



Recent ND developments and plans at UU

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INDEN meeting, October 29, 2018, Vienna

Parameters & Complexity



Outline



Schnabel, G., Sjöstrand, H., Construction of model defect priors inspired by dynamic time warping, WONDER 2018

Motivation of GP regression



Madal | Dafaat

Background + Signal

$$f(E) = a_1 + a_2 E + a_3 \exp\left(-\frac{(\mu - E)^2}{2\sigma^2}\right)$$

More general
$$f(E) = \sum_{k=1}^{\infty} a_k \sin(2\pi ck E)$$

Prior / Regularization

 $a_k \sim \mathcal{N}(0, 1/k)$

$$f(E) = \mathcal{M}_{\vec{p}}(E) + \delta(E) = \mathcal{M}_{\vec{p}}(E) + \sum_{k=1}^{\infty} a_k \sin(2\pi ck E)$$

Gaussian process

- infinite series
- normal prior on coeffs

Covariance matrix

<u>Covariance matrices</u> can represent a variety of things such as normalization uncertainties, linear trends, splines, Fourier series, polynomial expansions, white noise, etc.

$$y(x) = kx + d, \quad k \sim \mathcal{N}(0, \delta_k^2), \quad d \sim \mathcal{N}(0, \delta_d^2)$$

Observations $(\vec{y}_{exp}, \vec{x}_{exp})$

$$\vec{p} = \binom{k}{d} = AS^T \left(SAS^T + B\right)^{-1} \vec{y}_{exp}$$

$$\vec{y}_{pred} = S_{pred} \vec{p} = \left(\vec{x}_{pred}, \vec{1}\right) \binom{k}{d}$$

$$B = \begin{pmatrix} \varepsilon_1^2 & 0 & 0 \\ 0 & \varepsilon_2^2 & 0 \\ 0 & 0 & \ddots \end{pmatrix}$$

$$\kappa(x_1, x_2) := Cov[y(x_1), y(x_2)] = \delta_k^2 x_1 x_2 + \delta_d^2$$

 $K_{\text{pred,exp}} = \kappa(\vec{x}_{\text{pred}}, \vec{x}_{\text{exp}}) \quad K_{\text{exp,exp}} = \kappa(\vec{x}_{\text{exp}}, \vec{x}_{\text{exp}})$

$$\vec{y}_{\text{pred}} = K_{\text{pred,exp}} K_{\text{exp,exp}}^{-1} \vec{y}_{\text{exp}}$$



Power of GP

Powerful concept

Directly parametrize covariance matrix and work implicitly with an infinite number of parameters/basis functions!

$$\kappa(\boldsymbol{x}_1, \boldsymbol{x}_2) = \delta^2 \exp\left(-rac{(\boldsymbol{x}_1 - \boldsymbol{x}_2)^2}{2\lambda^2}
ight)$$



Sample from prior (
$$\delta = \lambda = 1$$
)

Sample from posterior



Energy-dependent parameters



Schnabel, G., Sjöstrand, H., Construction of model defect priors inspired by dynamic time warping, WONDER 2018

Energy-dependent model parameters

- Some parameters energy dependent (e.g., optical potential)
- Use GPs to fine-tune energy dependence to get a better reproduction of data
- Better physics or <u>vehicle to</u>
 <u>treat model defects</u>



Helgesson, P., Sjöstrand, H., 2018. Treating model defects by fitting smoothly varying model parameters: Energy dependence in nuclear data evaluation. Annals of Nuclear Energy 120, 35–47. https://doi.org/10.1016/j.anucene.2018.05.026

Synthetic data study

- Model: "Pseudo-TALYS" (⁵⁶Fe like data)
- Sampled truth:
- $f_{true}(x) = f(x, \beta) (1 + \xi(x))$
 - $-\beta$ and $\xi(x)$ sampled
 - \Rightarrow Varying model defect, $\xi(x)$
- Sampled experimental data

Found: Energy-dependent much more reasonable uncertainties.



Comparison of correlations



Global fit standard TALYS **Local fit** energy-dependent parameters augmented with GPs

Globally informed defect priors



 $k(E, E') = \delta^2 \exp\left(-\frac{1}{2}\frac{(E - E')^2}{\lambda^2}\right)$

Dynamic time warping GP

$$k(E, E') = \delta(E)\delta(E') \exp\left(-\frac{1}{2}\left(m(E) - m(E')\right)^2\right)$$

$$\delta(E) = \sum_{i=1}^{99} \left(\frac{E_{i+1} - E}{E_{i+1} - E_i} \mathbf{y}_i + \frac{E - E_i}{E_{i+1} - E_i} \mathbf{y}_{i+1} \right) \mathcal{I}_{(E_i \le E < E_{i+1})}(E)$$
$$m(E) = \sum_{i=1}^{99} \left(\frac{E_{i+1} - E}{E_{i+1} - E_i} \mathbf{z}_i + \frac{E - E_i}{E_{i+1} - E_i} \mathbf{z}_{i+1} \right) \mathcal{I}_{(E_i \le E < E_{i+1})}(E)$$





Happy! Got promoted to a function!

Global prior construction (n,p) reactions as examples



Resulting defect prior



energy [MeV]

Global defect (n,tot)



Marlike maxim with (n,tot) data





Remark

Optimization was guided by allowing more flexibility at lower than at higher energies.

> Link to animation [GIF] Link to animation [MP4]

Correlation matrices of defect (n,tot)



Ideally: All of them (BMA)

Poor man's BMA [again ⁵⁶Fe update (n,p) and (n,tot)]



Poor man's BMA [again ⁵⁶Fe update (n,p) and (n,tot)]



Correlation structure



energy [MeV]

⁵⁶Fe differential cross sections (n, ...)



Comparison update (def/nodef)



Consistent parameters



Treatment of inconsistent data



Schnabel, G., Sjöstrand, H., Construction of model defect priors inspired by dynamic time warping, WONDER 2018

Inconsistent data = trouble

Proton-Neutron total cross



Fit of

$$\boldsymbol{\sigma}_{\text{fit}}(E) = \frac{\sum_{i=1}^{M} y_i \mathcal{N}\left(E \mid x_i, \lambda^2\right)}{\sum_{j=1}^{M} \mathcal{N}\left(E \mid x_j, \lambda^2\right)}$$

to the neutron-proton total cross section using just statistical uncertainties B_{stat}

Problems

Final fit underestimates uncertainty

Associated $\chi^2/N \approx 16$ too large

Without visual inspection we do not know why

Large amount of data

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Database as of: 2017-04-

Number of ENTRY	21574	experimental works
Number of SUBENT	150976	data tables
Number of Datasets	167857	data tables of reactions
Number of Datapoints	14739297	total number of data points

Example: EXFOR Database

- Around 15 million data points
- No covariance matrices for many measurements
- Direct fitting of models/functions not reasonable

▲ Request #194 Results: Reactions: 203 Datasets: 827							
Data Selection							
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Output: X4+ EXFOR Bibliography TAB C4 PlotC4 Plot: Quick-plot (cross-sections) ungroup Advanced plot [how-to] using C5 and convert ratios to or Narrow incident energy (contingal) e() Min:							
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n Display Year Author-1 Energy range,eV Points Reference							
□ 1) 🛈 🔎 (3-LI-7(N,N+T)2-HE-4,,SIG)/(26-FE-56(N,P)25-MN-56,,SIG) C4: MF=3 MT=?							
Quantity: [CS] Cross section							
1 + 1 X4 X4+ X4± T4 Cov 1987 S.M.Qaim+ 1.00e7 1.05e7 2 + J,NSE,96,52,87							
C 2) 😨 🔎 (26-FE-0(N, INL)26-FE-0, PAR, DA)=(26-FE-56(N, INL)26-FE-56, PAR, DA, , A) C4: MF=4 MT=?							
Quantity: [DAP] Partial differential cross section d/dA							
2 + 1 X4 X4+ X4± T4 1968 E.Barnard+ 9.37e5 1.50e6 226 + J,NP/A,118,321,196810							
3 + 1 X4 X4+ X4+ T4 1.05e6 1.18e6 50							
3 3 0 2 (26-FE-0(N, INL) 26-FE-0, PAR, DA., LEG/RS) = (26-FE-56(N, INL) 26-FE-56, PAR, DA., LEG/RS/A) C4: MF=4							
Quantity: [DAP] Leg.coef.fit part1.4pi/Sig d/dA=1+Sum(a(L)P(L))							
4 + 1 X4 X4+ X4+ T4 1968 E.Barnard+ 1.09e6 1.31e6 6 + J.NP/A.118.321.196810							
4 0 0 (26-FE-0, N. INL) 26-FE-0, PAR, SIG) = (26-FE-56 (N. INL) 26-FE-56, PAR, SIG, A) C4: MF=? MT=?							
3 3 9 $(26-EE-0.0)$ $3/25-MN-56$ Dar Da $(3+/26-EE-56.0)$ $2N/26-EE-57$ Dar Da C A) $(4+ME=4-MT=7)$							
(3) (3) $(26-EE-0)$ (1) $(26-EE-56)$ Dar Da $(3+1/26-EE-56)$ (20) $(26-EE-56)$ Dar Da (-3) (-4) $(ME=4)$ $(ME=7)$							
3) 3 (20-FE-34 (R, INL) 20-FE-34, FAR, DA, G, A) + (20-FE-36 (N, 2N) 20-FE-35, FAR, DA, G, A) C4: MF=4 MT=?							
□ 10) 🕹 🛩 (20-FE-54 (N, INL) 20-FE-54, PAR, SIG, G, A) + (26-FE-56 (N, 2N) 26-FE-55, PAR, SIG, G, A) C4: MF=? MT=?							
11) U → (26-FE-54(N,P)25-MN-54,,SIG)/(26-FE-56(N,P)25-MN-56,,SIG) C4: MF=3 MT=?							

Empirical Bayesian approach $\mathbf{B} = \begin{bmatrix} \mathbf{B}_1 \\ \mathbf{B}_2 \\ & \ddots \end{bmatrix} \quad \vec{\sigma}_{exp} = \begin{pmatrix} \vec{\sigma}_{exp,1} \\ \vec{\sigma}_{exp,2} \\ & \vdots \end{pmatrix}$

Suggestion of a reasonable parametrization (others are possible!)

Additional normalization error (e.g. sample thickness, calibration, ...)

$$\tilde{\mathbf{B}}_i = \mathbf{B}_i + \kappa_i^2 \vec{\sigma}_{\exp,i} \vec{\sigma}_{\exp,i}^T$$

 $\pi_1(\vec{p}_{\text{true}}, \vec{\kappa} \mid \vec{\sigma}_{\text{exp}}, \vec{p}_0, \mathbf{A}_0) \propto \ell(\vec{\sigma}_{\text{exp}} \mid \vec{p}_{\text{true}}, \tilde{\mathbf{B}}(\vec{\kappa})) \times \pi_0(\vec{p}_{\text{true}} \mid \vec{p}_0, \mathbf{A}_0)$

Criteria for choice of prior

- Simple parametrization
- "Uninformative"
- Favor sparse solutions

Schnabel, G., 2017. Fitting and Analysis Technique for Inconsistent Nuclear Data, Proc. of M&C 2017 (arXiv:1803.00960).



 $\times \pi_0$

Schematic application



TABLE I. Posterior maxima κ based on the prior distributions specified in eqs. (50) to (52). For the pdfs ρ_N and ρ_L , results based on different values of δ are presented. Square brackets denote that the respective κ_i was fixed at zero. The index *i* refers to the experiment data set, see fig. 2. The value χ^2/N is the result of eq. (19) divided by the number of data points. Relative likelihoods ℓ are stated for the case ρ_L with $\delta = 0.13$.

Recent: Integral adjustment

• We add an extra uncertainty to each experiment.

$$\sigma_{B,J}^{2} = \sigma_{E}^{2} + \sigma_{stat}^{2} + \sigma_{defects}^{2} + \sigma_{other}^{2} + \sum_{\substack{\text{overall } p \\ \text{where } p \neq J}} \sigma_{ND,p}^{2}$$
$$\sigma_{B,l,J}^{2} = \sigma_{E}^{2} + \sigma_{stat}^{2} + \sigma_{extra,l}^{2} + \sigma_{extra,common}^{2}$$

• σ_{extra} found by maxzimizing L: $L = \frac{1}{\sqrt{(2\pi)^N |\text{cov}_{\text{stat,exp}, \text{extra}}|}} \sum_i e^{\left(\frac{-\chi_i^2}{2}\right)}$



¹Curtesy of Steven Van Der Marck

Sjöstrand, H., Schnabel, G., Helgesson P., Monte Carlo integral adjustment of nuclear data libraries – experimental covariances and inconsistent data, WONDER 2018

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Some results



Benchmark uncertaintes [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Fully correlated
No ML: Reported uncertaintes	100	160	300	170	80	0
Uptated uncertaintes	153	204	300	580	390	0
With correlation	267	329	333	591	409	257

Outlook

- Perform an evaluation of 56Fe with GPs on parameter side1
- Interface recent methodological developments with TALYS/TENDL
- Continue development of methodology for integral adjustment