Assessing the Robustness of VBMC for Extracting Parameters in Differential Equations

Alia Valentine, Grace Rojo, Anna Rittenhouse

Michigan State University, Massachusetts Institute of Technology, Clark Atlanta University
Advisors: Rachel Kurchin, Gerald Wang, David Offner, Carnegie Mellon University

Bayes' Theorem

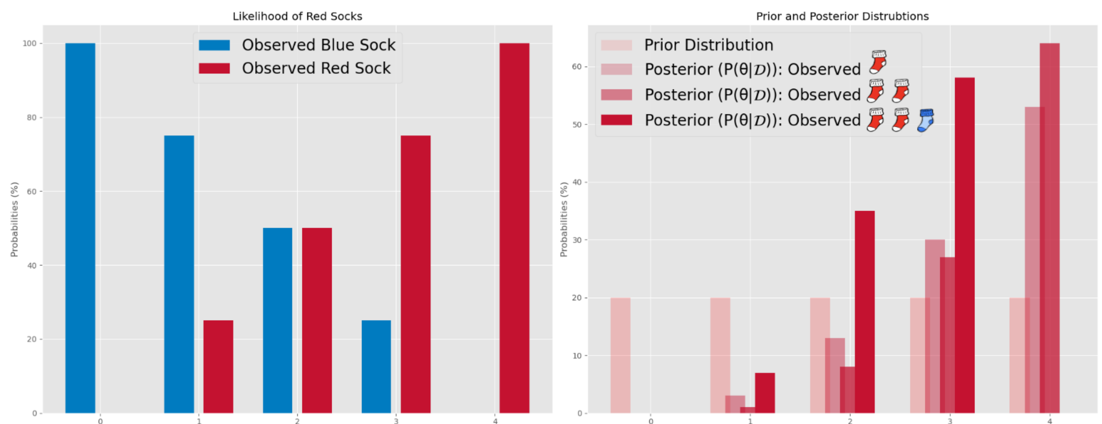
Theorem 1 (Bayes' Theorem) *Given a dataset $\mathcal{D}$ and model parameters $\boldsymbol{\theta} \in \mathbb{R}^D$, we compute*

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

where $p(\boldsymbol{\theta}|\mathcal{D})$ is the posterior, $p(\mathcal{D}|\boldsymbol{\theta})$ is the likelihood of the model of interest, $p(\boldsymbol{\theta})$ is the prior over parameters, and $p(\mathcal{D})$ is the model evidence.

Example: Sock Problem

There are four red or blue socks. We want to know how many are red with no prior knowledge. Our data set is observing a sock's color, and our parameters are the number of red socks.

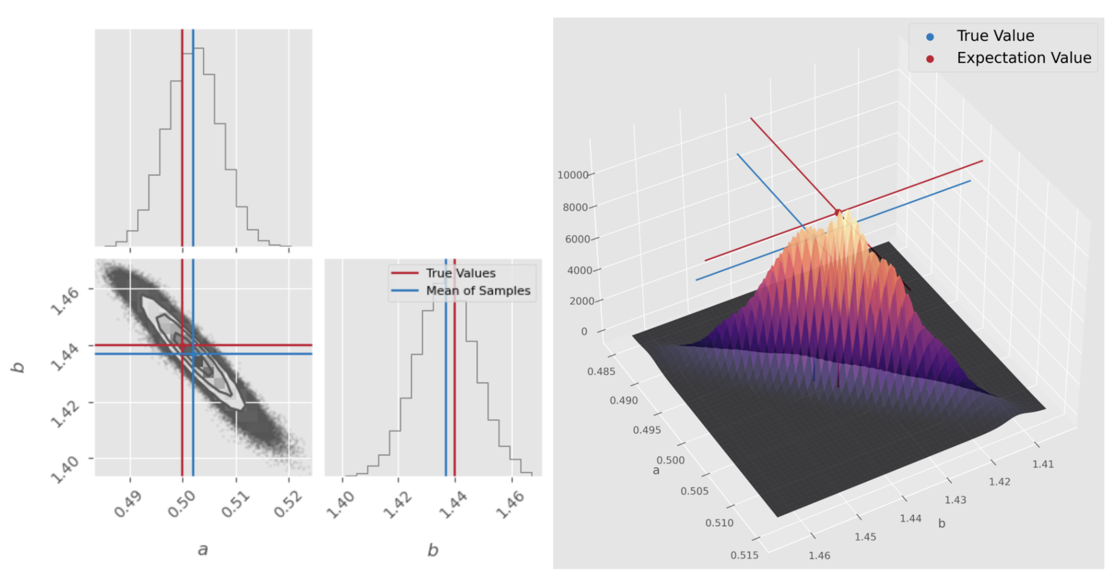


VBMC

Variational Bayesian Monte Carlo (VBMC) is an inference algorithm that returns a variational posterior probability density function (PDF) and lower bound of the model evidence (ELBO) for a black-box log-likelihood of interest.

VBMC Algorithm

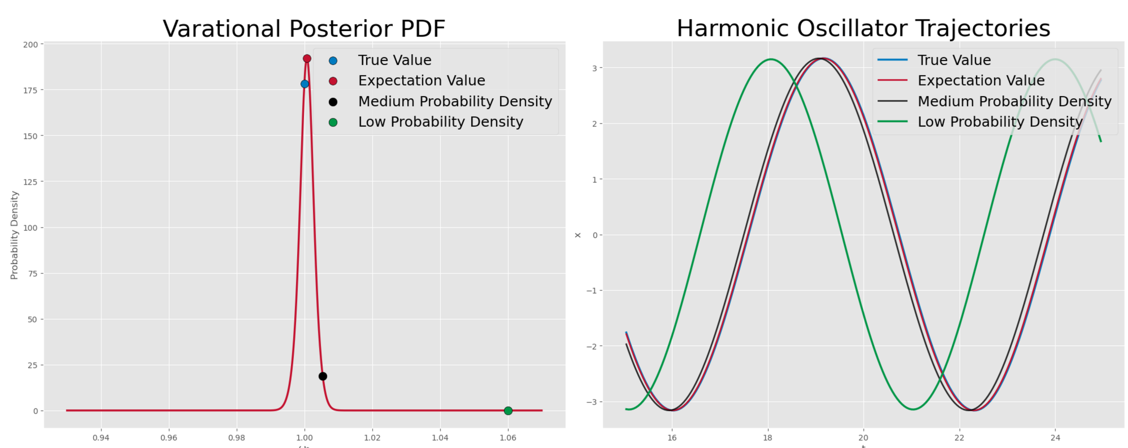
1. Sample from log-likelihood function, initially randomly, then according to an acquisition function
2. Train Gaussian process on these samples
3. Optimize ELBO via stochastic gradient descent
4. Update variational posterior (VP)
5. Repeat 1-3 until converged and return VP



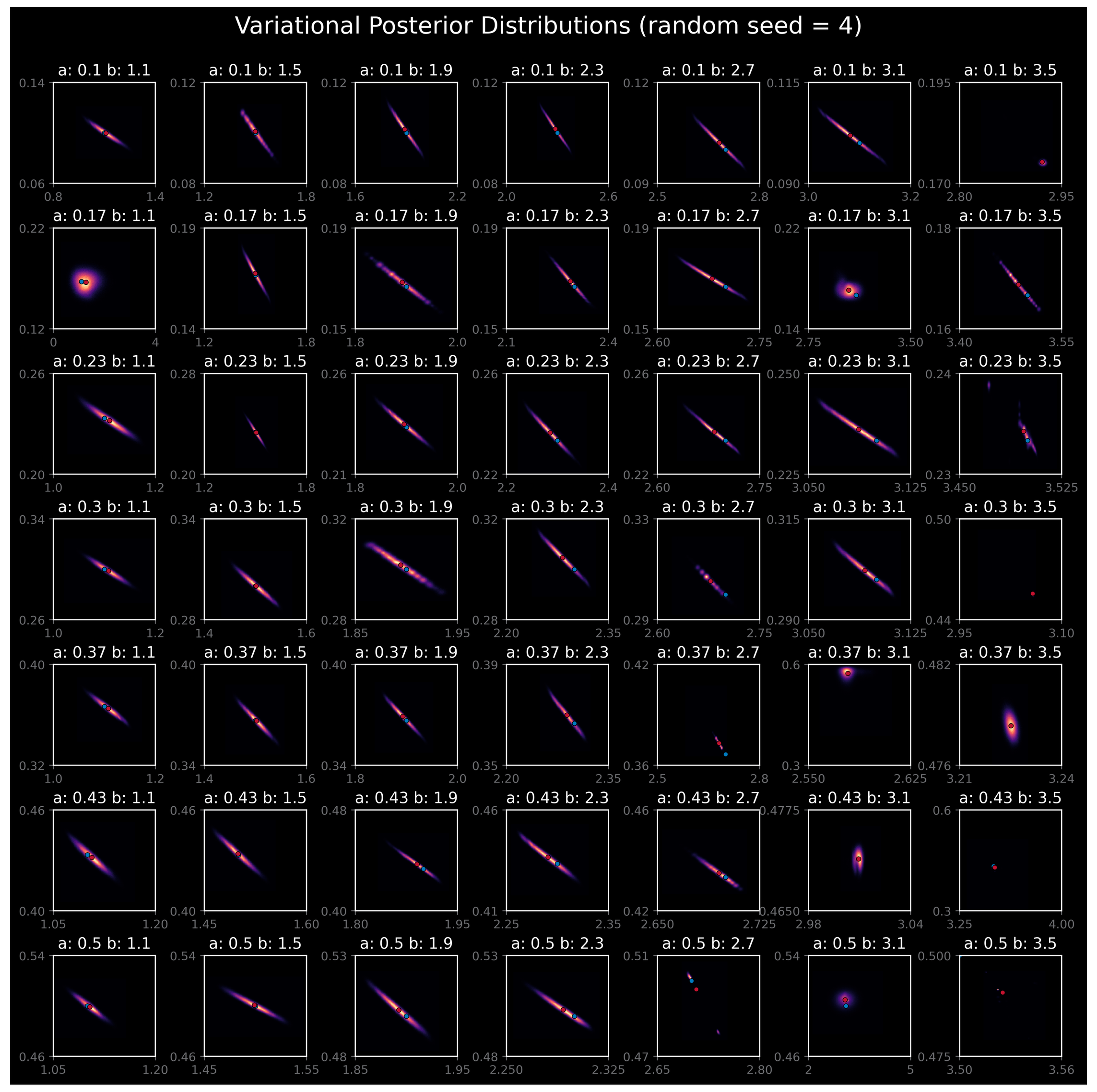
Differential Equations

We are concerned with how well VBMC can predict parameters of Ordinary Differential Equations. Here $\mathcal{D}$ is a set of trajectories and $\boldsymbol{\theta}$ is a vector of parameters of said ODEs.

Example: Simple Harmonic Oscillator (SHO): $\ddot{x} = -\omega_0^2 x$



Example: Anharmonic Oscillator: $\ddot{x} = -x - ax^b$



Assessing the Robustness

How does one measure 'how accurate' a result is when it's a distribution?

Definition 2 (Delaunay) *A triangulation is Delaunay if, when we take the circumcircle of any triangle in it (the unique circle going through its vertices), no point of our set lies inside (in the interior) of that circle.*

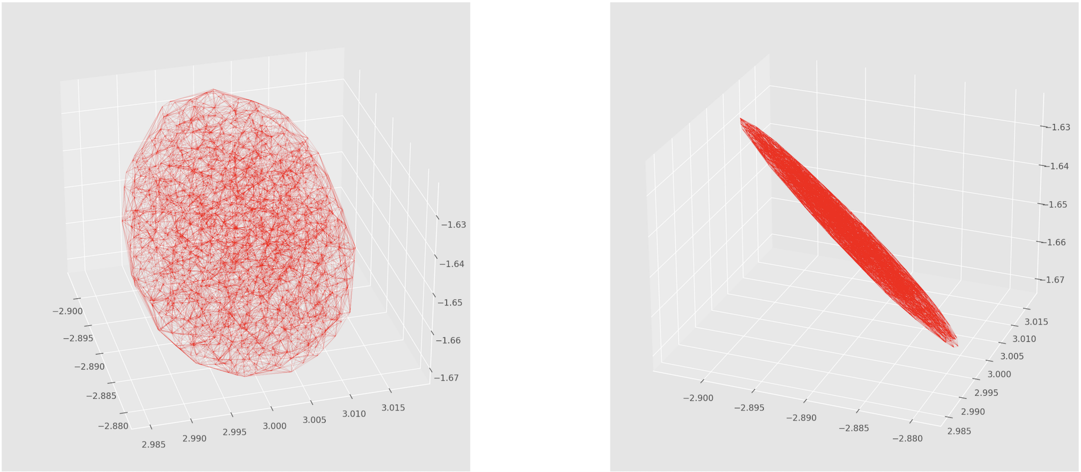
Definition 3 (Concave Hull) *A concave hull is a (possibly) non-convex polygon that contains all the input points. For a set of points there is a sequence of hulls of increasing concaveness, which is determined by a numeric target parameter.*

Comparing Metrics for Assessing Robustness

Metric	Definition	Pros	Cons
Euclidean	The Euclidean distance between the true params and $\mathbb{E}[\boldsymbol{\theta}]$	Computationally inexpensive	$\mathbb{E}[\boldsymbol{\theta}]$ is uninformative when the parameters are dependent upon each other
Concave Hull	Integrates the VP using a concave hull over specific* samples	Accurate in low dim	Computationally expensive; doesn't work in high dim
D-dim Delaunay Integration	Integrates the VP over specific* samples using Delaunay triangulation	Scales well in all dim	'Doesn't internally handle clusters' EDIT

*Have probability density larger than some $c \in [0,1]$ times the probability density of the true value

Example: Delaunay triangulation of SEIR Model in 3-dim, $c = .9$ (Integration returned 0.017)



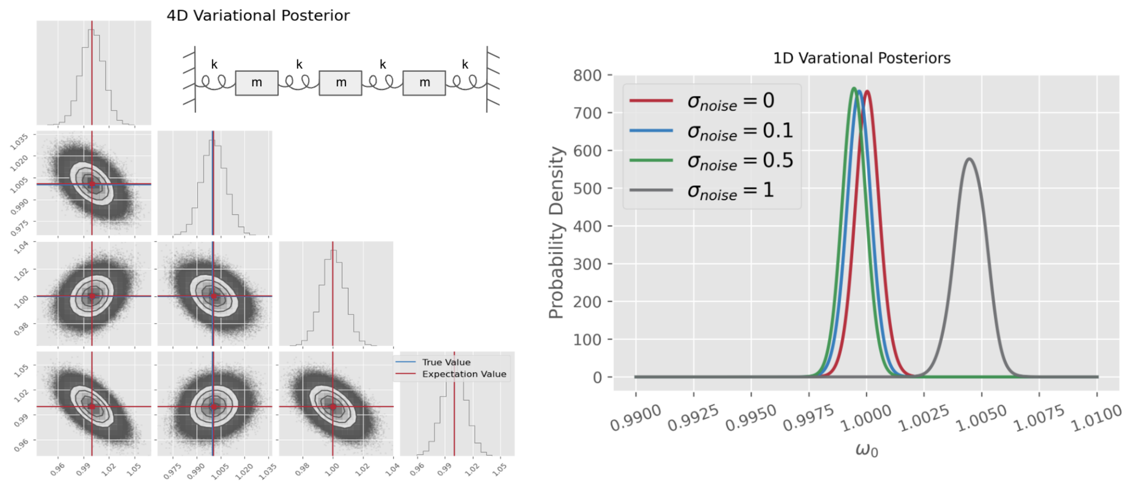
Example: Delaunay triangulation of 3 linearly coupled SHOs in 3-dim, $c = 1$ (Integration returned 0.999)

Results

VBMC Strengths

- Able to extract simple relationships between parameters
- Able to handle noisy datasets

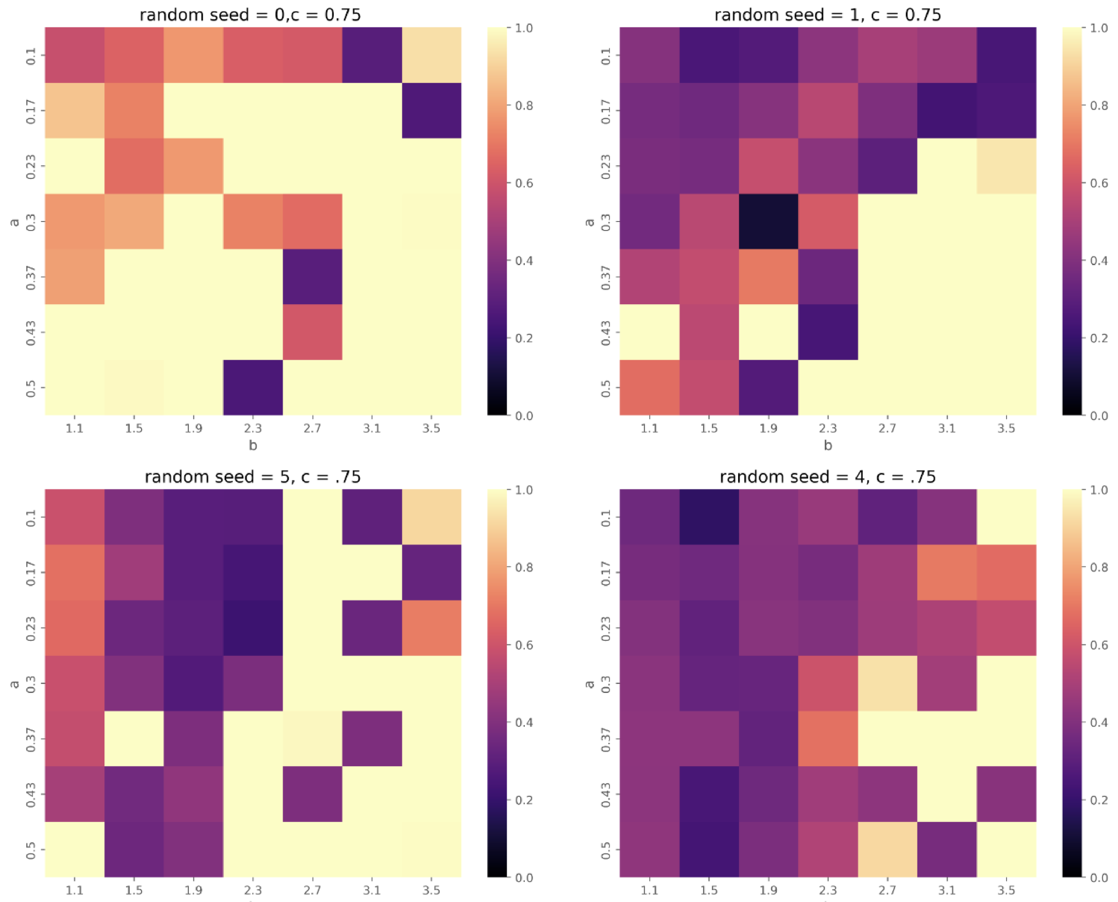
Examples: Normal modes; SHO with varying noise



VBMC Weaknesses

- Sensitive to randomness, due to random sampling in the initial stage
- Not able to conclusively find distinct parameters that belong to different manifolds

Example: Heatmap of $\ddot{x} = -x - ax^b$; color is the number returned from D-dim Delaunay Integration



References & Acknowledgements

Special thanks to our mentors for their guidance. This material is based upon work supported by the National Science Foundation under Grant No. 2244348.

LaTeX TikZposter