

## **Probabilistic methods for nuclear data**

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## **Short bio**

- **Studied physics at TU Vienna**
- **PhD in nuclear data evaluation 2015**
- Postdoc at CEA Saclay (2015-2018) and Uppsala University (2018-2019)
- Since 2020 nuclear physicist at Nuclear Data Section of the IAEA dealing with nuclear data library projects, method and code development



## **Challenge #1: Mars rover**



A self-driving vehicle should follow a predefined path on Mars



ghost car



#### **Assumptions**:

Vehicle *approximately* aware of initial position and knows *approximately* speed and direction of movement at any point in time afterwards.

#### **Task:**

Determine current position by  $x_0 = x_{old} + v^* \Delta t$  and adjust speed and direction to stay on desired trajectory

#### **Problem:**

Uncertainty about position puts the rover at risk to fall into a deep crater and get damaged

## **Truth-Estimate divergence**



[Link to movie](http://www.nucleardata.com/storage/presentations/PHENIICS_fest_2017/movies/kalman_robot_error_increase.mp4)

#### **Make use of GPS**



[Link to movie](http://www.nucleardata.com/storage/presentations/PHENIICS_fest_2017/movies/kalman_robot_gps.mp4)

#### **Challenge #2: Face reconstruction**



Taken from the A&T face dataset



#### **Nuclear data**

Probabilities of various nuclear interactions involving the atomic nuclei, e.g., cross sections.







- Radiation dosimetry
- Radiation protection
- Radioactive waste management
- Astrophysics
- Nuclear medicine
- Fusion research
- ...









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Shielding

## **Challenge #3: Nuclear data evaluation**



#### **Two formulas for (at least) three applications**

$$
\vec{p}_1 = \vec{p}_0 + \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} (\vec{\sigma}_{\text{exp}} - M_{\text{lin}} [\vec{p}_0])
$$

$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} \mathbf{S} \mathbf{A}_0
$$

#### **Outline**

Why those equations? Where do they come from?



Application of these formulas to different inference problems

On the way, we will encounter two data science methods



#### **Jaynes Robot**

#### **Hypotheses**

H1: It rained H2: It did not rain





#### **Observations**

O1: The ground is wet O2: The ground is dry





Edwin Thompson Jaynes 1922-1998



#### **Which hypothesis is true?**

Probability Theory The Logic of Science E. T. JAYNES

**CAMBRIDGE** 

## **Consistency with Aristotelian logic**

#### **Hypothesis**



If  $A$  is true, then  $B$  is true  $\boldsymbol{A}$  is true

Therefore,  $B$  is true

#### **Consistency with common sense**

#### **Hypothesis**



 $B$  is true

Therefore,  $A$  becomes more plausible

More

#### **Desiderata**

(I) Degrees of Plausibility are represented by real numbers

(II) Qualitative Correspondence with common sense

(IIIa) If a conclusion can be reasoned out in more than one way, then every possible way must lead to the same result.

(from E.T. Jaynes, Probability Theory: The Logic of Science)



Scanned at the American stitute of Physics

Richard Threlkeld Cox 1898-1991

## **Desiderata / Cox theorem**

(I) Degrees of Plausibility are represented by real numbers

(II) Qualitative Correspondence with common sense

(IIIa) If a conclusion can be reasoned out in more than one way, then every possible way must lead to the same result.

(from E.T. Jaynes, Probability Theory: The Logic of Science)



canned at the American stitute of Physics

Richard Threlkeld Cox 1898-1991

**Computation rules of probability theory follow**

e.g., product rule

 $P(H, O) = P(O | H)P(H)$ 

## **The statistical split**

#### Frequentist statistics **Bayesian statistics**



Ronald Fisher





Egon Pearson



Thomas Bayes



#### Pierre-Simon Laplace

Jerzy Neyman \*

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## **Bayesian update formula**



Thomas Bayes

 $P(H|O) \propto P(O|H)P(H)$ 

- **H** hypothesis (e.g., "It rained")
- **O** observation (e.g., "Floor wet")
- **P(H)** probability of hypothesis to be true
- **P(O|H)** probability to make observation O given hypothesis H is true
- **P(H|O)** probability of hypothesis H given we observed O



1701-1761 Pierre Simon Laplace 1749-1827

#### **Multivariate normal distribution**

$$
\mathcal{N}(\vec{x} \,|\, \vec{x}_0, \mathbf{A}_0) = \frac{1}{\sqrt{(2\pi)^N |\mathbf{A}_0|}} \exp\left(-\frac{1}{2} \left(\vec{x} - \vec{x}_0\right)^T \mathbf{A}_0^{-1} \left(\vec{x} - \vec{x}_0\right)\right)
$$





#### **Covariance matrix**



A covariance matrix captures linear relationships and uncertainties

#### **Putting everything together (at the example of linear regression)**



$$
y(x) = kx + d
$$

## **Putting everything together (prior knowledge "P(H)")**



$$
y(x) = kx + d
$$

 $k \propto \mathcal{N}(0, \delta_k^2)$ 

 $d \propto \mathcal{N}(0, \delta_d^2)$ 

 $\pi(\vec{p}) = \mathcal{N}(\vec{p} | \vec{p}_0, \mathbf{A}_0)$ 

 $\vec{p}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ 

$$
\mathbf{A}_0 = \begin{pmatrix} \delta_k^2 & 0 \\ 0 & \delta_d^2 \end{pmatrix}
$$

## **Putting everything together (likelihood "P(O|H)")**



 $f(\vec{\sigma}_{\text{exp}} | \vec{p}) = \mathcal{N}(\vec{\sigma}_{\text{exp}} | M_{\text{lin}}[\vec{p}], \mathbf{B})$ 

$$
\vec{\sigma}_{\exp} = \begin{pmatrix} \sigma_{\exp,1} \\ \sigma_{\exp,2} \\ \vdots \end{pmatrix} \qquad \qquad \mathbf{B} = \begin{pmatrix} \varepsilon_1^2 & 0 & 0 \\ 0 & \varepsilon_2^2 & 0 \\ 0 & 0 & \ddots \end{pmatrix}
$$

## **Putting everything together (likelihood "P(O|H)")**



# $f(\vec{\sigma}_{\text{exp}} | \vec{p}) = \mathcal{N}(\vec{\sigma}_{\text{exp}} | M_{\text{lin}}[\vec{p}], \mathbf{B})$

$$
\vec{\sigma}_{\exp} = \begin{pmatrix} \sigma_{\exp,1} \\ \sigma_{\exp,2} \\ \vdots \end{pmatrix} \qquad \qquad \mathbf{B} = \begin{pmatrix} \varepsilon_1^2 & 0 & 0 \\ 0 & \varepsilon_2^2 & 0 \\ 0 & 0 & \ddots \end{pmatrix}
$$



Counting statistics  $\rightarrow$  Poisson distribution

 $counts_i$  $\varepsilon_i =$ 

## **Putting everything together (likelihood "P(O|H)")**



#### **Generalized Least Squares (GLS) in a nutshell**



$$
\vec{p}_1 = \vec{p}_0 + \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} (\vec{\sigma}_{\text{exp}} - M_{\text{lin}} [\vec{p}_0])
$$

$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} \mathbf{S} \mathbf{A}_0
$$

"GLS formulas"

#### **And the result?**



## **Important insight about models**

"All models are wrong but some are useful"

- George E. P. Box



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Ice cream or pizza?





Reality



#### **How to deal with a deficient model (or to come up with a good one)?**

$$
y(x) = a_0 + a_1 x + a_2 x^2
$$

$$
a_0 \propto \mathcal{N}(0, \delta_{a_0}^2)
$$
  
\n
$$
a_1 \propto \mathcal{N}(0, \delta_{a_1}^2)
$$
  
\n
$$
a_2 \propto \mathcal{N}(0, \delta_{a_2}^2)
$$
  
\n
$$
\vec{p}_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
$$
  
\n
$$
\mathbf{A}_0 = \begin{pmatrix} \delta_{a_0}^2 & 0 & 0 \\ 0 & \delta_{a_1}^2 & 0 \\ 0 & 0 & \delta_{a_2}^2 \end{pmatrix}
$$

But what if it is too difficult to find a good analytic function?

#### **Surrogate approach**

#### **Assumptions**:

- Access to a good physics model
- Ability to perform hundreds to thousands of model calculations using different parameter values in good time
- Each model calculation yields predictions on a dense mesh and we can use linear interpolation between mesh points



#### **Surrogate approach basic idea**



 $\pi(\vec{p}_{\text{true}} | \vec{\sigma}_{\text{exp}}, M) \propto f(\vec{\sigma}_{\text{exp}} | \vec{p}_{\text{true}}, M) \pi(\vec{p}_{\text{true}} | M)$ 

#### **Surrogate approach construction of M sur**

1) draw ensemble  $\vec{p}_1 \vec{p}_2, \vec{p}_3, \ldots, \vec{p}_n$  from prior distribution  $\pi(\vec{p}_{\text{true}} | M)$ 2) use nuclear model to calculate  $\vec{\sigma}_1 = M[\,\vec{p}_1\,], \vec{\sigma}_2 = M[\,\vec{p}_2\,], \ldots$ 

3) estimate multivariate normal distribution in observation space

$$
\vec{\sigma}_0 = \frac{1}{n} \sum_{i=1}^n \vec{\sigma}_i \qquad \mathbf{A}_0 = \frac{1}{n} \sum_{i=1}^n (\vec{\sigma}_i - \vec{\sigma}_0)(\vec{\sigma}_i - \vec{\sigma}_0)^T \qquad M_{\text{sur}}[\sigma_{\text{true}}] = \mathbf{S} \vec{\sigma}_{\text{true}}
$$



**Generalized Least Squares formulas**

$$
\begin{aligned} \mathbf{A}_1 &= \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} \mathbf{S} \mathbf{A}_0 \\ \vec{\sigma}_1 &= \vec{\sigma}_0 + \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} (\vec{\sigma}_{\text{exp}} - M_{\text{sur}}[\vec{\sigma}_0]) \end{aligned}
$$

## **Application to nuclear data evaluation face reconstruction**



We have a sample of model predictions faces

#### **Representation of faces**



#### **All the matrices in their glory details**

**Prior belief**

$$
\vec{x}_0 = \frac{1}{N} \sum_{i}^{400} \vec{f}_i \qquad \mathbf{A}_0 = \frac{1}{N} \sum_{i}^{400} (\vec{f}_i - \vec{x}_0) (\vec{f}_i - \vec{x}_0)^T
$$
\n**Observation**\n
$$
\vec{y} = \begin{pmatrix} o_{12} \\ o_{28} \\ \vdots \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} 0.1^2 & 0 & \dots \\ 0 & 0.1^2 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 & 1 & \dots & 0 & \dots \\ 0 & 0 & \dots & 1 & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix} \quad \vec{x} = \begin{pmatrix} r_{11} \\ \vdots \\ r_{21} \\ r_{22} \\ \vdots \end{pmatrix}
$$
\n
$$
\text{improved estimate}
$$
\n
$$
\vec{x}_1 = \vec{x}_0 + \mathbf{A}_0 \mathbf{S}^T \left( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \right)^{-1} (\vec{y} - \mathbf{S} \vec{x}_0)
$$
\n
$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T \left( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \right)^{-1} \mathbf{S} \mathbf{A}_0
$$

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## **Example result**

Observation (5%) Prediction Criginal

#### **Ok, let's do also nuclear data evaluation with this approach**



#### **But what if...**



… we don't have a good physics model nor a comprehensive database

… we don't know a good analytic function to be used as model

#### **Idea: Use a function to construct covariance matrices**



$$
\mathbf{y} \sim \mathcal{N}(\vec{m}, \mathbf{K})
$$

$$
\vec{m} = \begin{pmatrix} \mu(x_1) \\ \mu(x_2) \\ \mu(x_3) \\ \vdots \end{pmatrix} \qquad \mathbf{K} = \begin{pmatrix} \kappa(x_1, x_1) & \kappa(x_1, x_2) & \kappa(x_1, x_3) & \dots \\ \kappa(x_2, x_1) & \kappa(x_2, x_2) & \kappa(x_2, x_3) & \dots \\ \kappa(x_3, x_1) & \kappa(x_3, x_2) & \kappa(x_3, x_3) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}
$$

#### **Covariance function**

Specify a function that yields the covariance between function values  $f(x_1)$  and  $f(x_2)$  for any possible pair  $x_1$  and  $x_2$ . This function is called a **covariance function**.

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

Specify another function μ(**x**) that yields the center value of the process at location **x**. This function is called a **mean function**.

$$
\mu(\mathbf{x})=0
$$

#### **Different covariance functions and the prior knowledge they induce**



#### **Gaussian process regression**

#### **Powerful concept**

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

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





## **Computational mesh and experimental mesh**

Introduce computational mesh **U** and experimental mesh **V**



#### **A few covariance matrices**

$$
\mathbf{K}_{UU} = \begin{pmatrix}\n\kappa(x_{U,1}, x_{U,1}) & \kappa(x_{U,1}, x_{U,2}) & \kappa(x_{U,1}, x_{U,3}) & \cdots \\
\kappa(x_{U,2}, x_{U,1}) & \kappa(x_{U,2}, x_{U,2}) & \kappa(x_{U,2}, x_{U,3}) & \cdots \\
\kappa(x_{U,3}, x_{U,1}) & \kappa(x_{U,3}, x_{U,2}) & \kappa(x_{U,3}, x_{U,3}) & \cdots \\
\vdots & \vdots & \vdots & \ddots\n\end{pmatrix}
$$
\n
$$
\mathbf{K}_{VV} = \begin{pmatrix}\n\kappa(x_{V,1}, x_{V,1}) & \kappa(x_{V,1}, x_{V,2}) & \kappa(x_{V,1}, x_{V,3}) & \cdots \\
\kappa(x_{V,2}, x_{V,1}) & \kappa(x_{V,2}, x_{V,2}) & \kappa(x_{V,2}, x_{V,3}) & \cdots \\
\kappa(x_{V,3}, x_{V,1}) & \kappa(x_{V,3}, x_{V,2}) & \kappa(x_{V,3}, x_{V,3}) & \cdots \\
\vdots & \vdots & \vdots & \ddots\n\end{pmatrix}
$$
\n
$$
\mathbf{K}_{UV} = \begin{pmatrix}\n\kappa(x_{U,1}, x_{V,1}) & \kappa(x_{U,1}, x_{V,2}) & \kappa(x_{U,1}, x_{V,3}) & \cdots \\
\kappa(x_{U,2}, x_{V,1}) & \kappa(x_{U,2}, x_{V,2}) & \kappa(x_{U,1}, x_{V,3}) & \cdots \\
\kappa(x_{U,3}, x_{V,1}) & \kappa(x_{U,3}, x_{V,2}) & \kappa(x_{U,3}, x_{V,3}) & \cdots \\
\vdots & \vdots & \vdots & \ddots\n\end{pmatrix}
$$

## **Applying the GLS formulas**

Use GLS formulas:

$$
\vec{p}_1 = \vec{p}_0 + \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} (\vec{\sigma}_{\text{exp}} - M_{\text{lin}} [\vec{p}_0])
$$

$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T (\mathbf{S} \mathbf{A}_0 \mathbf{S} + \mathbf{B})^{-1} \mathbf{S} \mathbf{A}_0
$$



Make the following assignments:

$$
\mathbf{A}_0 \to \mathbf{K}_{UU}
$$
  

$$
\vec{p}_0 \to \vec{m}_U
$$

$$
M_{\text{lin}}[\vec{p}_0] \to \vec{m}_V
$$

$$
\mathbf{SA}_0 \mathbf{S}^T \to \mathbf{K}_{VV}
$$

$$
\mathbf{SA}_0 \to \mathbf{K}_{VU}
$$

#### **GPs constrained with observations**



The posterior covariance matrix encodes more than just uncertainties!

#### **GPs constrained with observations**



## **Comparison to neural networks**



2  $\mathbf{1}$ 

Both approaches …

- … are methods for classification and regression
- … are universal function approximators

Neural networks …

- … scale better to large data sets
- … are able to capture non-local features
- … are difficult to interpret

GP processes …

- … are statistical methods from the ground up (uncertainties)
- … facilitate the incorporation of prior assumptions
- … interface well with existing nuclear data evaluation methods

## **Summary**

- Two formulas for inference for at least three applications (GLS)
- Presented an argument to motivate the use of Bayesian statistics
- Employed the multivariate normal distribution
- Generalized Least Squares method applied in different ways
- Finally, we talked about Gaussian process regression which can be regarded as special case of Bayesian GLS if we discretize the function (or vice-versa)

## **Bonus: Mars rover**



**Task**: An automated vehicle should follow a predefined path on Mars



ghost car



#### **Hypothetical approach**:

**a)** Vehicle is aware of initial position and its speed and direction of movement at any point in time afterwards. **b)** Determine current position by  $x_0 = x_{old} + v^* \Delta t$ **c)** Adjust speed and direction to stay on desired trajectory

#### **Problems**:

Neither initial position nor speed nor direction are perfectly known. This introduces uncertainty about the current position.

**State and error propagation**:

$$
\vec{x}_0 = \vec{x}_{\mathrm{old}} + \vec{v}\Delta t \quad \mathbf{A}_0 = \mathbf{A}_{\mathrm{old}} + \mathbf{V}\Delta t^2
$$

#### **Update equations**

Prior belief

 $\vec{x}_0 = \vec{x}_{old} + \vec{v}\Delta t$   $\mathbf{A}_0 = \mathbf{A}_{old} + \mathbf{V}\Delta t^2$ 

**Observation** 

 $\vec{y}$  ... GPS position estimate  $\mathbf{B} = \begin{pmatrix} 20^2 & 0 \\ 0 & 20^2 \end{pmatrix}$   $\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ 

Improved estimate

$$
\vec{x}_1 = \vec{x}_0 + \mathbf{A}_0 \mathbf{S}^T \Big( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \Big)^{-1} (\vec{y} - \mathbf{S} \vec{x}_0)
$$

$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T \Big( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \Big)^{-1} \mathbf{S} \mathbf{A}_0
$$

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## **Using a laser guidance system**



Prior belief

$$
\vec{x}_0 = \vec{x}_{old} + \vec{v}\Delta t \quad \mathbf{A}_0 = \mathbf{A}_{old} + \mathbf{V}\Delta t^2
$$

**Observation** 

 $\vec{y}$  ... horizontal position estimate

$$
\mathbf{B} = \left(0.2^2\right) \quad \mathbf{S} = \left(1 \quad 0\right)
$$

Improved estimate

$$
\vec{x}_1 = \vec{x}_0 + \mathbf{A}_0 \mathbf{S}^T \Big( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \Big)^{-1} (\vec{y} - \mathbf{S} \vec{x}_0)
$$

$$
\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T \Big( \mathbf{S} \mathbf{A}_0 \mathbf{S}^T + \mathbf{B} \Big)^{-1} \mathbf{S} \mathbf{A}_0
$$

## **Using a laser guidance system**



[Link to movie](http://www.nucleardata.com/storage/presentations/PHENIICS_fest_2017/movies/kalman_robot_gps_laser.mp4)

#### **References**

- E. T. Jaynes "Probability Theory: The Logic of Science" (first chapters available online for free)
- C. E. Rasmussen & C. K. I Williams, "Gaussian processes for Machine Learning", <http://www.gaussianprocess.org/gpml/>
- GitHub repository with the scripts and videos of this presentation: <https://github.com/gschnabel/compnuc-workshop-2022>