The Bayesian Analysis of Nuclear Dynamics Framework

Özge Sürer, Moses Chan

On behalf of BAND collaboration

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Outline

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BAND Framework

BAND Framework

- Reliable predictions for experimentally inaccessible environments
- Uncertainty quantification by creating an extendible software base
- Cyberinfrastructure framework is Bayesian
- Suite of codes will serve a broad community of nuclear physicists

BAND Framework

https://bandframework.github.io

https://github.com/bandframework/bandframework

Check out the tools and examples in BAND Framework v0.2! And stay tuned for additional capabilities in v0.3!

BAND Framework v0.2

- Tools:
  - `surmise`: Surrogate model interface for calibration, uncertainty quantification, and sensitivity analysis
  - `SaMBA`: Sandbox for Mixing via Bayesian Analysis
- Examples:
  - QGP Bayes: Tutorial on Bayesian analysis of QGP simulations
  - BRICK: Bayesian R-matrix Inference Code Kit
  - BFRESCOX: Emulation and Bayesian model calibration of coupled-channels treatment of nuclear reactions

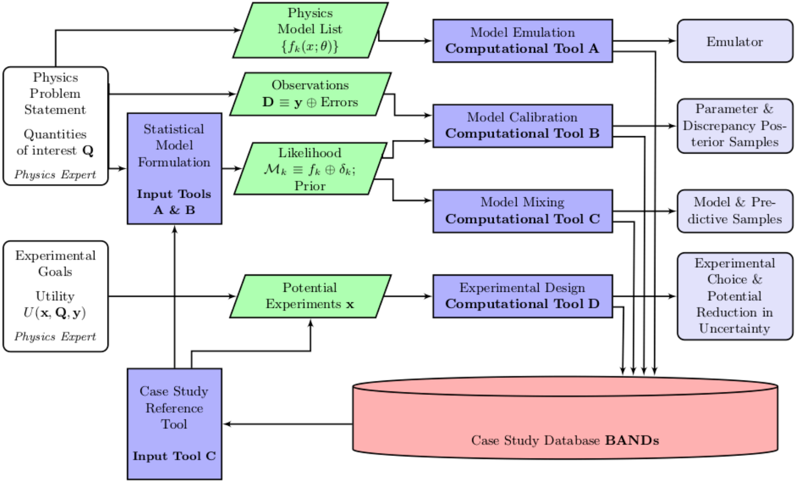
We welcome contributions (tools, examples, and suggestions) to the BAND Framework from the community!

What to expect in BAND Framework v0.3

- Tools:
  - `ROSE`: Reduced Order Scattering Emulator
  - `Taweret`: Python interface to support variety of BMM models
  - `BMEX`: Bayesian Mass Explorer
  - `parmoo`: Python library for parallel multiobjective simulation optimization
- Examples:
  - `VAH`: Bayesian calibration of Viscous Anisotropic Hydrodynamic Simulations of Heavy-Ion collisions

We welcome contributions (tools, examples, and suggestions) to the BAND Framework from the community!

BAND Framework



Model Emulation

Simulators

- In almost all fields of science, technology, industry and policy making, people use mechanistic models to simulate real-world processes
  - For understanding, prediction, control
- Usually implemented in computer codes
  - Often very computationally expensive
- There is a growing realization of the importance of uncertainty in simulator predictions
  - Can we trust them?
  - Without any quantification of output uncertainty, it is easy to dismiss them

Example

Frescox

Scattering code Frescox for coupled-channels calculations

FRESCO FRXY version 7.1 at https://github.com/LLNL/Frescox LLNL-CODE-811517

This directory contains four sub-directories: source, man, test and util.

The source/ directory contains : Fortran files .f, *fx*.def files for separate machines

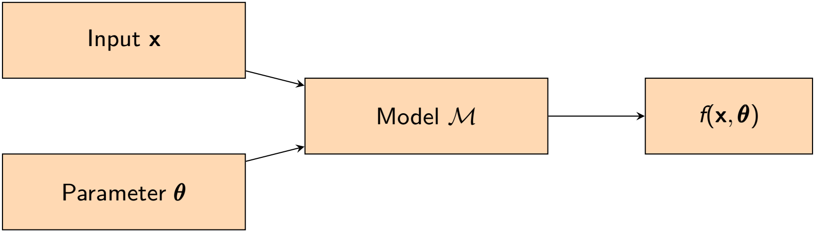
Code | Blame | Executable File · 63 lines (52 loc) · 2.07 KB

```
ca48(d,p)ca49 @ 10 MeV, Daehnick;
NAMELIST
 &FRESCO hcm=0.1 rmatch=20 rintp=0.20 hnl=0.1 rnl=4.0 centre=-0.4
         jtmin=0.0  jtmax=30 absend=-1.0
         thmin=0.00 thmax=180.00 thinc=1.00
         iter=1 nnu=36
         chans=1 xstabl=1
         elab=10 /

 &PARTITION namep='d'  massp=2.014 zp=1
              namet='Ca48'  masst=47.95 zt=20 nex=1  /
```

```
frescox < frescox_inputs/D1048cadp.in > frescox_outputs/D1048cadp.out
```

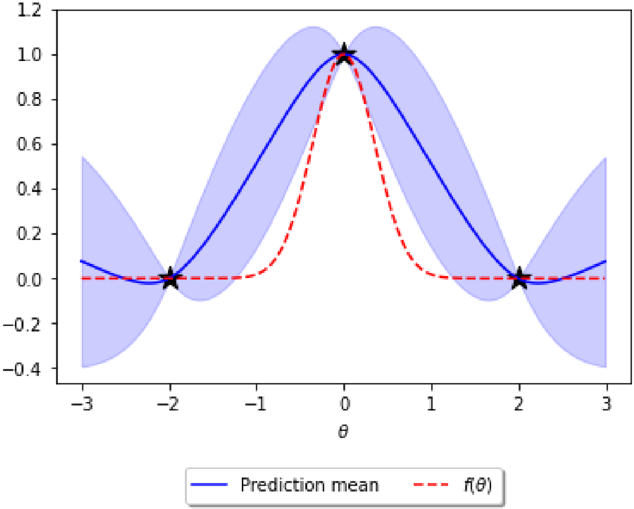
Model Emulation



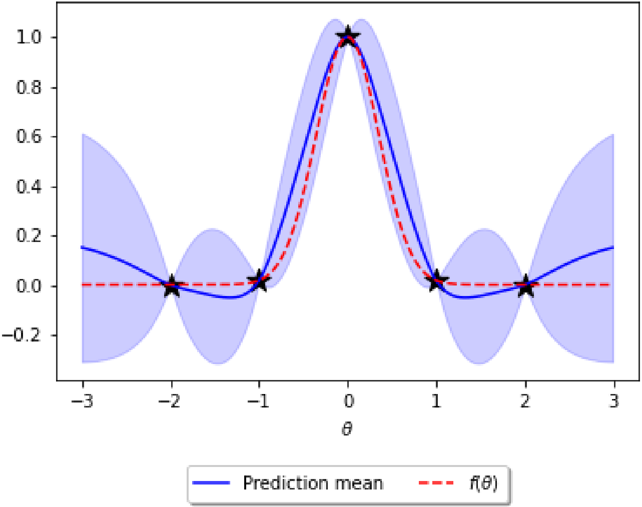
Problem of Complex Models

- If the simulator takes more than a few seconds to run, anything requiring the simulation model becomes computationally infeasible
  - We need a more efficient technique
- Gaussian process (GP) representation
  - Considers $f(\cdot)$ as a random process
  - Represent it as a GP
- Training runs
  - Run simulator for sample of $(\mathbf{x}, \boldsymbol{\theta})$ values
- Then what?
  - Use the emulator to make inference about other things of interest

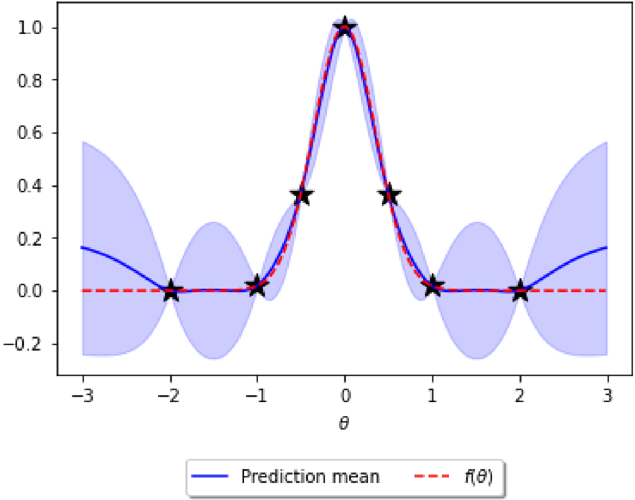
GP with 3 simulation runs



GP with 5 simulation runs



GP with 7 simulation runs

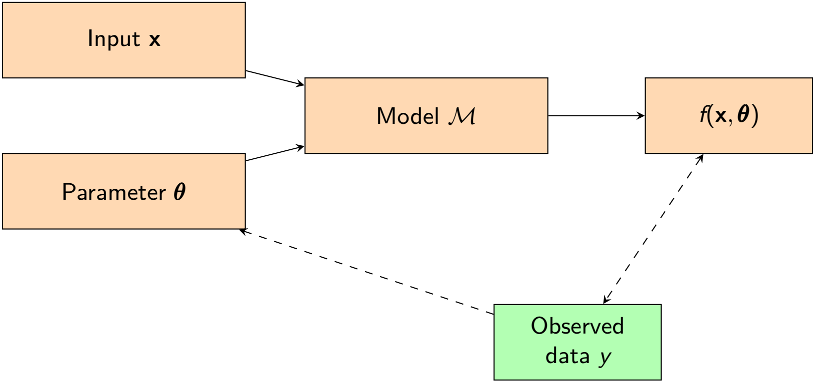


Reduced Basis Methods for emulation with ROSE

The Bayesian Mass Explorer, BMEX

Model Calibration

Model Calibration



Model Calibration

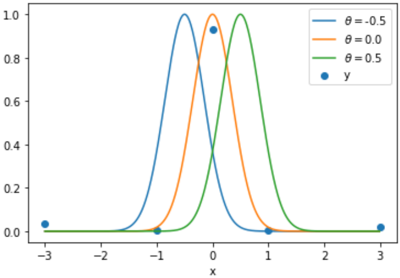
- Seek parameter vector(s) $\boldsymbol{\theta} \in \mathbb{R}^p$ to align simulator outcomes with data
- Physical observation from the real system y can be modeled using the expensive simulation $f(\mathbf{x}, \boldsymbol{\theta})$

$$y(\mathbf{x}) = f(\mathbf{x}, \boldsymbol{\theta}) + \epsilon, \qquad \epsilon \sim \mathrm{N}(\mathbf{0}, \sigma^2)$$

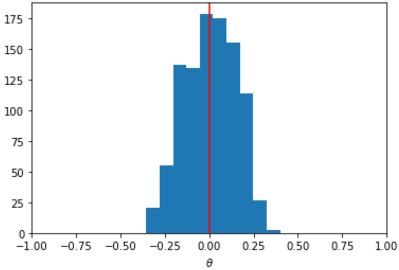
- Given the likelihood $p(\mathbf{y}|\boldsymbol{\theta})$, the posterior distribution is computed by using Bayes' rule

$$\underbrace{p(\boldsymbol{\theta}|\mathbf{y})}_{\text{posterior}} \propto \tilde{p}(\boldsymbol{\theta}|\mathbf{y}) = \underbrace{p(\mathbf{y}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta})}_{\text{prior}}$$

  - Prior $p(\boldsymbol{\theta})$ can be computed for any $\boldsymbol{\theta}$ (i.e., independent of simulation)
  - Likelihood requires expensive simulator evaluation for a given $\boldsymbol{\theta}$



1.0
0.8
0.6
0.4
0.2
0.0
−3
−2
−1
0
1
2
3
x
θ = -0.5
θ = 0.0
θ = 0.5
y



175
150
125
100
75
50
25
0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
θ

surmise: Designed for Emulation and Calibration Flexibility

https://surmise.readthedocs.io

```
pip install surmise==0.1.1
```

```
emulator(x=x, theta=theta, f=f, method='PCGP', args=args)
```

```
emulator(x=x, theta=theta, f=f, method='PCGPwM', args=args)
```

```
calibrator(emu=emu, y=y, x=x, thetaprior='uniform', method='bayes', args={'samp
```

Research Article

Constructing a simulation surrogate with partially observed output

Moses Y.H. Chan, Matthew Plumlee & Stefan M. Wild

Received 10 Dec 2021, Accepted 27 Apr 2023, Accepted author version posted online: 03 May 2023

Bayesian calibration of viscous anisotropic hydrodynamic simulations of heavy-ion collisions

Dananjaya Liyanage,[1] Özge Sürer,[2,3] Matthew Plumlee,[3,4] Stefan M. Wild,[3,5] and Ulrich Heinz[1]

Bayes goes fast: Uncertainty quantification for a covariant energy density functional emulated by the reduced basis method

Pablo Giuliani[1,2*†], Kyle Godbey[1*†], Edgard Bonilla[3*], Frederi Viens[2,4*] and Jorge Piekarewicz[5*]

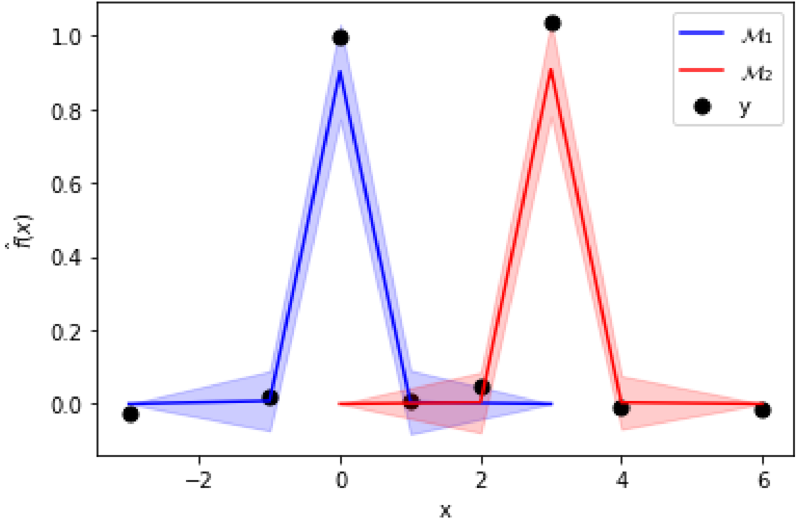
Uncertainty quantification in breakup reactions

Ö. Sürer, F. M. Nunes, M. Plumlee, and S. M. Wild

Phys. Rev. C **106**, 024607 – Published 11 August 2022

Model Mixing

Model Mixing



Ongoing Mixing Projects

Model Mixing Using Bayesian Additive Regression Trees

John C. Yannotty, Thomas J. Santner, Richard J. Furnstahl, and Matthew T. Pratola

Interpolating between small- and large-g expansions using Bayesian model mixing

A. C. Semposki, R. J. Furnstahl, and D. R. Phillips
Phys. Rev. C **106**, 044002 – Published 20 October 2022

Dan Liyanage

Alexandra Semposki

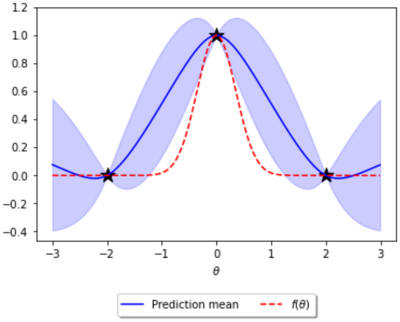
John Yannotty

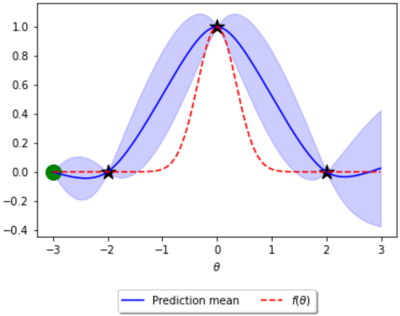
Bayesian Model Mixing using Taweret

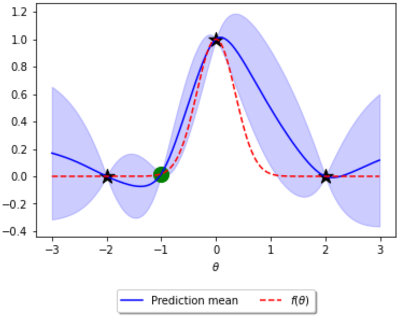
Experimental Design

Experimental Design

- Optimally design a computer experiment
  - How to select the inputs at which to compute the simulation output to achieve specific goals
- Optimally design a physical experiment
  - Unknown calibration parameters can be estimated from real data by conducting physical experiments


θ
Prediction mean
f(θ)


θ
Prediction mean
f(θ)


θ
Prediction mean
f(θ)

Tue:

Sequential Bayesian experimental design for calibration of expensive physics models	*Ozge Sürer*
Crow 201, Washington University in St. Louis	11:30 - 12:00

Short talk: Bayesian calibration of viscous anisotropic hydrodynamic simulations of heavy-ion collisions
Dananjaya Liyanage

W:

Machine learning for nuclear physics	*Witek Nazarewicz*
Crow 201, Washington University in St. Louis	11:00 - 11:45

Th:

Overview of emulators for nuclear physics	*Dick Furnstahl*
Crow 201, Washington University in St. Louis	09:00 - 09:30
Quantification for a covariant energy density functional emulated by the reduced basis method	*Pablo Giuliani*
Crow 201, Washington University in St. Louis	11:30 - 12:00
Short Talk: Reduced Basis Methods and Scattering	*Daniel Odell*
Crow 201, Washington University in St. Louis	16:00 - 16:15

F:

Excavating insights from sparse data with statistics and machine learning	*Kyle Godbey*
Crow 201, Washington University in St. Louis	09:30 - 10:00

BAND

Bayesian Analysis of Nuclear Dynamics

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