!

- **Please see the various SAMMY test cases to compare results from one method to another**
- **One test that has not been systematically done is to simultaneously use several different types of parameters as PUPs**
  - **Check your results carefully to be sure they make sense**
  - **As always, tell me if you uncover problems**
- **Also not extensively tested – PUPs in INPut file**
  - **This *should* work, but look carefully at LPT file to be sure**

PUP'd parameters are indicated by <38> instead of (38), for example.

Limitations on PUPs?

- **Not available yet:**
  - **Off-diagonal covariance matrices for PUPs**

$$P' - P = M'Y \qquad M' = \left(W + M^{-1}\right)^{-1}$$

$$Y = G^t V^{-1}(d - t) \qquad W = G^t V^{-1} G$$

$$V = v + g\,\boxed{m}\,g^t$$

  - **(To be implemented as the need arises)**

Fitting Procedure – IDC

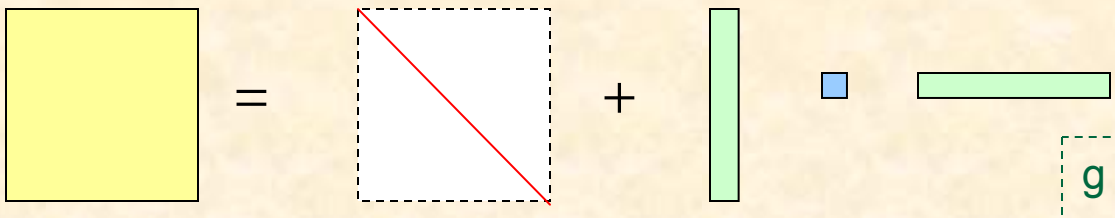
- **Inverting the data covariance matrix V**
  - **Explicitly**
    - **Large number of numbers**
      - **Takes time**
      - **Takes storage**
      - **Becomes inaccurate**
  - **Implicitly**
    - **Use matrix algebra to simplify**

Data Covariance Matrix, symbolically

Statistical part

Systematic part

$$V = v + g\ m\ g^t$$



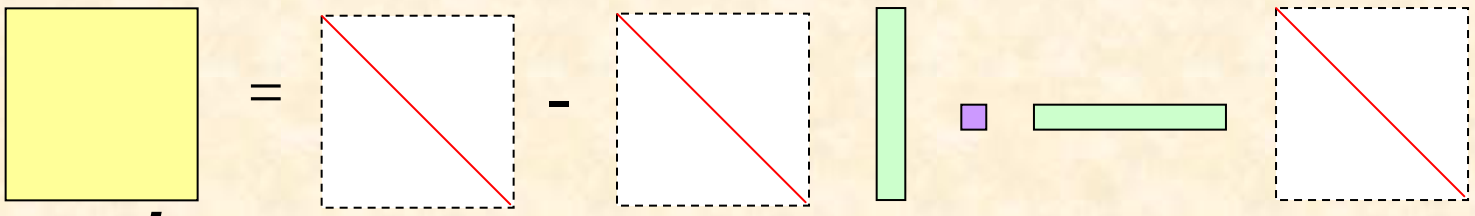
g = sensitivity for data-reduction parameters
m = cov matrix for d-r par

where

- **size of box may be considered to be logarithmic**
  - **large ~ thousands (or 10 K or 100 K)**
  - **small ~ very few (5? 10?)**
- **dashed box with diagonal line indicates diagonal matrix**
- **solid box indicates non-diagonal matrix**

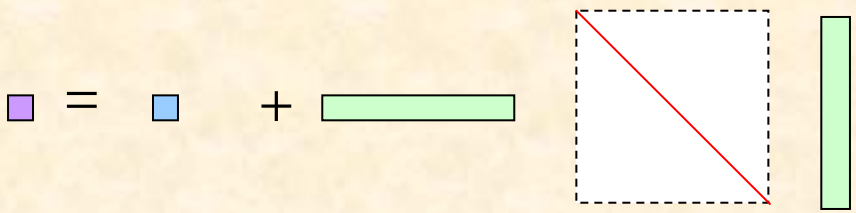
Inverse of Data Covariance Matrix, symbolically

$$V^{-1} = (v + g\ m\ g^t)^{-1}$$
$$= v^{-1} - v^{-1} g\,(m^{-1} + g^t v^{-1} g)^{-1} g^t v^{-1}$$
$$= v^{-1} - v^{-1} g\ Z^{-1}\ g^t v^{-1}$$



where

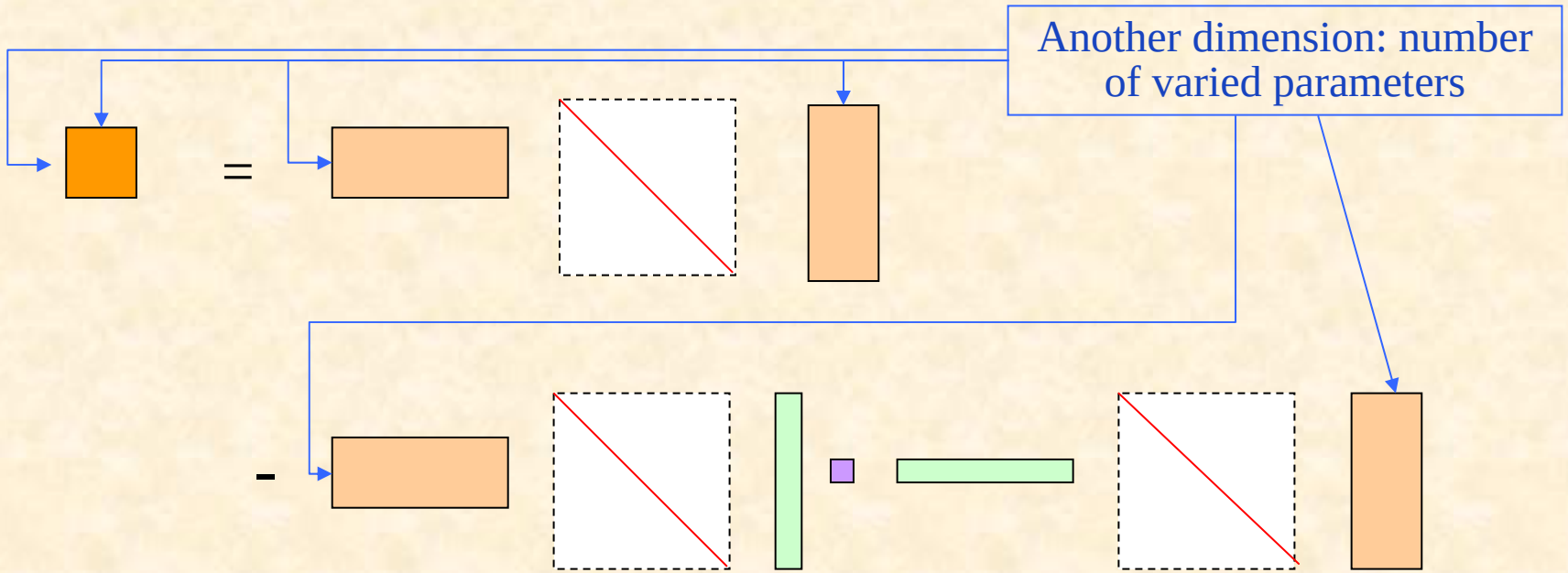
$$Z = m^{-1} + g^t v^{-1}\ g$$



Quantities needed in Bayes' equations: W

$$W = G^t V^{-1} G$$

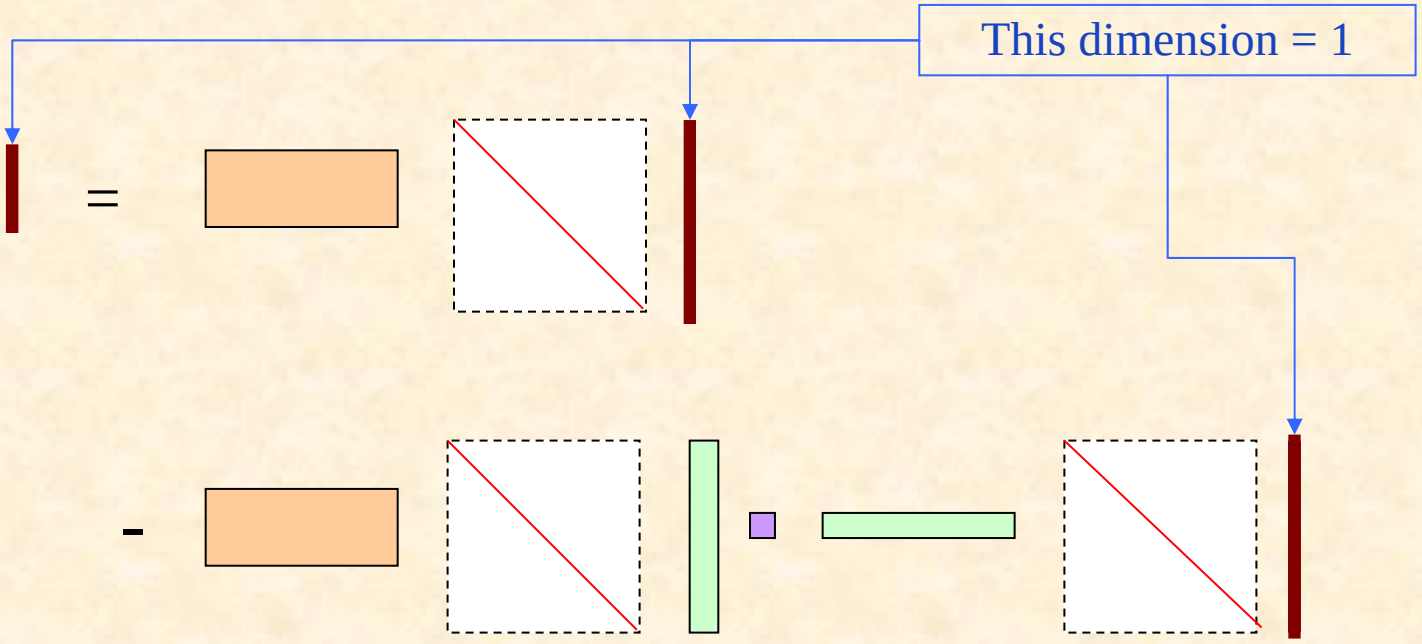
$$= G^t v^{-1} G - G^t v^{-1} g Z^{-1} g^t v^{-1} G$$



Quantities needed in Bayes' equations: Y

$$Y = G^t V^{-1} (D - T)$$

$$= G^t v^{-1} (D - T) - G^t v^{-1} g Z^{-1} g^t v^{-1} (D - T)$$



Why bother with all these arrays?

Matrices in *W* and *Y* are easier to invert than *V* –

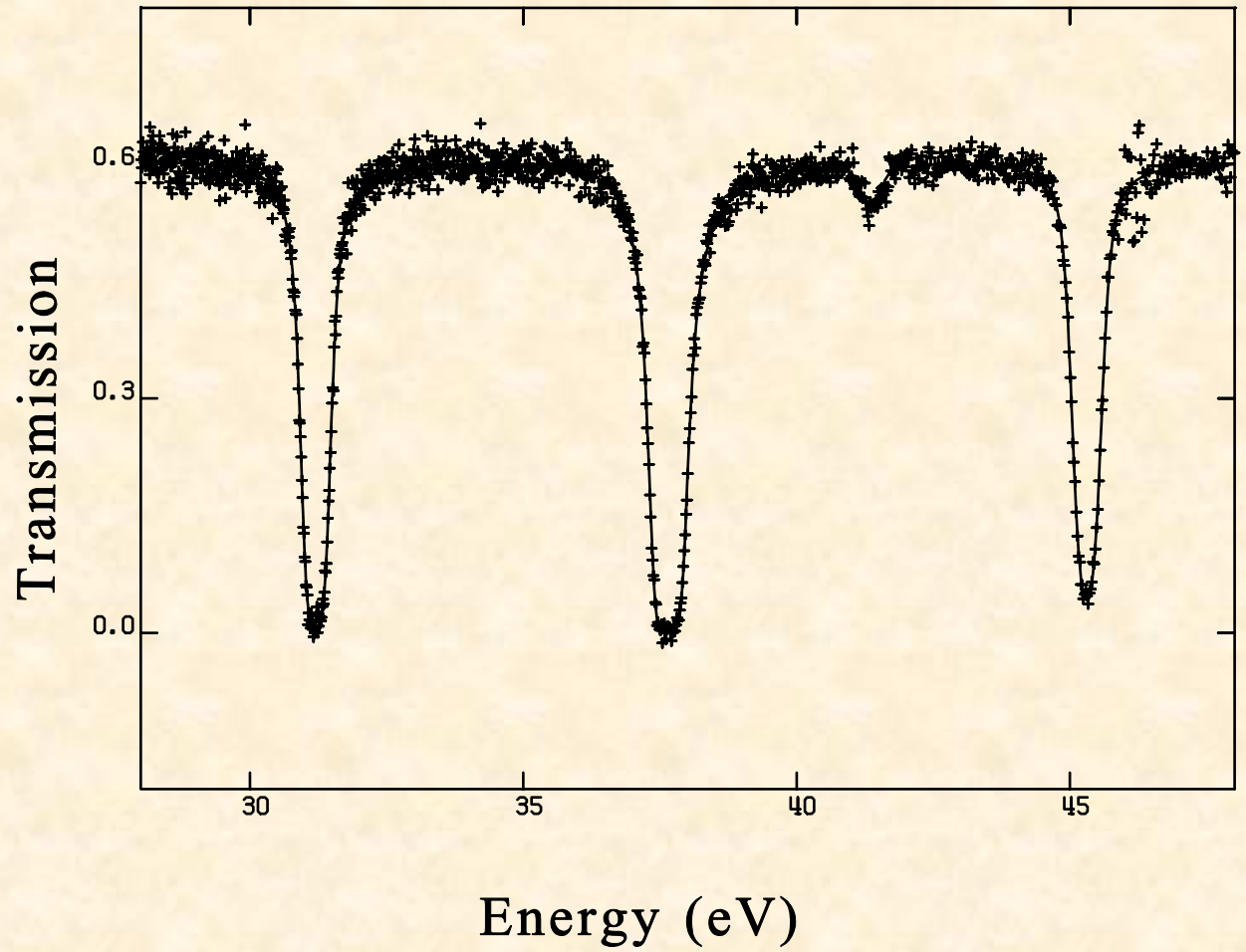
- ***v*** **is large but diagonal**
  - **(size ~ thousands of data points)**
- ***m*** **is small and often diagonal**
  - **(size ~ tens of data-reduction parameters)**
- ***Z*** **is off-diagonal but small**
  - **(size ~ tens)**

– which leads to savings in

- **computation time (never calculate *V* or V^{-1})**
- **computer memory (never store *V* or V^{-1})**
- **numerical accuracy and stability (fewer round-off problems)**

Example from SAMMY Test Case tr140: ^{129}I transmission data

Geel data provided by Gilles Noguere, Cadarache



Example, continued

1245 experimental data points;
[full data set has 32660 data points]
9 data-reduction parameters;
655 resonances; 9 varied parameters in this example

	Description of data covariance treatment for this run	Cpu time for Bayes solver (sec)	Total cpu time (sec)	Array size
a	only statistical errors	0.03	14	254 K
b	statistical plus systematic, only on diagonal	0.03	14	254 K
c	explicit data cov matrix	16.46 = x 500	59	1800 K = x 6
d	IDC matrix	0.06 = x 2	14	267 K = x 1

Note: c & d give essentially the same results provided c is done carefully

In SAMMY, **implicit data covariance (IDC) matrices** can be used for

- ~~**normalization and background correction factors**~~
- **user-supplied implicit data covariance** new
  - **external code can be used to generate pieces (*g* and *m*)**
- **propagated-uncertainty parameters (PUPs)** newer

Caveat

- **Methodology described here implicitly assumes that values for data-reduction parameters are accurate**
  - **Values will not be updated**

- **Nevertheless, final results may reflect inaccuracy in input values for those parameters**
  - **as seen, for example, in studies of mistakes-in-measuring-backgrounds**

Caveat # 2

- **This methodology assumes that Bayes' Equations are correct**
  - **Bayes' Equations are based on the implicit assumption that the parameters obey Gaussian statistics**
  - **That assumption does not hold in general**
  - **Nevertheless that assumption appears to be approximately correct often enough that the equations are useful**