Assessing the Robustness of VBMC for Extracting Parameters in Differential Equations

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Bayes' Theorem

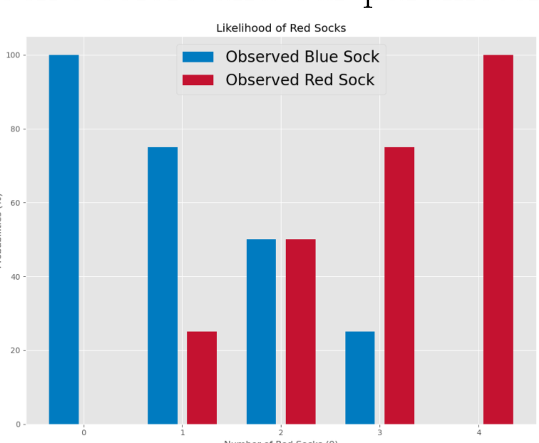
Theorem 1 (Bayes' Theorem) *Given a dataset $\mathcal{D}$ and model parameters $\boldsymbol{\theta} \in \mathbb{R}^D$, we compute*

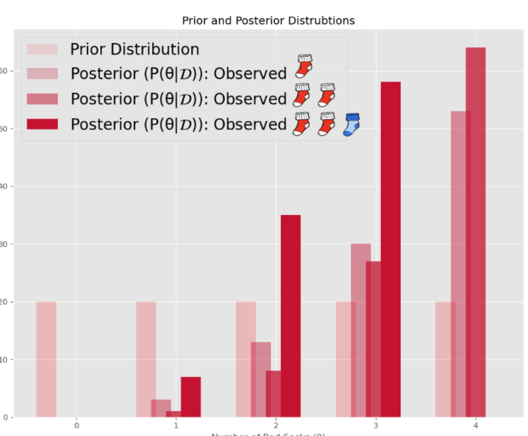
$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{D})}, \qquad p(\mathcal{D}) = \int p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$

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 dataset is observations of sock's colors and our parameters are the number of red socks.



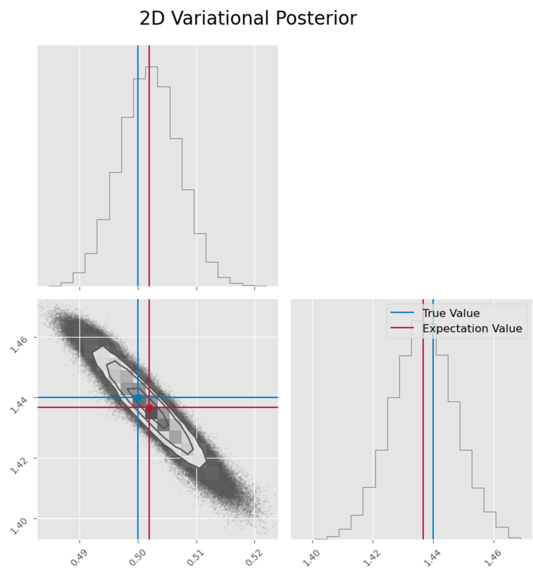


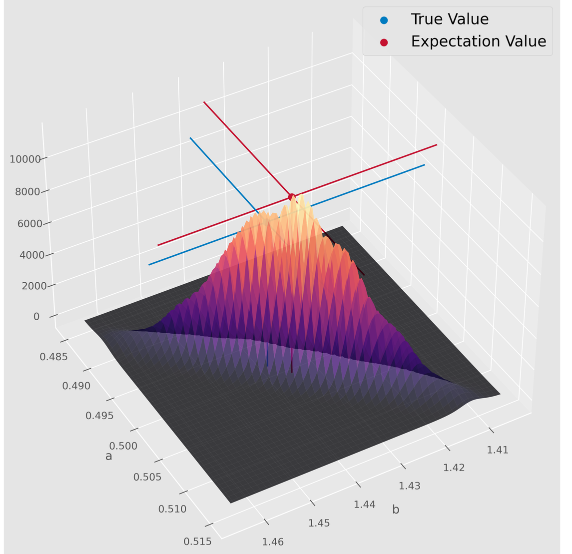
VBMC

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

VBMC Algorithm

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

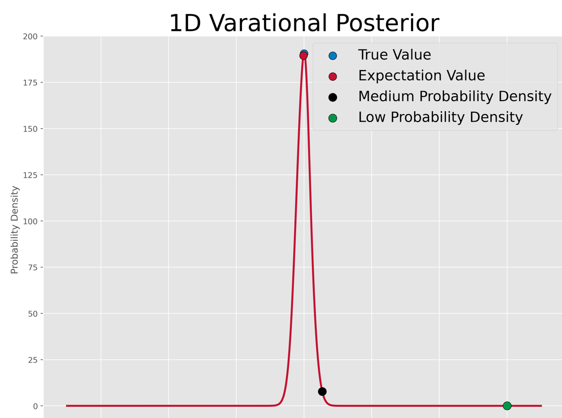


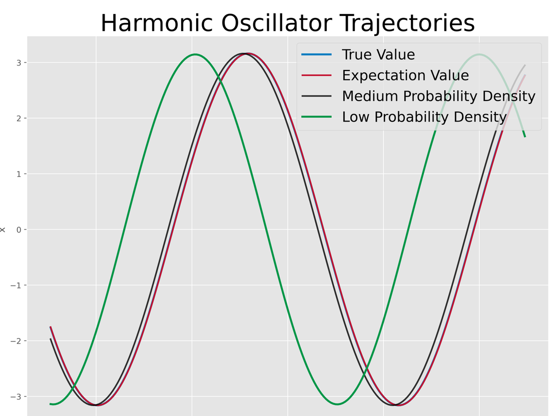


Differential Equations

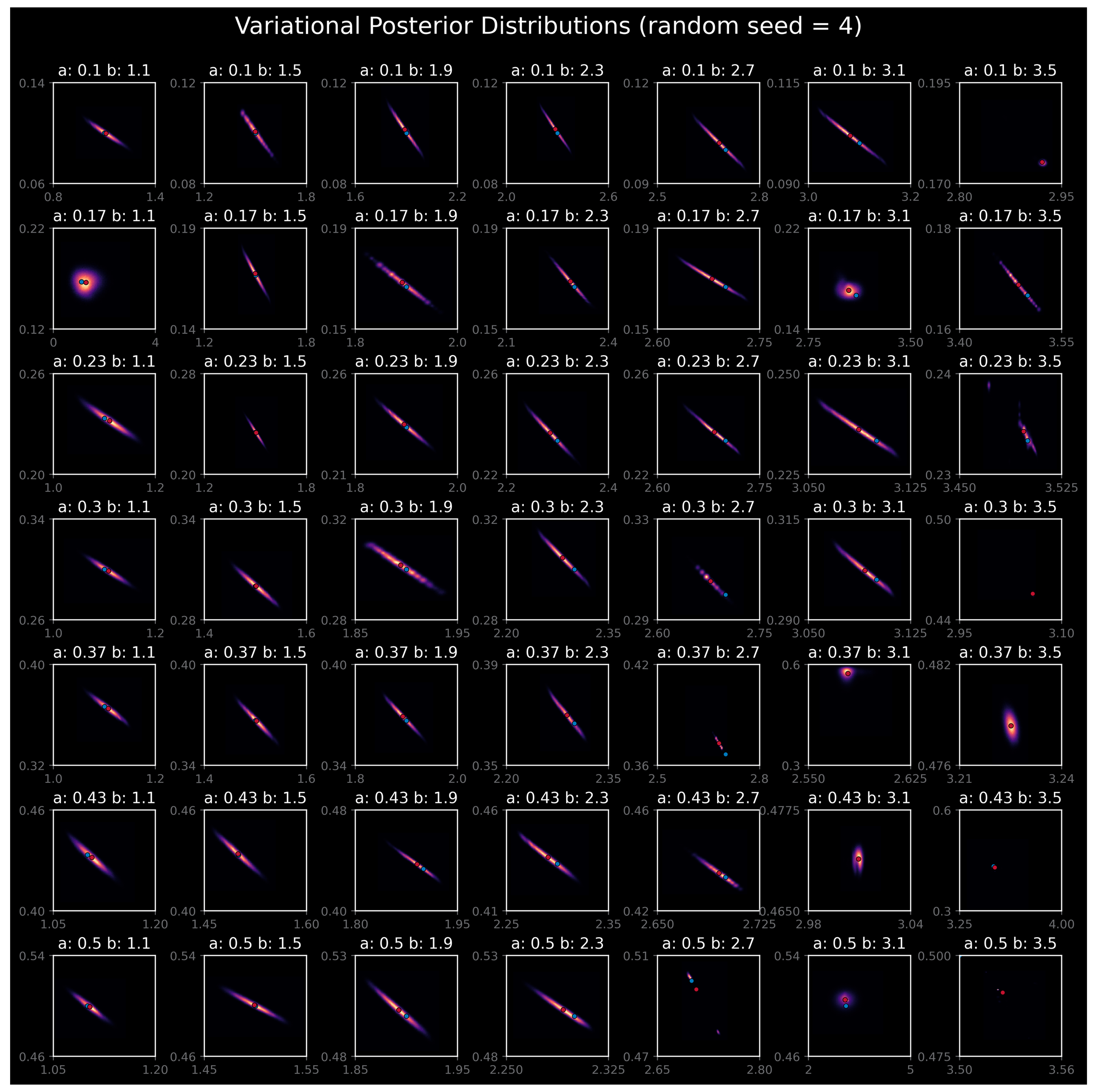
We are concerned with how well VBMC can predict parameters, and relationships between them, in Ordinary Differential Equations (ODEs). In this context, $\mathcal{D}$ is a set of ODE trajectories and $\boldsymbol{\theta}$ is a vector their parameters.

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





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



Assessing Robustness

How does one measure how 'good' a result is when that result is 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.*

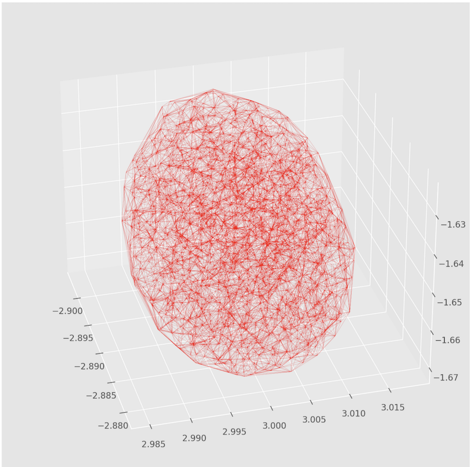
Definition 3 (Concave Hull) *A concave hull is a (possibly) non-convex polygon that contains all the input points. For a set of points there is a sequence of hulls of increasing concaveness, which is determined by a numeric target parameter.*

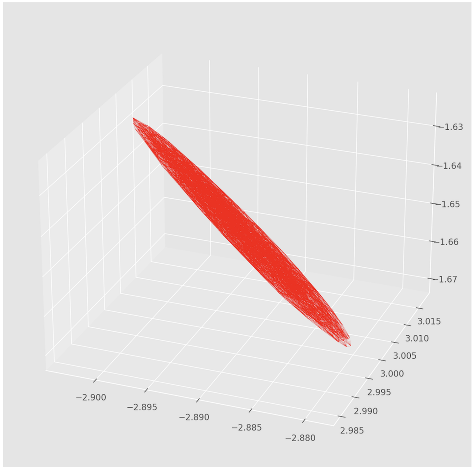
Comparing Metrics for Assessing Robustness

Metric	Definition	Pros	Cons
Euclidean	Euclidean distance between true parameters and $\mathbb{E}[\boldsymbol{\theta}]$	Computationally inexpensive	$\mathbb{E}[\boldsymbol{\theta}]$ is uninformative when parameters depend on each other
Concave Hull (CH)	Integral of VP using a concave hull created from samples*	Accurate in low dim	Computationally expensive; doesn't work in high dim
D-dim Delaunay Integration	Integral of VP using a Delaunay triangulation of samples*	Works well in high dim; shorter runtime than CH	Handles unintentional clusters poorly

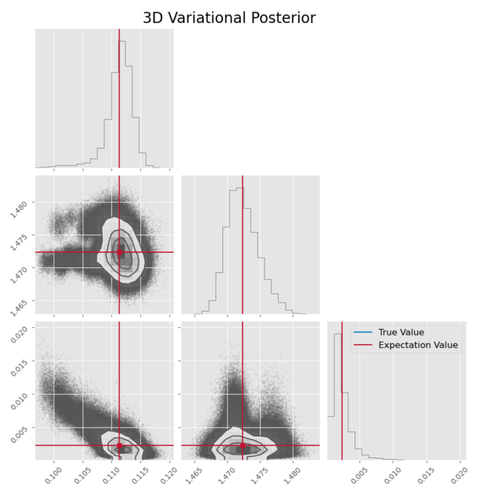
*With probability density larger than some $c \in [0, 1]$ times the probability density of the true value

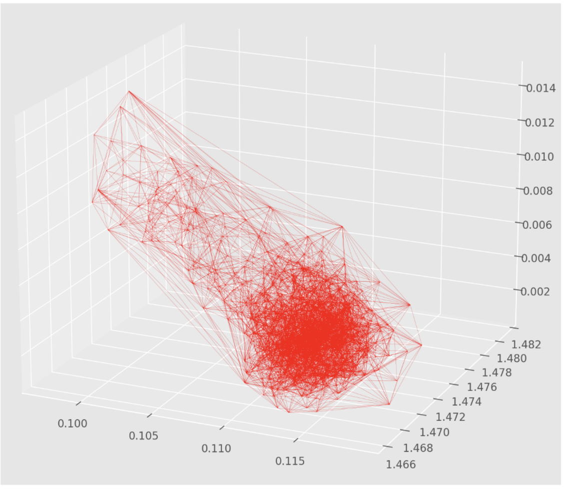
Example: Delaunay triangulation of SEIR Model in 3-dim, $c = .9$ (Integration returned 0.017)





Example: Delaunay triangulation of 2 linearly coupled SHOs in 3-dim, $c = 1$ (Integration returned 0.999)



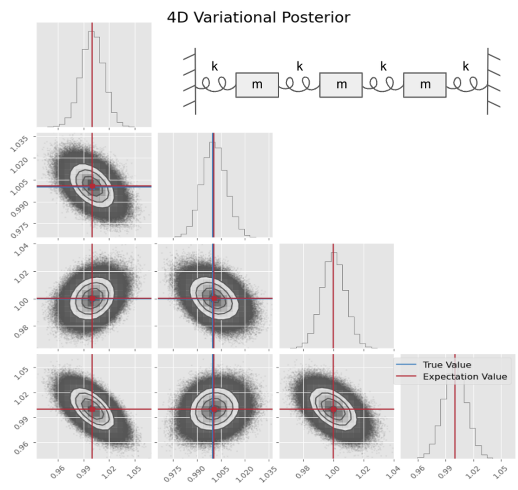


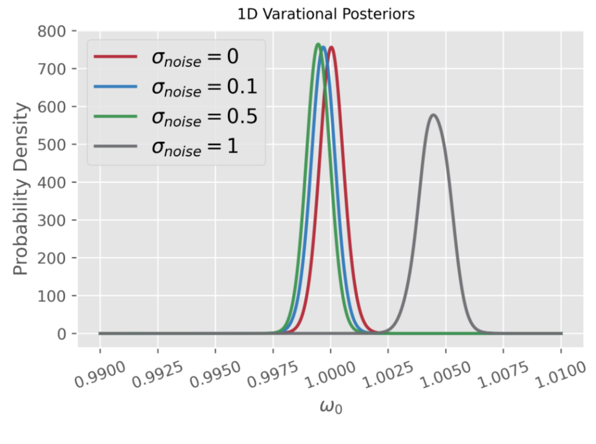
Results

VBMC Strengths

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

Examples: Normal modes; SHO with varying noise

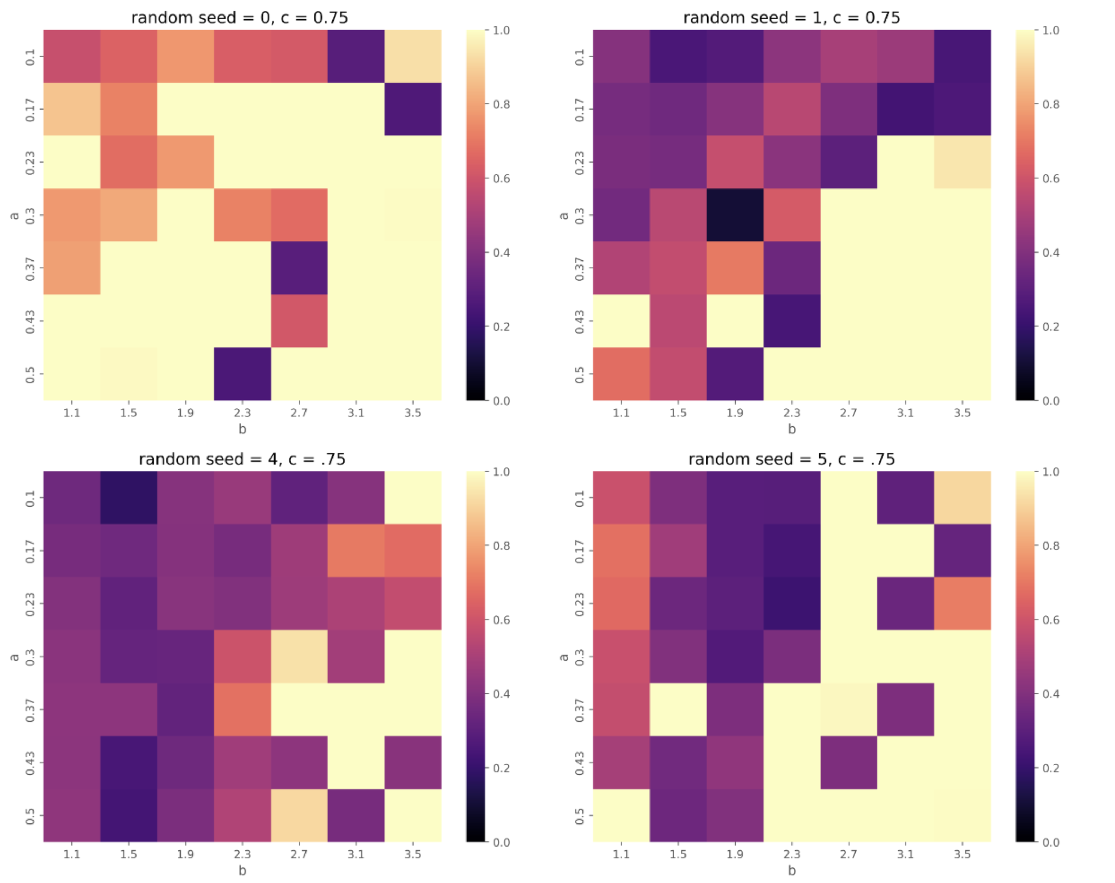




VBMC Weaknesses

- 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

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