Covariance update for light elements

Cross Section Evaluation Working Group
Covariance Committee
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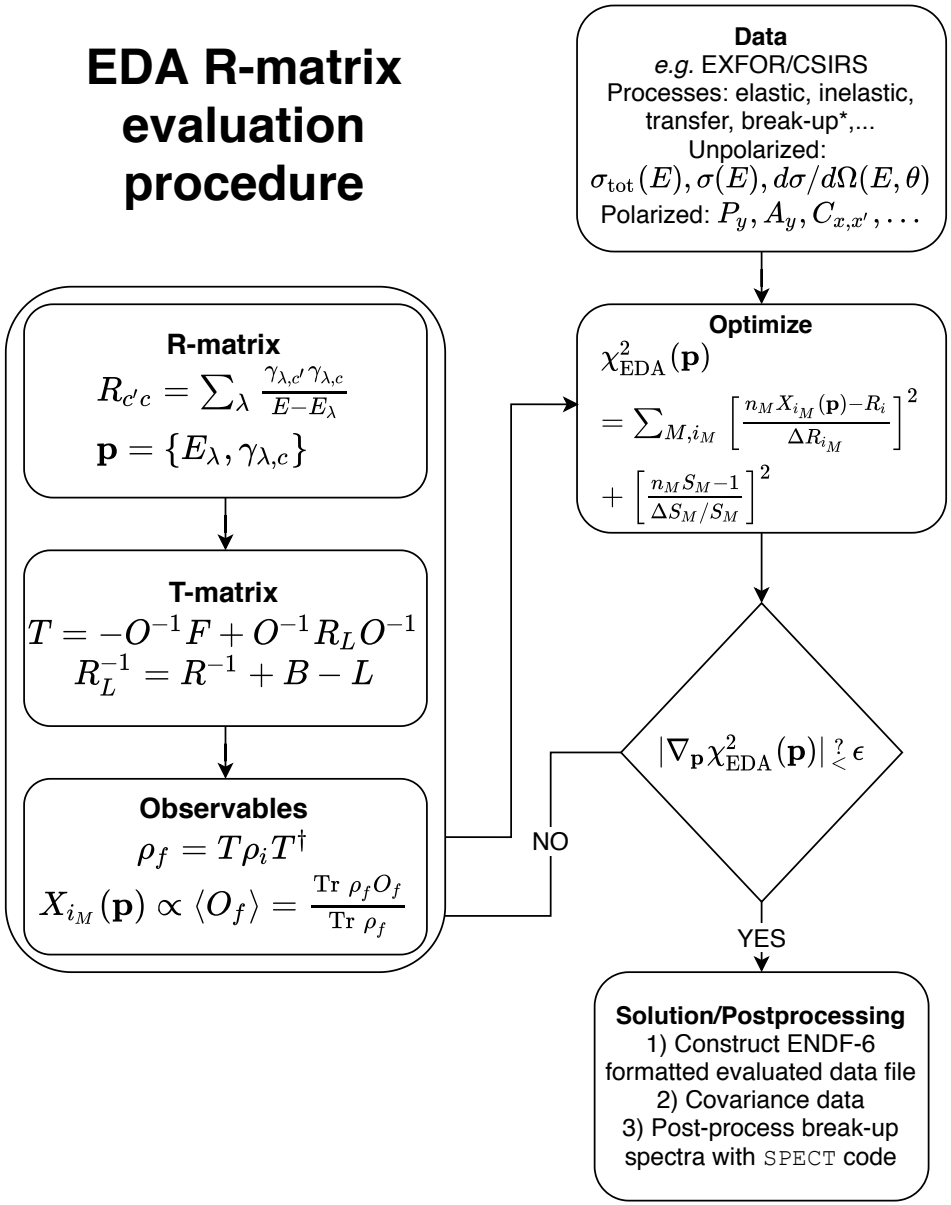
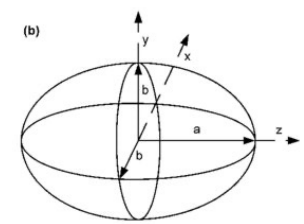
Evaluation flowchart



Parameter uncertainty from χ^2

The Old Way gives too-small uncertainty

- At a solution: $\left.\frac{\partial \chi^2}{\partial p}\right|_{\hat{p}} \approx 0 \qquad \chi^2(p) \approx \chi^2(\hat{p}) + \sum_{\alpha,\beta=1}^{N_p} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$



- Variations at $\hat{p}$:

$$\delta\chi^2(p) = \chi^2(\hat{p} + \delta p) - \chi^2(\hat{p})$$
$$= \delta p_1 A \delta p_1 + \delta p_1 B \delta p_2 + \delta p_2 B^T \delta p_1 + \delta p_2 D \delta p_2$$

- Change in χ^2 when $\{p_2\}$ change, re-optimize $\delta\chi^2$ w.r.t. $\{p_1\}$

$$\delta\chi^2(p_1 + \delta p_1^{min}, p_2 + \delta p_2) = \sum_{\alpha,\beta=N_1+1}^{N_2} \delta p_{2,\alpha} \tilde{D}^{-1}_{\alpha\beta} \delta p_{2,\beta}$$

- $\tilde{D}$: restriction of C to $\{p_2\}$-subspace

$$\delta\chi^2 = \frac{(\delta p_0)^2}{C_{00}} \implies \delta p_0 = (C_{00})^{1/2} \iff \delta\chi^2 = 1$$

- <u>NB</u>: the $\delta\chi^2 = 1$ hypersurface's average distance shrinks with incr. N_p

Parameter variance

- At a solution $\left.\frac{\partial \chi^2}{\partial p}\right|_{\hat{p}} \approx 0$ $\quad \chi^2(p) \approx \chi^2(\hat{p}) + \sum_{\alpha,\beta=1}^{N_p} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$

- Assuming a normal distribution

$$P_c(p|y) = \frac{1}{\det C^{1/2} (2\pi)^{N_p/2}} e^{-\frac{1}{2}\left[\chi^2(p) - \chi^2(\hat{p})\right]},$$

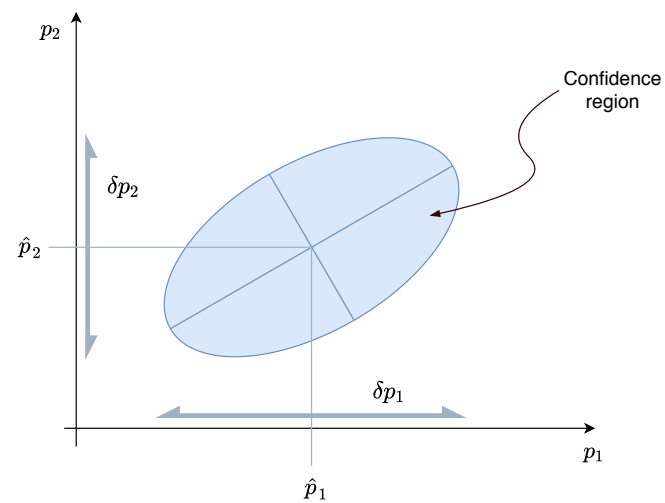
$$\langle (\delta p_\alpha)^2 \rangle = \int_{-\infty}^{\infty} dp_1 \cdots \int_{-\infty}^{\infty} dp_{N_p}\, P_c(p|y) (\delta p_\alpha)^2 = C_{\alpha\alpha}$$

- Change in chi-squared $\quad \delta p_\mu = (C_{\alpha\alpha})^{1/2} \delta_{\mu\alpha}$

$$\delta\chi^2(p) = \chi^2(\hat{p} + \delta p) - \chi^2(\hat{p}) = \sum_{\alpha,\beta} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$$

$$\delta\chi^2(\delta p_\mu) = C_{\mu\mu} C^{-1}_{\mu\mu} = 1 - \sum_{\beta \neq \mu} (C_{\mu\beta})^2 < 1$$

- <u>NB</u>: adding redundant params can lower $\delta\chi^2(\delta p_\mu)$



Uncertainties from chi-squared minimization

Data Covariances from R-Matrix Analyses of Light Nuclei

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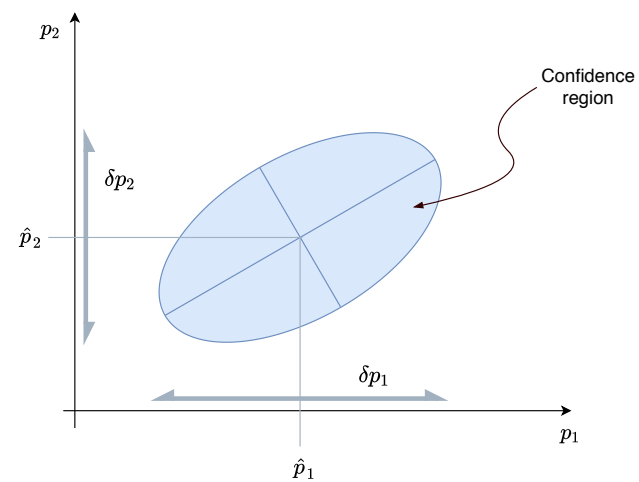
$$\chi^2_{\rm EDA}(\mathbf{p}) = \sum_{M,i_M} \left[\frac{n_{i_M} X_{i_M}(\mathbf{p}) - R_{i_M}}{\delta R_{i_M}}\right]^2 + \left[\frac{n_M S_M - 1}{\delta S_M / S_M}\right]^2 \left\{ \begin{array}{rl} M & : \text{experimental setup} \\ i & : \text{observable} \\ R_{i_M}, \delta R_{i_M} & : \text{relative measurement, uncert.} \\ X_{i_M} & : \text{calc'd observable} \\ n_M & : \text{normalization} \end{array} \right.$$

<u>Uncertainty determination comparison:</u>

1) previous: $\delta\chi^2 = 1 \implies$ Uncertainties too small; scaling: $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$
2) improved:

$$P(\delta\chi^2 | k \text{ DOF}) = \frac{1}{2^{k/2}\Gamma(k/2)} \int_0^{\delta\chi^2} dt\, t^{k/2-1} e^{-t/2} = \text{CL}(68\%: 1-\sigma;\ 95\%: 2-\sigma; \ldots)$$

Better scaling: $\delta p_i \sim (N_p C_{ii})^{1/2}$



Observable error propagation

Covariance matrix

The parameter covariance matrix is $\mathbf{C}_0 = 2\mathbf{G}_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\chi^2(\mathbf{p}) = \chi_0^2 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0)$$
$$= \chi_0^2 + \Delta\chi^2.$$

$$\begin{cases} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

$$\boxed{\begin{aligned} \mathrm{cov}[\sigma_{\mathrm{i}}(E)\sigma_j(E')] &= \left[\nabla_{\mathbf{p}}\sigma_{\mathrm{i}}(E)\right]^{\mathrm{T}}\mathbf{C}_0\left[\nabla_{\mathbf{p}}\sigma_{\mathrm{j}}(E')\right]\Big|_{\mathbf{p}=\mathbf{p}_0} \\ &= \Delta\sigma_{\mathrm{i}}(E)\Delta\sigma_{\mathrm{j}}(E')\rho_{ij}(E,E'). \end{aligned}}$$

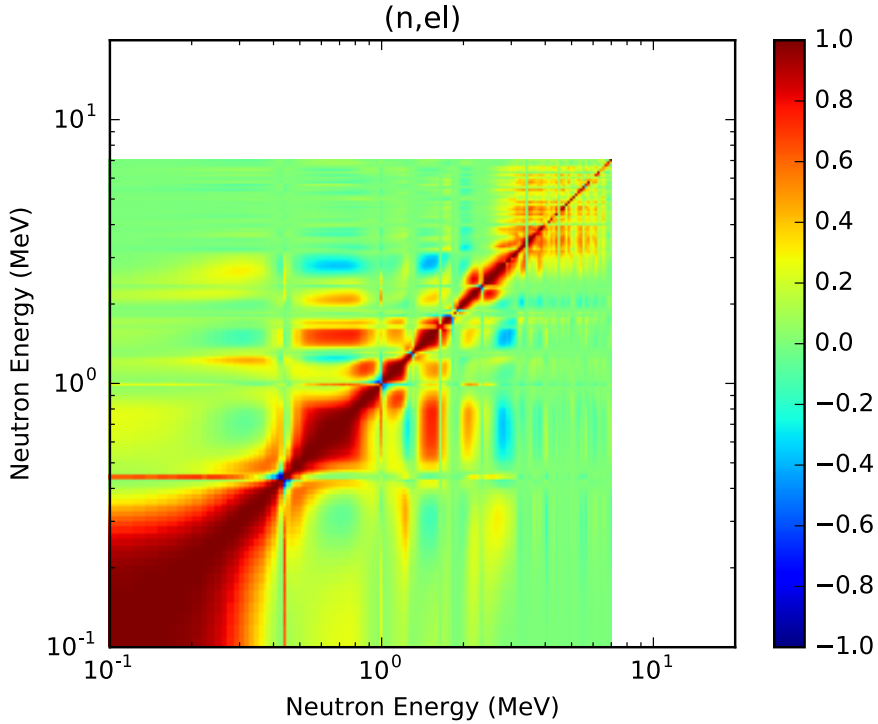
observable uncertainties

correlation coefficient

Example covariance

- ^{17}O system
  - (n,el)
  - correlation matrix
    - elements (-1.0,1.0)

ENDF/B-VIII.0



Fin

Thank you

Covariances for ENDF/B-VIII.1

Anticipated; time-permitting

- CP induced
  - `p-001_H_001.endf`
  - `p-002_He_004.endf`
  - `d-002_He_003.endf`
  - `t-002_He_004.endf`
  - `a-006_C_013.endf`
- n induced
  - `n-003_Li_006.endf`
  - `n-004_Be_009.endf`
  - `n-008_O_016.endf`