Measurement Error Variances in FRAM: Item-specific Bias As One Contributor To Dark Uncertainty

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Item-specific bias in FRAM. Data set 1 of 8 shown here.

490 measurements on 33 working standards (mass spec assigned nominal values)

FRAM's main task: Infer percentages of Pu isotopes.

Result: this is second top-down study where FRAM exhibits item-specific bias.

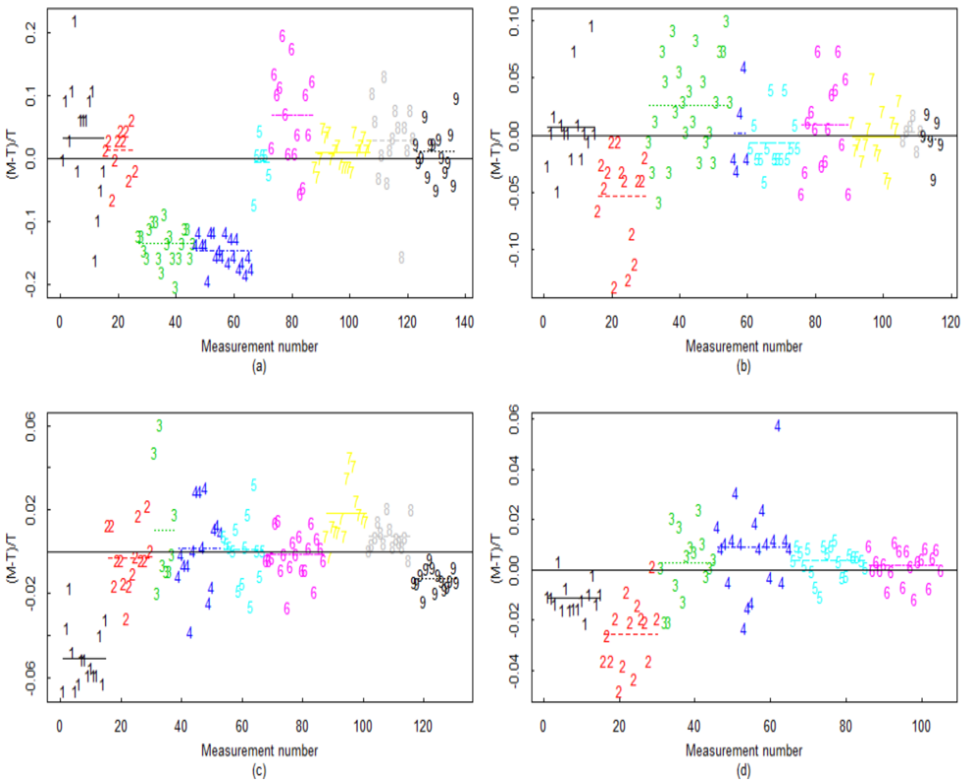
Total RSD is still acceptably small, but want to understand item-specific bias

FRAM's bottom-up RSD estimate of total RSD δ_T is approx. 10% larger than $\delta_R \rightarrow$ bottom-up RSD estimate is too small.

$$I = True(1 + B_I + S_I + R_I)$$

$$S_I \sim N(0, \delta_{SI})$$

$$R_I \sim N(0, \delta_{RI})$$



$$\hat{\delta}_R^2 = \frac{1}{ng - g} \sum_{j=1}^{g} \sum_{k=1}^{n} \left(Y_{jk} - \bar{Y}_j\right)^2$$

$$\hat{\delta}_S^2 = \frac{\sum_{j=1}^{g} \left(\bar{Y}_j - \bar{\bar{Y}}\right)^2}{(g-1)} - \frac{\hat{\delta}_R^2}{n}$$

3 Topics: item-specific bias, ABC, peak area estimation

1. Item-specific bias

$$\hat{\delta}_R^2 = \frac{1}{ng-g}\sum_{j=1}^{g}\sum_{k=1}^{n}\left(Y_{jk}-\bar{Y}_j\right)^2$$

$$\hat{\delta}_S^2 = \frac{\sum_{j=1}^{g}\left(\bar{Y}_j-\bar{\bar{Y}}\right)^2}{(g-1)} - \frac{\hat{\delta}_R^2}{n}$$

Measurand	$\hat{\delta}_R$	$\hat{\delta}_S$	$\hat{\delta}_{Reff}$
1	3.4	4.5	5.6
2	0.2	0.2	0.3
3	1.6	1.1	1.9
4	0.3	0.6	0.7
5	NA	NA	NA
6	1.4	1.5	2.1
7	0.3	0.2	0.3
8	1.5	1.0	1.8

$$\hat{\delta}_T = \sqrt{\hat{\delta}_R^2 + \hat{\delta}_S^2}$$

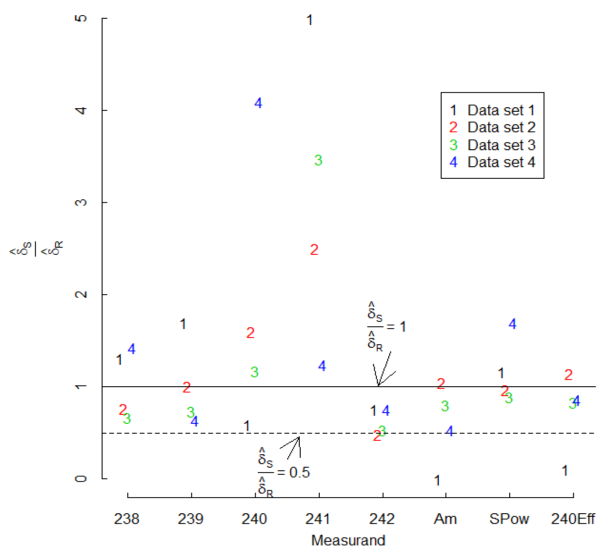
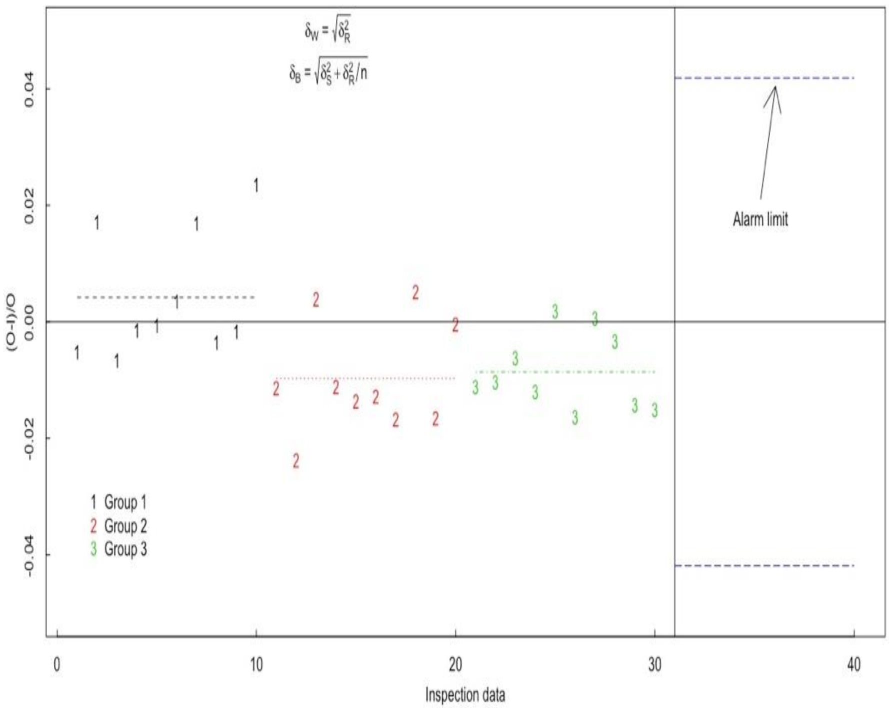
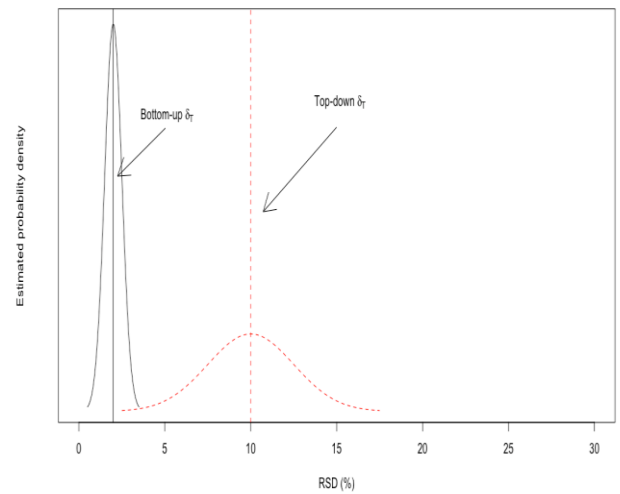


Table 1. Data set 1: Estimated RSDs in %. Plutonium, Planar Detector, 120–460 keV Analysis These estimated RSDs include the 3 mild outliers
The number of repeats for data set 1 for the 33 items are:15, 11, 20, 20, 6, 15, 20, 15, 15, 15, 15, 25, 5, 15, 15, 15, 6, 6, 15, 15, 8, 15, 14, 20, 14, 15, 15, 15, 15,
20,20,20, respectively.

Paired operator, inspector data: top-down UQ via Grubbs' estimation for (O-I)/O within and between periods

(O-I)/O data: total RSD in ITV: $\delta_T = \sqrt{\delta_R^2 + \delta_S^2}$. Long-term bias estimate has standard deviation $\delta_{\hat{B}} = \sqrt{\delta_R^2/_{ng} + \delta_S^2/_g}$ for *g* groups, *n* meas per group

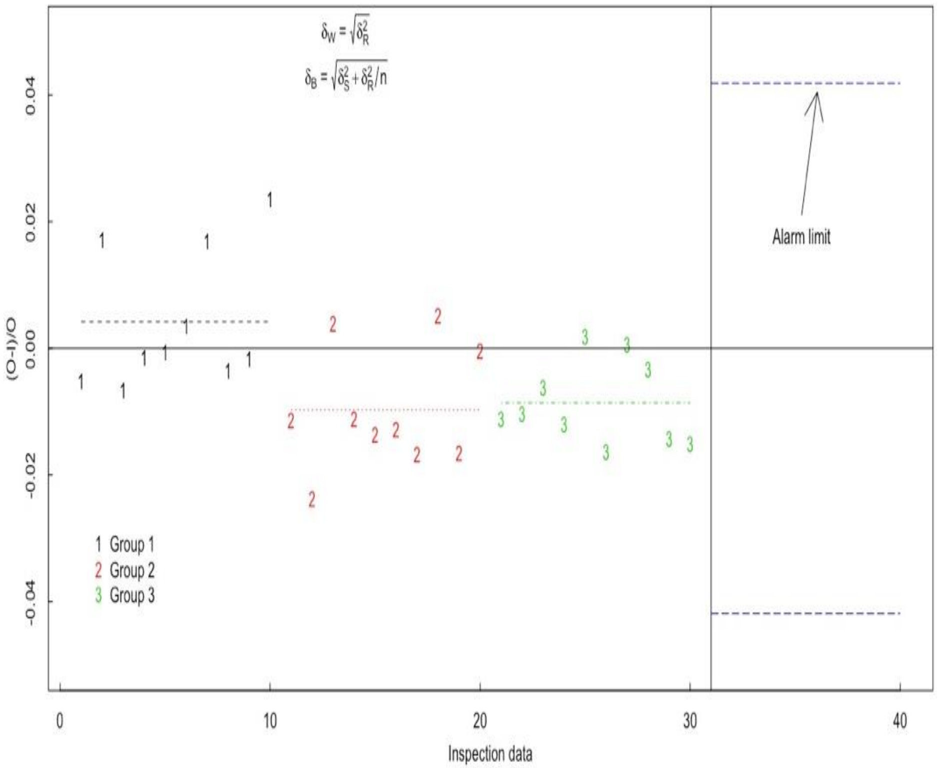




Approximate Bayesian Computation ABC used to estimate δ_T

Dark uncertainty: term to partly explain gap between top-down (Grubbs') and bottom-up RSD estimates

(O-I)/O data



$$I = True(1 + B_I + S_I + R_I)$$

$$S_I \sim N(0, \delta_{SI})$$
$$R_I \sim N(0, \delta_{RI})$$

δ_{RI} is the effective inspector random error AND:

item-specific bias is part of effective random error:

$$\delta_{Reffective} = \sqrt{\delta_{Rep}^2 + \delta_{item-spec}^2}$$

Item-specific bias is **not** currently included in FRAMs bottom-up RSD estimation.

2. ABC

ABC simulates data from a forward model such as

$M = True(1 + B + S + R)$ **for top down**

to approximate posterior probability density function (pdf) of model parameters such as δ_R as in usual Bayes, but does not require a likelihood.

In top down with $M = True(1 + B + S + R)$ there is a likelihood, but can still use ABC and ABC is robust with respect to misspecifying the likelihood.

ABC in nutshell: Specify model parameters B, $\boldsymbol{\delta_S}$, and $\boldsymbol{\delta_R}$ from prior.

Simulate many data sets using $M = True(1 + B + S + R)$.

For each simulated data set, compute summary statistics S using Y = (M-T)/T

S = {$\bar{\bar{Y}}, \hat{\delta}_R^2 = \frac{1}{ng-g}\sum_{j=1}^{g}\sum_{k=1}^{n}\left(Y_{jk} - \bar{Y}_j\right)^2 \;\; \hat{\delta}_S^2 = \frac{\sum_{j=1}^{g}\left(\bar{Y}_j - \bar{\bar{Y}}\right)^2}{(g-1)} - \frac{\hat{\delta}_R^2}{n}$ **}**

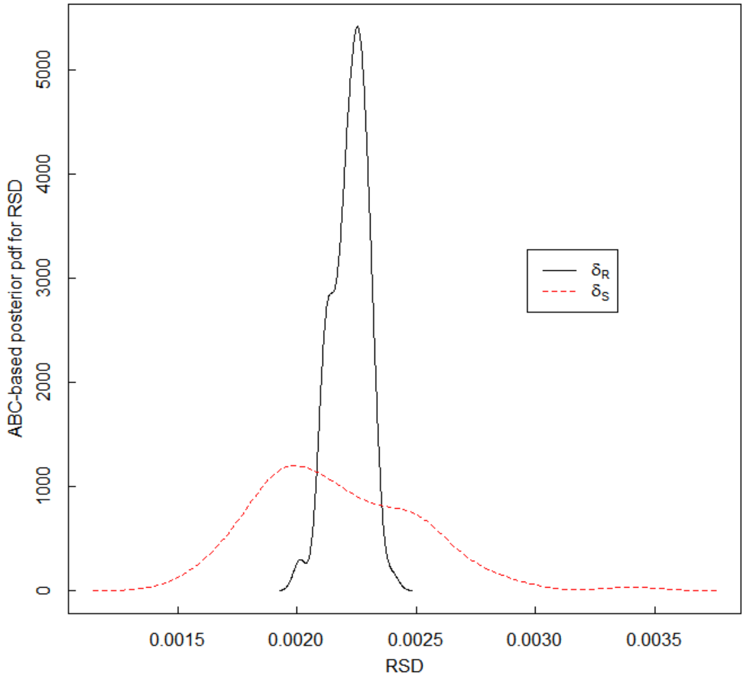
For test case, accept parameters B, $\boldsymbol{\delta_S}$, and $\boldsymbol{\delta_R}$ into posterior whose corresponding S have smallest distance to collection of simulated S's.

2. ABC

ABC simulates data from a forward model such as

$M = True(1 + B + S + R)$ **for top down**

to approximate posterior pdf of model parameters such as δ_S and δ_R



How to check whether ABC is working?

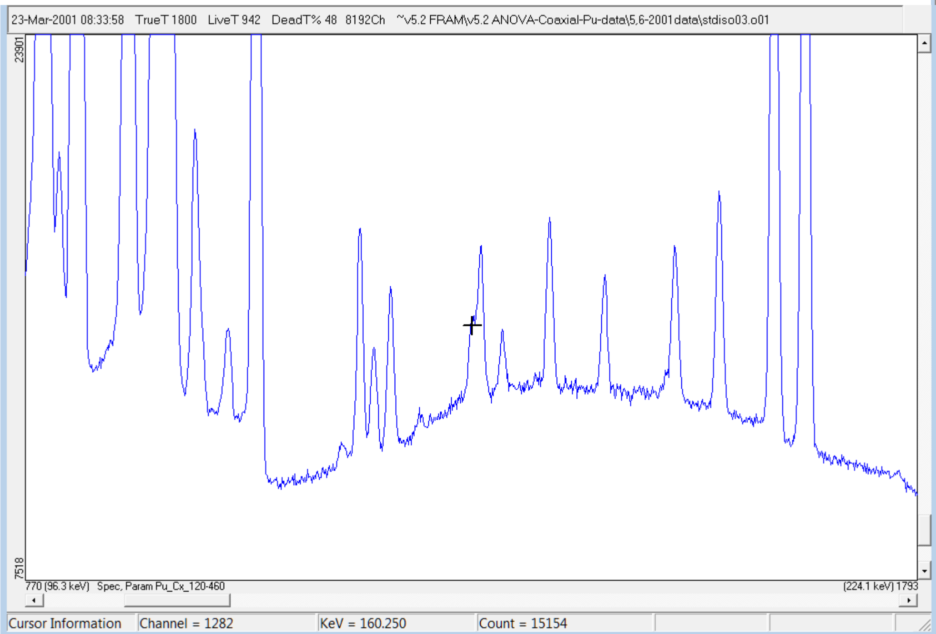
1) Do the nominal probability intervals agree with the true intervals?

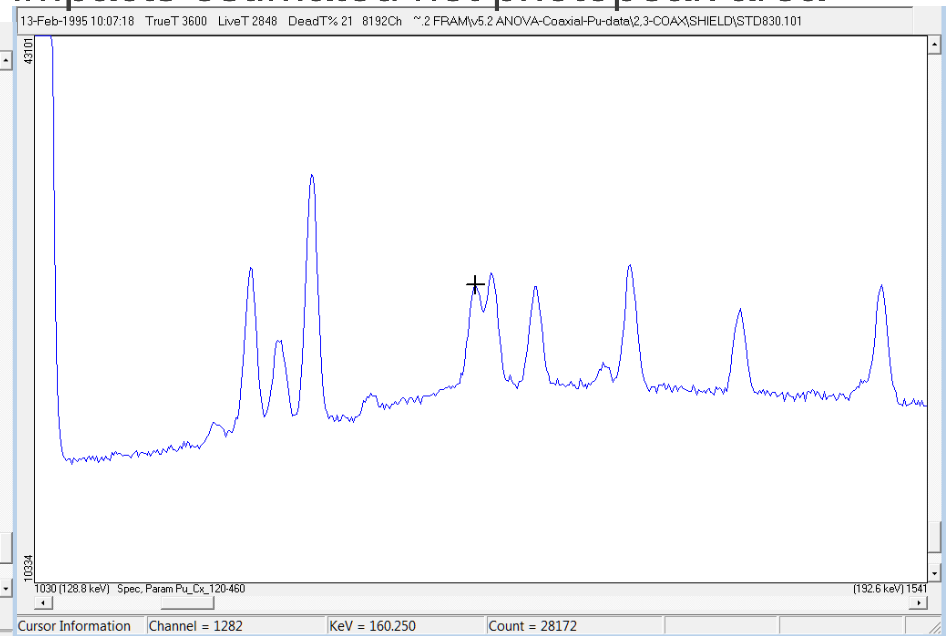
2) Is the SD of the RSD estimates well predicted?

If so, then evidence that ABC is well calibrated.

3. Item-specific bias in FRAM – net peak area estimation?

FRAM uses estimated photopeak areas. Example: near 160 keV
Impurities impact global curvature, which impacts estimated net photopeak area





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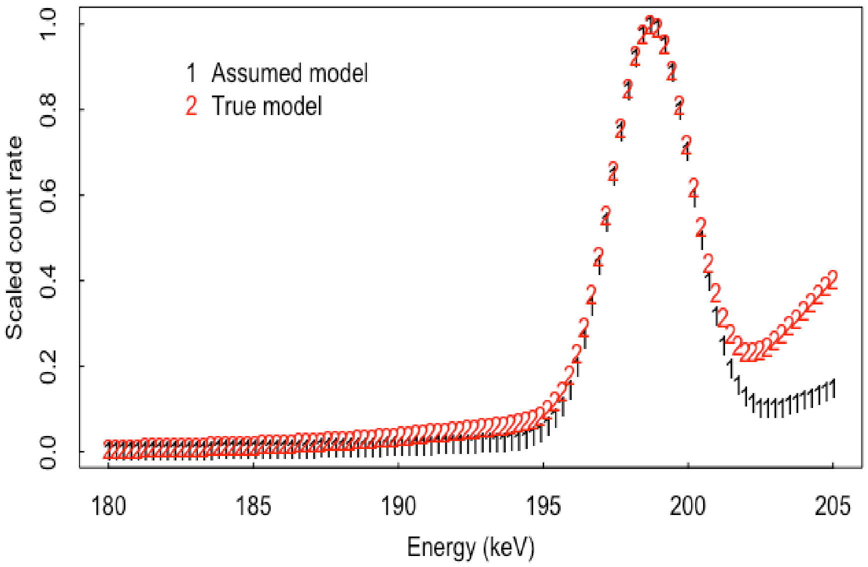
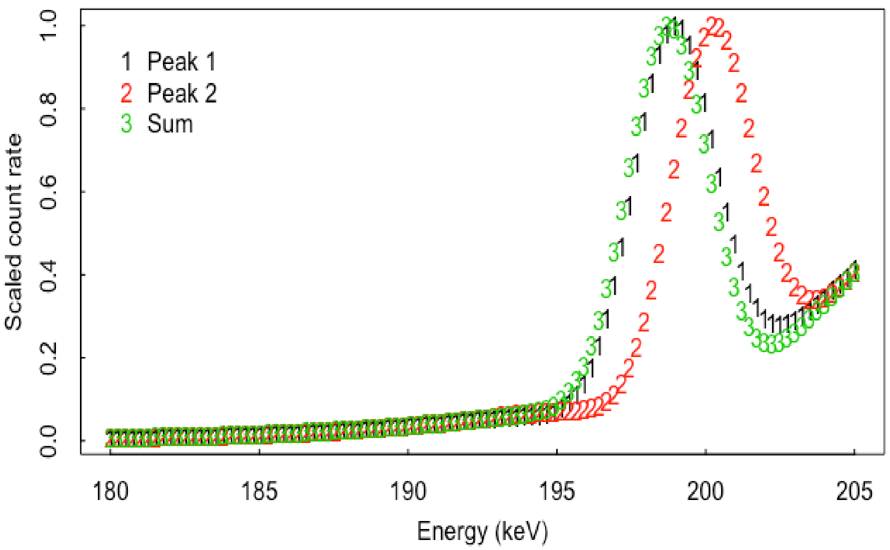




3. Item-specific bias in FRAM using ABC

Case 1. One assumed peak; one true peak. Assumed model is correct model.
Case 2. One assumed peak; one true peak. Assumed model is not the correct model.
Case 3. One assumed peak; two true peaks. Assumed model is the correct model.
Case 4. One assumed peak; two true peaks. Assumed model is not the correct model.
A large number (10^3) of simulated test cases were generated and ABC was applied.
For the 10^3 test cases, the average area estimate, average of true area, *t*-value, *p*-value for Cases 1-4 are listed in Table 1.

Table 1. Average area estimate, average of true area, t-value, and p-value for cases 1-4.

Case	Average area estimate	Average of true area	t-value	p-value
1	55.7	55.9	-0.57	0.57
2	51.5	55.4	-3.9	10^{-4}
3	56.4	57.5	-4.1	10^{-4}
4	51.3	55.9	-8.9	$<10^{-8}$

Summary

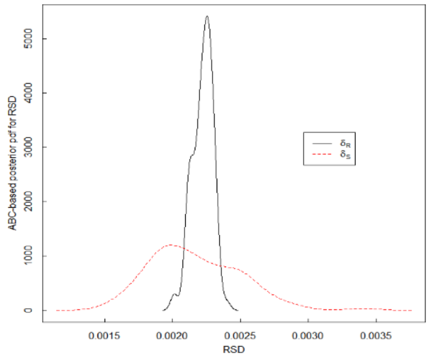
This is second large study that shows item-specific bias in FRAM. NOTE: FRAM's total RSD is still impressively small!

→ **Bayes estimators should have good frequentist properties**

1) **Nominal probability interval coverage should agree with actual**
2) **Estimated posterior standard deviation should agree with RMSE**

Bottom-up RSD estimates tend to be lower than top-down RSD estimates.

Seek understanding of errors in fielded assay methods



Item-specific biases (propagate like random errors). Example reason for item-specific biases: item-specific background and/or peak shape. Can be difficult to express likelihood, so approximate Bayesian computation (ABC).