Variational Bayesian Monte Carlo

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1. Introduction and motivation
2. Background
3. Variational Bayesian Monte Carlo
4. Experiments

1 Introduction and motivation

2 Background

3 Variational Bayesian Monte Carlo

4 Experiments

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Bayesian inference with expensive black-box statistical models

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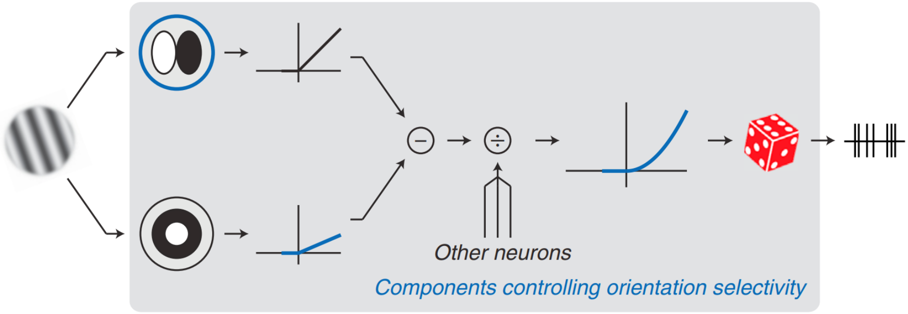
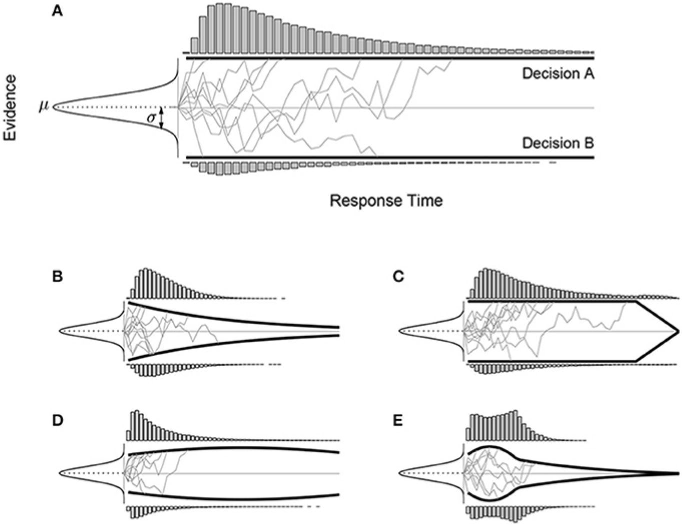
(Why Bayesian inference?)

Example: LN-LN neuronal model



from Goris et al., *Neuron* (2015)

Example: Drift-diffusion models



from Zhang et al., *Front Psychol* (2014)

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- Markov Chain Monte Carlo (MCMC)
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require

- many likelihood evaluations
- knowledge of the model (e.g., gradients, detailed structure)

Sketch solution

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- Fit *surrogate model* to likelihood evaluations
- Perform *approximate inference* with surrogate model
- Use *active sampling* to smartly evaluate likelihood landscape

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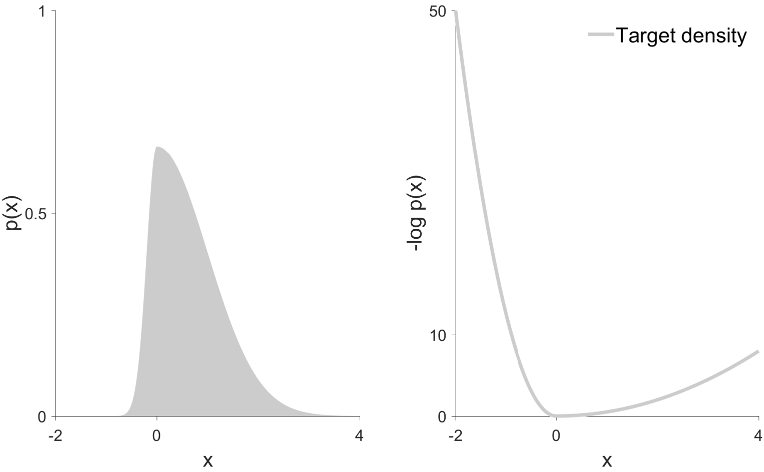
VI casts Bayesian inference into optimization + integration

Variational inference: example



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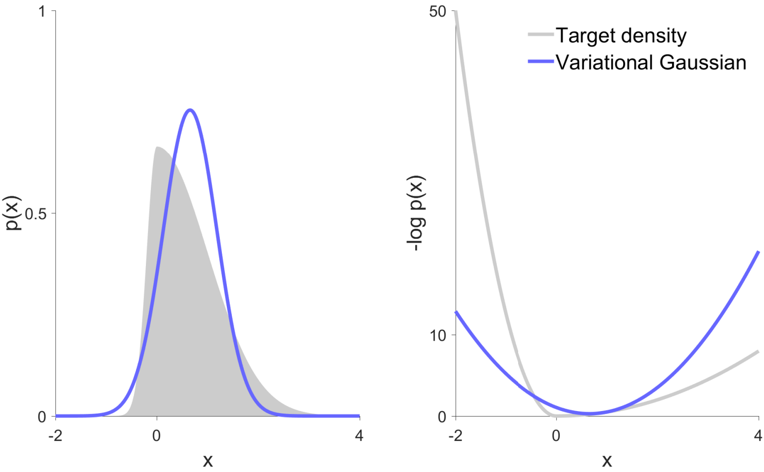

$$q_\phi(x) = \mathcal{N}\left(x, \mu, \sigma^2\right) \qquad \phi = \left(\mu, \sigma^2\right)$$

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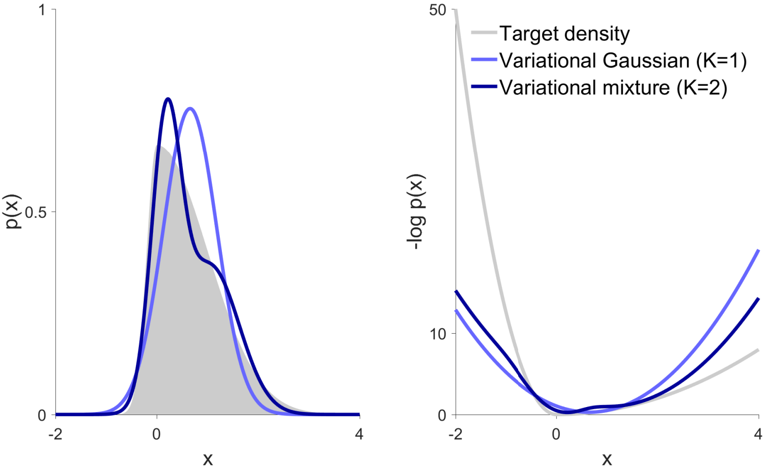

$$q_\phi(x) = \sum_{k=1}^{K} w_k \mathcal{N}\left(x, \mu_k, \sigma_k^2\right) \qquad \phi = \left(w_k, \mu_k, \sigma_k^2\right)_{k=1}^{K}$$

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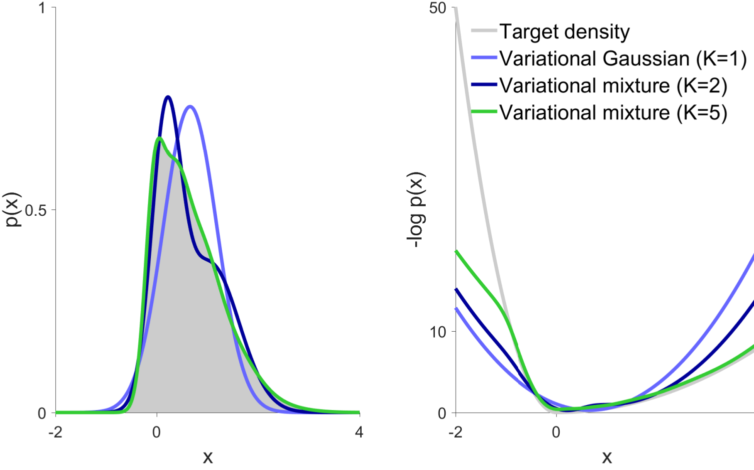

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- covariance function $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
  - exponentiated quadratic $\kappa_{EQ}(\boldsymbol{x}, \boldsymbol{x}') = \sigma_f^2 \exp\left[-\frac{1}{2}\sum_i \frac{(x_i - x_i')^2}{\ell_i^2}\right]$

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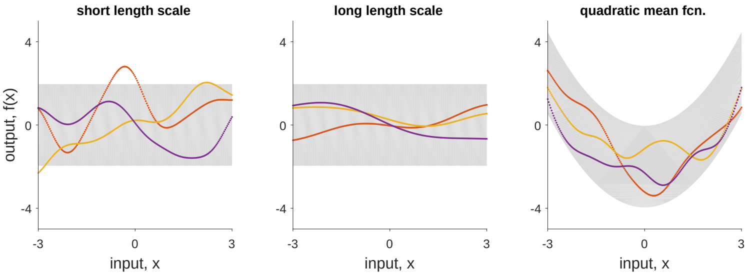

Posterior GPs

Training inputs $\mathbf{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$
Observed values $\boldsymbol{y} = (y_1 = f(\boldsymbol{x}_1), \ldots, y_n = f(\boldsymbol{x}_n))$
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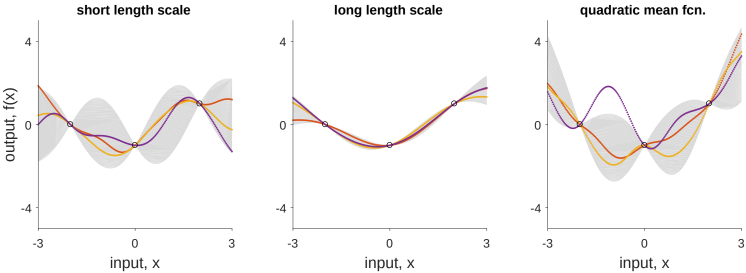

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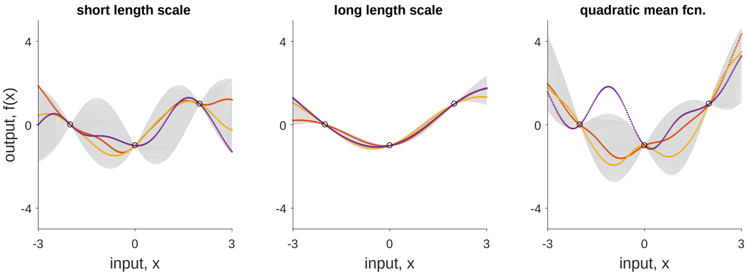

GP marginal likelihood $p(\boldsymbol{y}|\mathbf{X}, \psi)$

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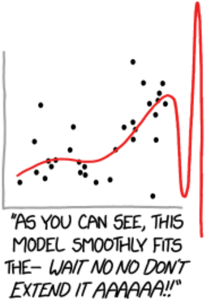
- Model mismatch



from `xkcd.com/2048`

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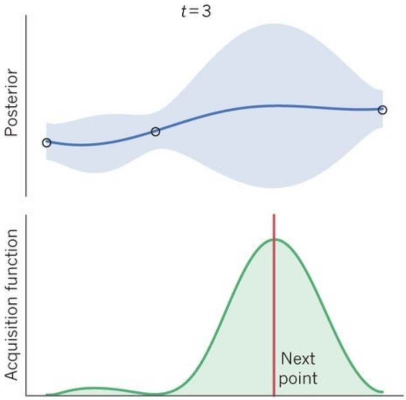

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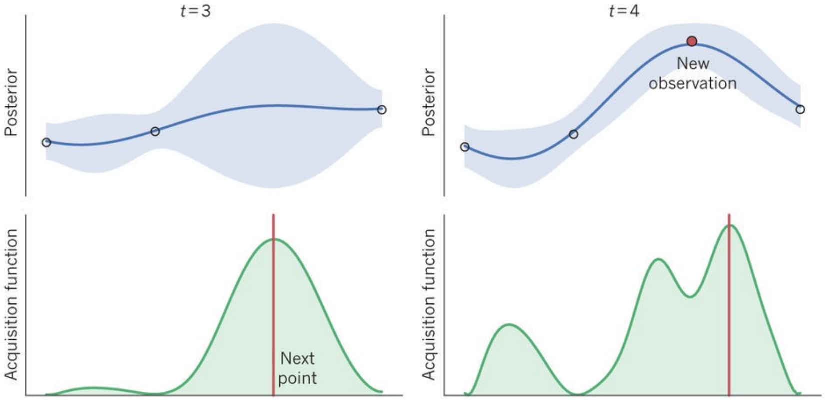

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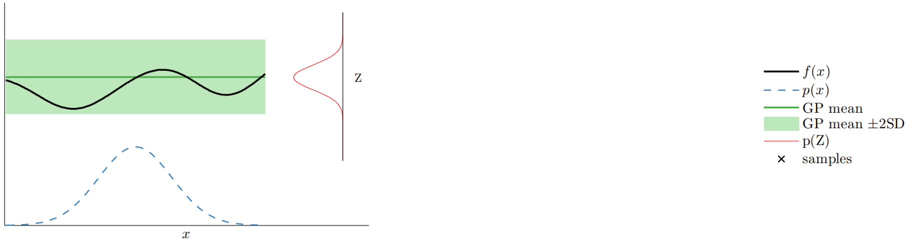

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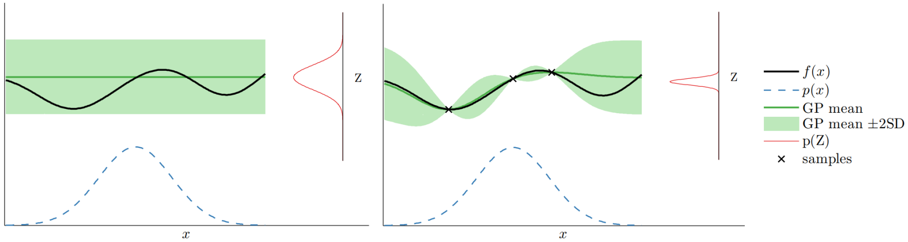

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- *Uncertainty sampling*: Maximize variance of integrand $p(\boldsymbol{x})f(\boldsymbol{x})$

Putting things together

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$$
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VI + BQ = VBMC

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VBMC in an nutshell

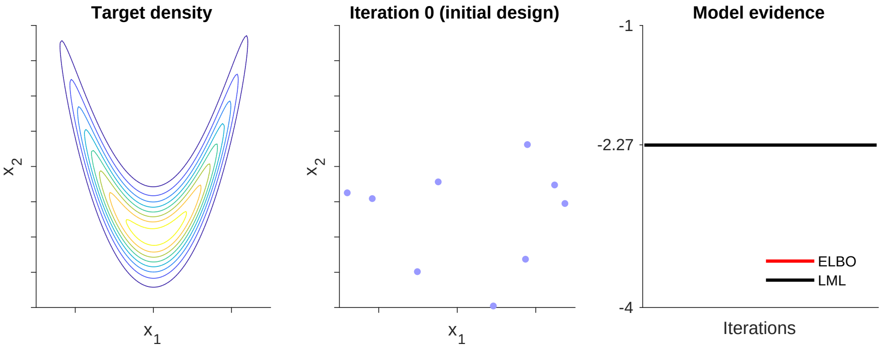
In each iteration t:

1. (Actively) sample new points, evaluate $f = \log p(\mathcal{D}|\boldsymbol{x}_{\text{new}})p(\boldsymbol{x}_{\text{new}})$
2. train GP model of the log joint f
3. update variational posterior q_{ϕ_t} by optimizing the ELBO

Loop until reaching termination criterion

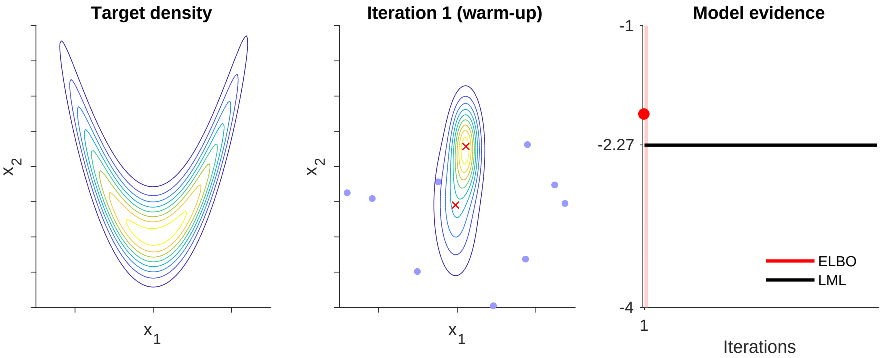
Acerbi, *NeurIPS* (2018)

VBMC demo



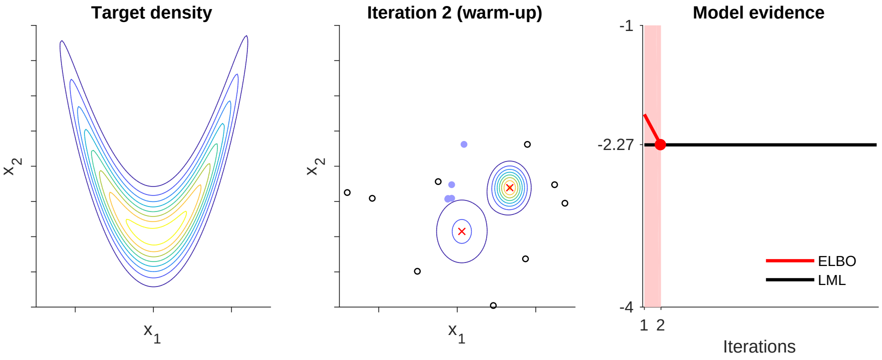
Target density
x 2
x 1
Iteration 0 (initial design)
x 2
x 1
Model evidence
-1
-2.27
-4
ELBO
LML
Iterations

VBMC demo



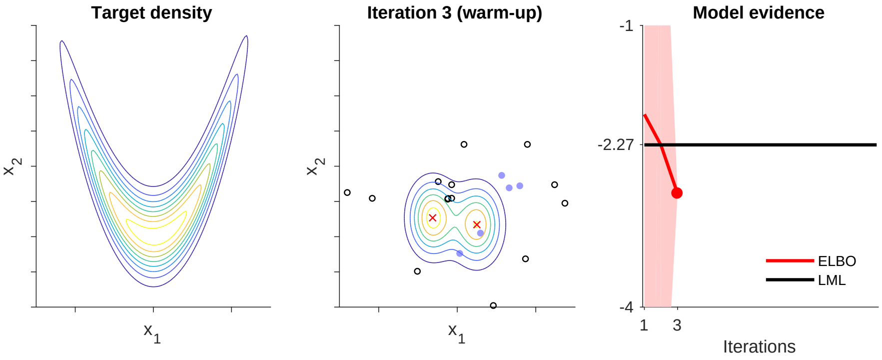
Target density
x_2
x_1
Iteration 1 (warm-up)
x_2
x_1
Model evidence
-1
-2.27
-4
1
Iterations
ELBO
LML

VBMC demo



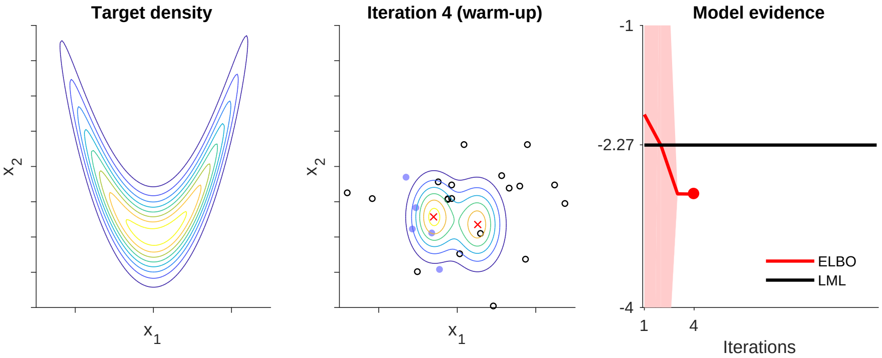
Target density
x2
x1
Iteration 2 (warm-up)
x2
x1
Model evidence
-1
-2.27
-4
1
2
Iterations
ELBO
LML

VBMC demo



Target density
x 2
x 1
Iteration 3 (warm-up)
x 2
x 1
Model evidence
-1
-2.27
-4
1
3
Iterations
ELBO
LML

VBMC demo



Target density
x_2
x_1
Iteration 4 (warm-up)
x_2
x_1
Model evidence
-1
-2.27
-4
1
4
Iterations
ELBO
LML

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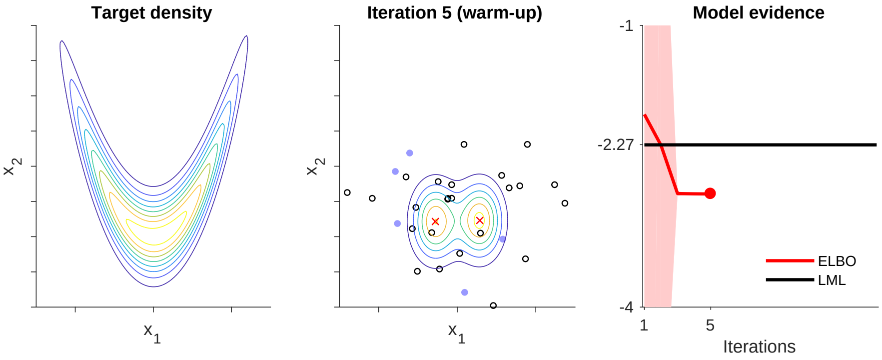
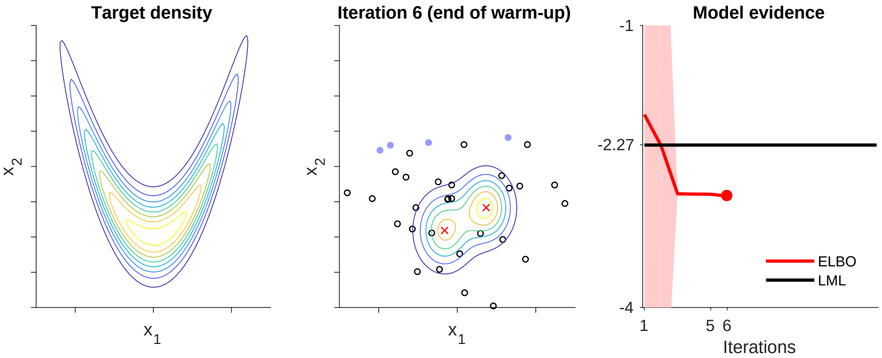


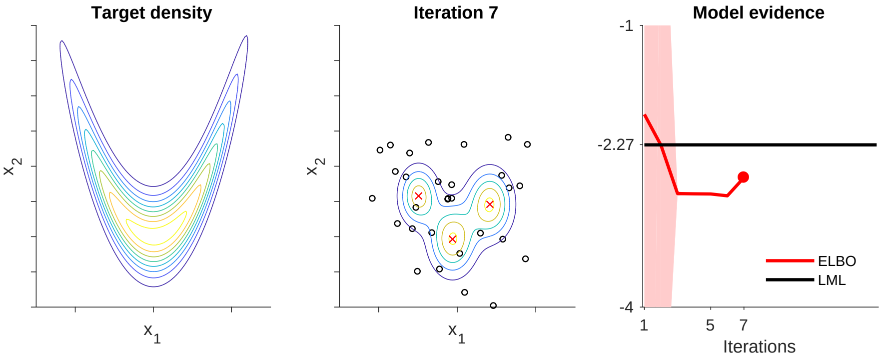
Target density
Iteration 5 (warm-up)
Model evidence
x_2
x_1
x_2
x_1
-1
-2.27
-4
1
5
Iterations
ELBO
LML

VBMC demo



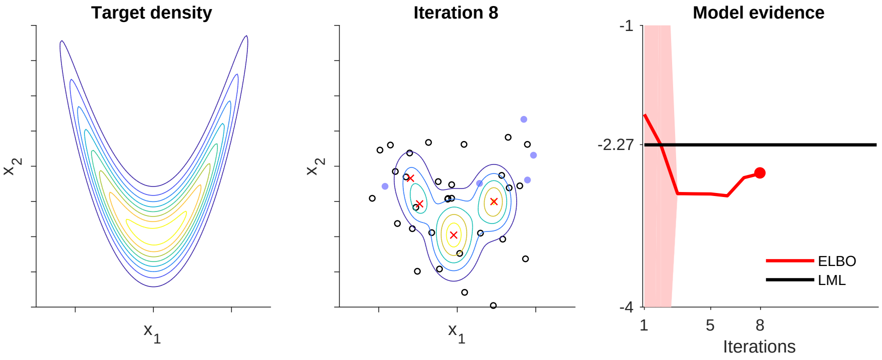
Target density
x2
x1
Iteration 6 (end of warm-up)
x2
x1
Model evidence
-1
-2.27
-4
1
5 6
Iterations
ELBO
LML

VBMC demo



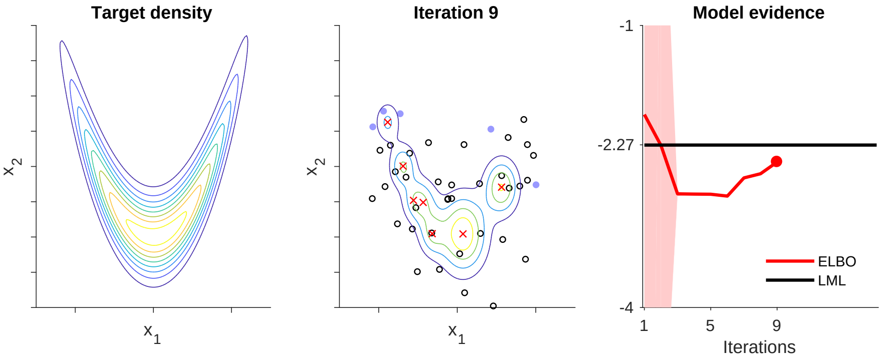
Target density
x 2
x 1
Iteration 7
x 2
x 1
Model evidence
-1
-2.27
-4
1
5
7
Iterations
ELBO
LML

VBMC demo



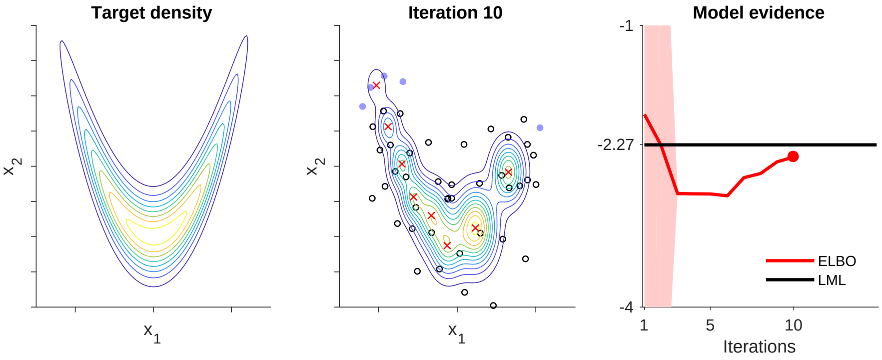
Target density
x_2
x_1
Iteration 8
x_2
x_1
Model evidence
-1
-2.27
-4
1
5
8
Iterations
ELBO
LML

VBMC demo



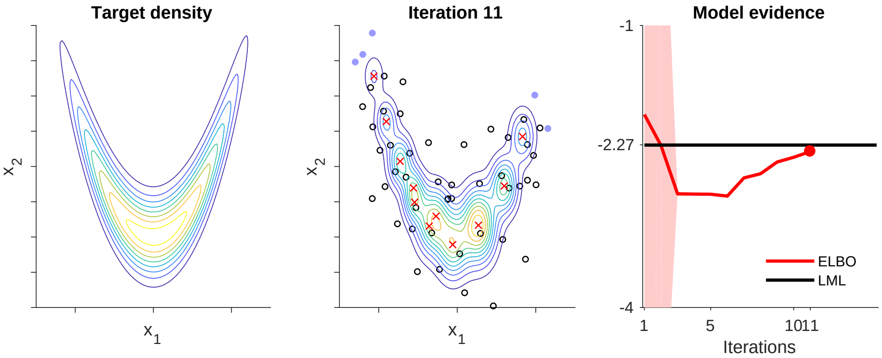
Target density
Iteration 9
Model evidence
x2
x1
x2
x1
-1
-2.27
-4
1
5
9
Iterations
ELBO
LML

VBMC demo



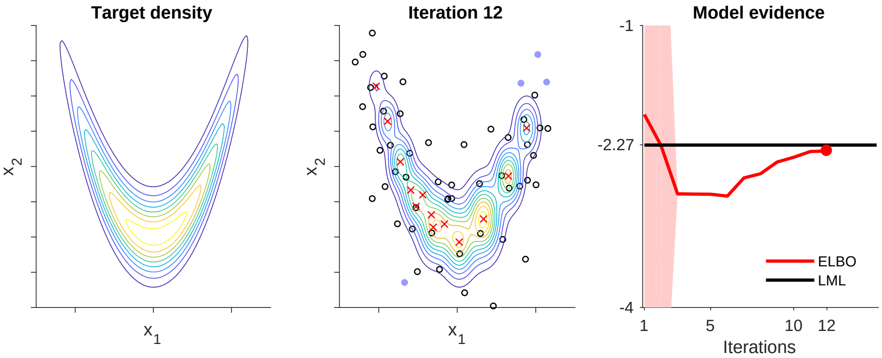
Target density
Iteration 10
Model evidence
x_2
x_1
x_2
x_1
-1
-2.27
-4
1
5
10
Iterations
ELBO
LML

VBMC demo

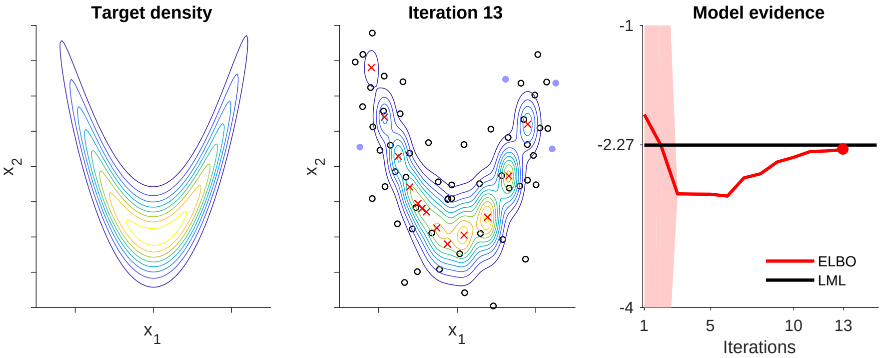


Target density
x_2
x_1
Iteration 11
x_2
x_1
Model evidence
-1
-2.27
-4
1
5
1011
Iterations
ELBO
LML

VBMC demo

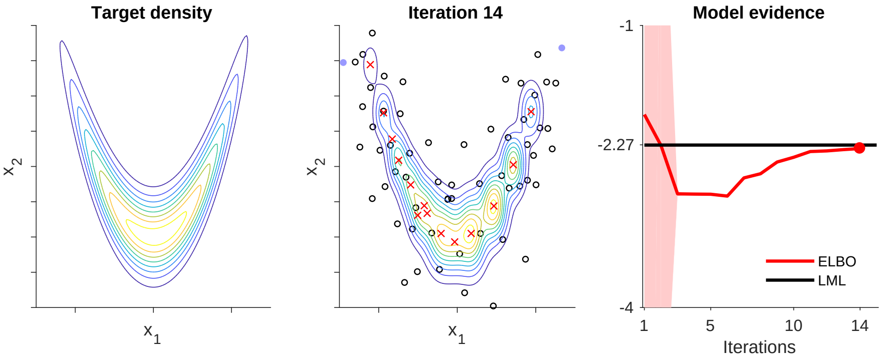

Target density
Iteration 12
Model evidence
x_2
x_1
x_2
x_1
-1
-2.27
-4
1
5
10
12
Iterations
ELBO
LML

VBMC demo



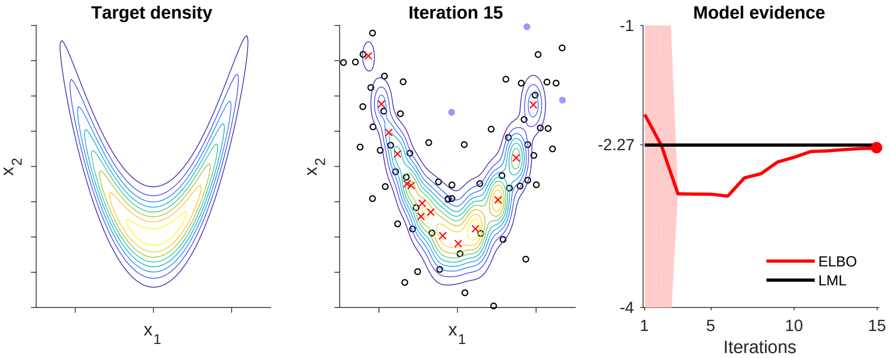
Target density
x2
x1
Iteration 13
x2
x1
Model evidence
-1
-2.27
-4
1
5
10
13
Iterations
ELBO
LML

VBMC demo



Target density
x_2
x_1
Iteration 14
x_2
x_1
Model evidence
-1
-2.27
-4
1
5
10
14
Iterations
ELBO
LML

VBMC demo



Target density
x2
x1
Iteration 15
x2
x1
Model evidence
-1
-2.27
-4
1
5
10
15
Iterations
ELBO
LML

Variational posterior

$$q_\phi(\boldsymbol{x}) = \sum_{k=1}^{K} w_k \mathcal{N}\left(\boldsymbol{x}; \boldsymbol{\mu}_k, \sigma_k^2 \boldsymbol{\Sigma}\right), \quad \boldsymbol{\Sigma} \equiv \text{diag}[{\lambda^{(1)}}^2, \ldots, {\lambda^{(D)}}^2]$$

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- $\boldsymbol{x} \in \mathbb{R}^D$
- $\phi \equiv (w_1, \ldots, w_K, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \sigma_1, \ldots, \sigma_K, \boldsymbol{\lambda})$
- $K(D+2)+D$ parameters
- K is changed adaptively each iteration

Gaussian process representation

$$f(\boldsymbol{x}) = \log p(\mathcal{D}|\boldsymbol{x})p(\boldsymbol{x})$$

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Sample over GP hyperparameters (later optimize)

Variational optimization

$$\mathrm{ELBO}(\phi, f) = \int q_{\phi}(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x} + \mathcal{H}[q_{\phi}(\boldsymbol{x})]$$

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Optimize with SGD (Adam; Kingma & Ba, 2014)

Active sampling

Optimize *acquisition function*: $\boldsymbol{x}_{\text{next}} = \arg\max_{\boldsymbol{x}} a(\boldsymbol{x})$

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$\Longrightarrow$ Prospective uncertainty sampling: $a_{\text{pro}}(\boldsymbol{x}) = V(\boldsymbol{x}) q_\phi(\boldsymbol{x}) \exp\left(\overline{f}(\boldsymbol{x})\right)$

Algorithmic details

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Expected Lower Confidence Bound (ELCBO)

$$\mathrm{ELCBO}(\phi, f) = \mathrm{ELBO}(\phi, f) - \beta_{LCB} \cdot \mathrm{SD}\left[\mathbb{E}_{\phi}\left[f\right]\right]$$

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- Termination criteria
  - Reliability index $\rho(t)$
  - Long-term stability: $\rho(t) \leq 1$ for n_{stable} iterations

1 Introduction and motivation

2 Background

3 Variational Bayesian Monte Carlo

4 Experiments

Experiment setup

Benchmark sets:

- Three families of synthetic functions ($D \in \{2, 4, 6, 8, 10\}$)
- Neuronal model with real data ($D = 7$)

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Procedure:

- Budget of $50 \times (D + 2)$ likelihood evaluations
- Metrics
  - Error wrt true log marginal likelihood (LML)
  - 'Gaussianized' symmetrized KL divergence between ground truth and posterior approximation (gsKL)

Algorithms

- VBMC-U (a_{us}) and VBMC-P (a_{pro})
- Simple Monte Carlo (SMC), annealed importance sampling (AIS)
- Bayesian Monte Carlo (BMC)
- Doubly-Bayesian quadrature (BBQ, BBQ*)
- WSABI, linearized (WSABI-L) and moment-matching (WSABI-M)
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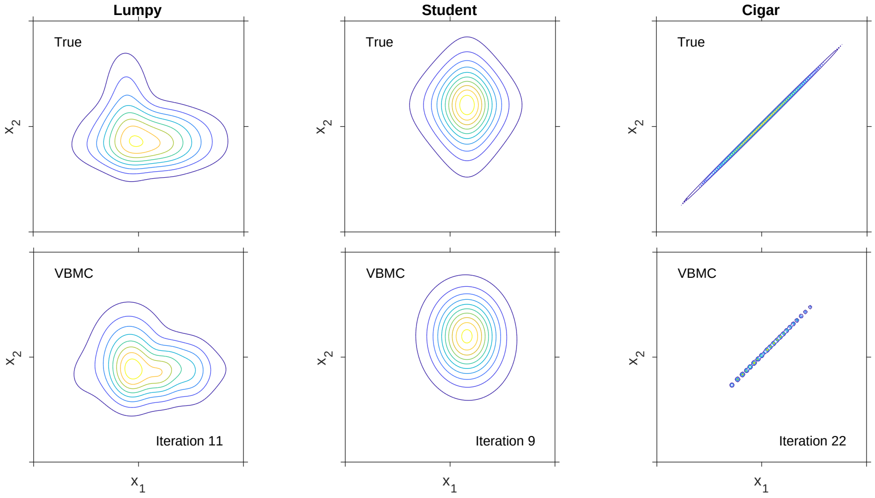
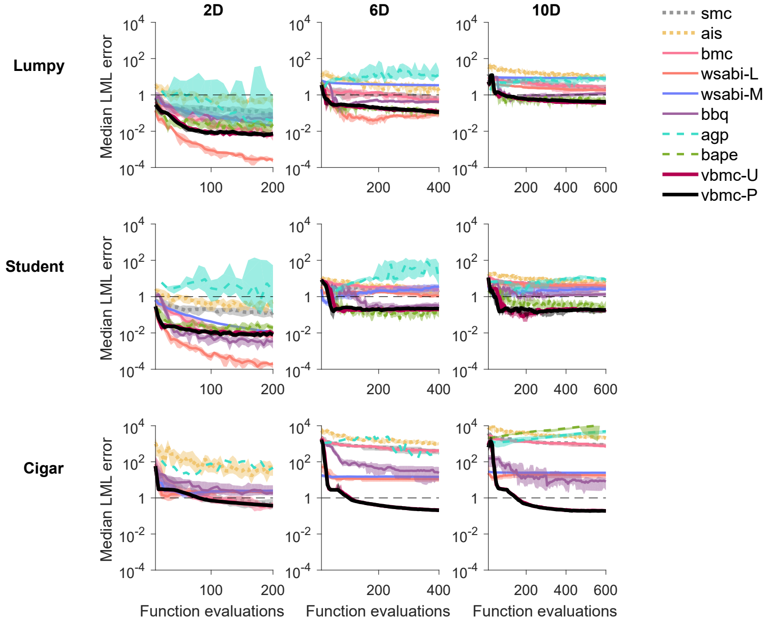
Synthetic target densities

Three families: *Lumpy*, *Student*, *Cigar* $\quad D \in \{2, 4, 6, 8, 10\}$



Synthetic target densities: Results



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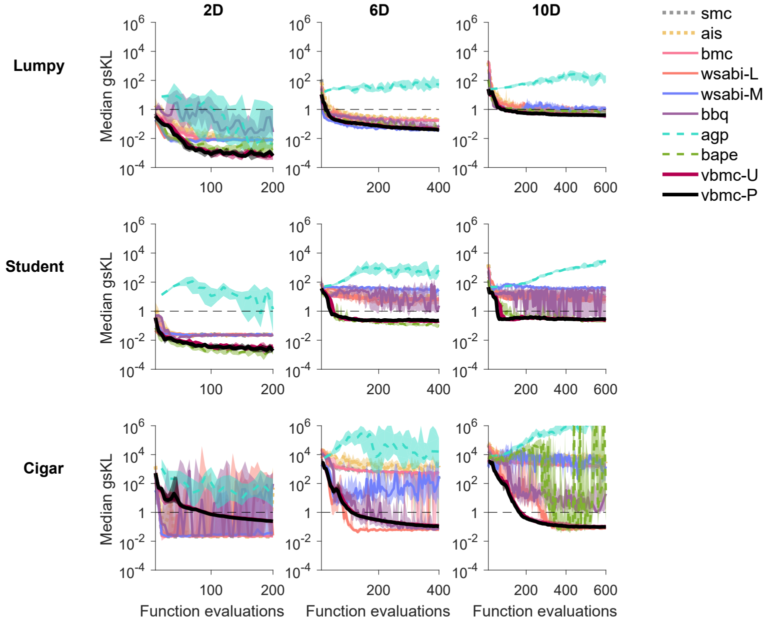
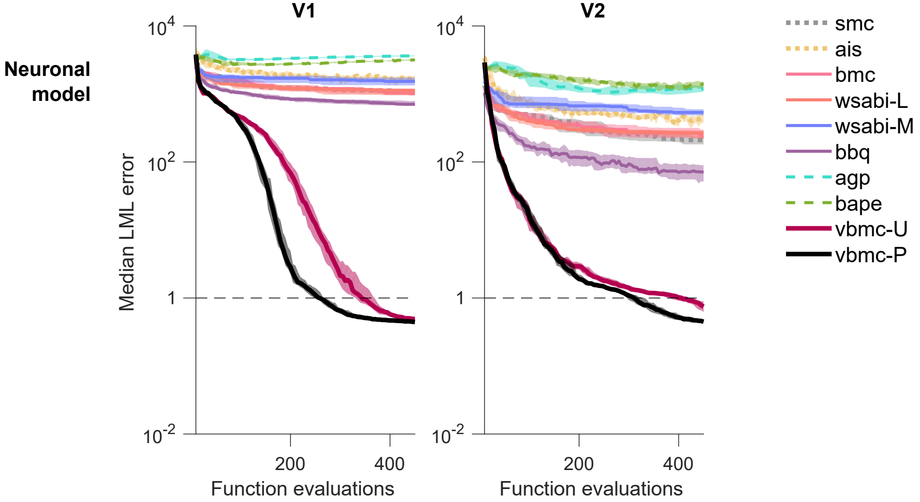


Neuronal model: Results

Two datasets: V1, V2 $\quad D = 7$



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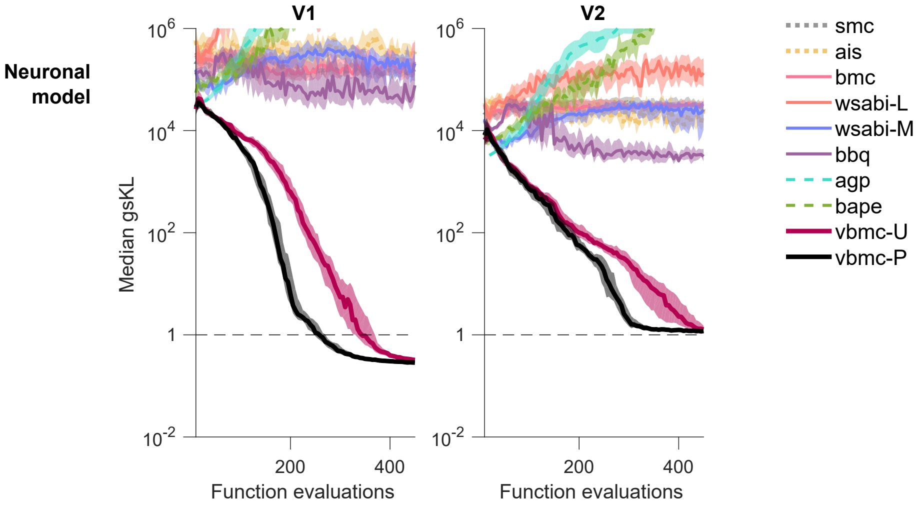
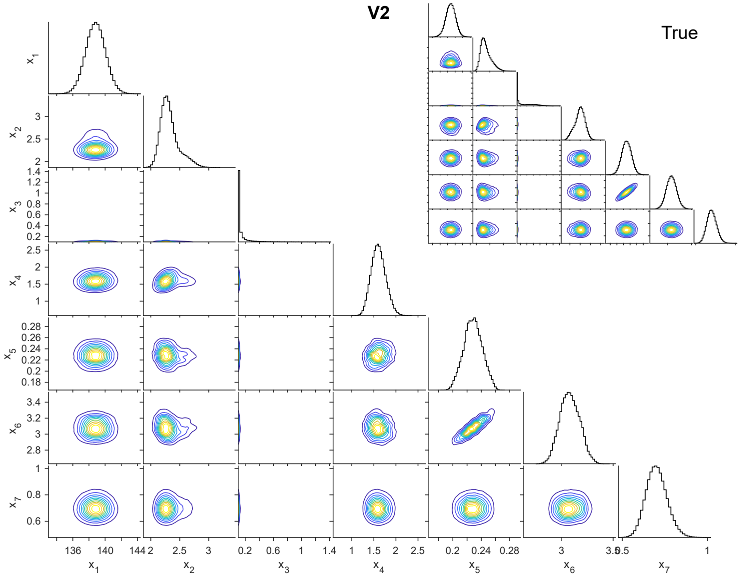
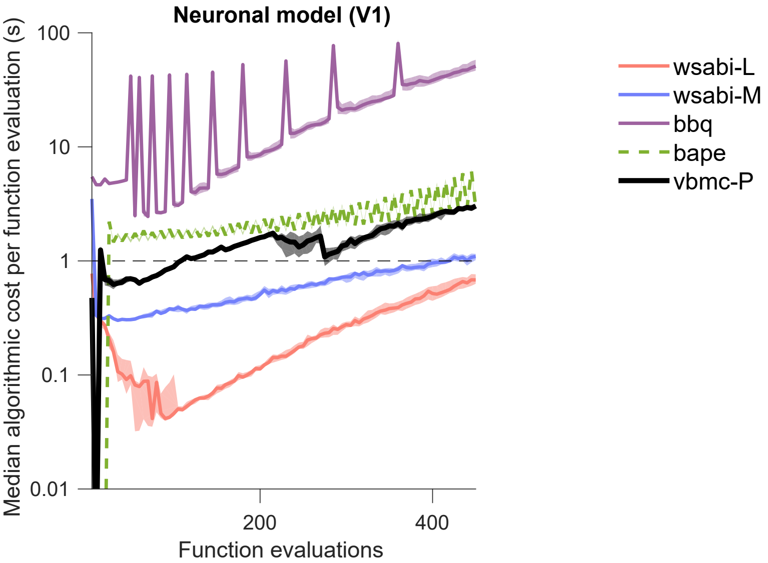


Neuronal model: VBMC



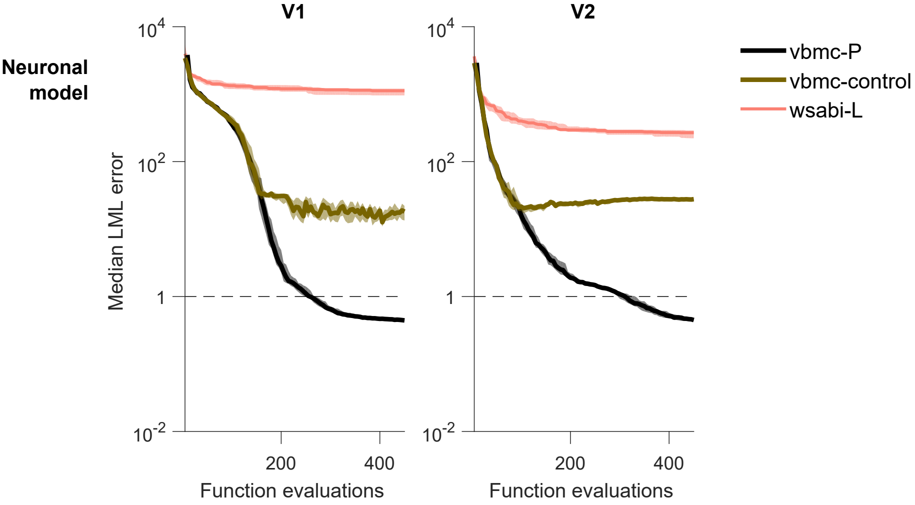
VBMC (iteration 52)

Computational cost



Control experiment

LML computed with WSABI-L on VBMC samples



What's the secret sauce?

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Other quadrature methods: (BMC, BBQ, WSABI)

$$Z = \int p(\boldsymbol{x}) p(\mathcal{D}|\boldsymbol{x}) d\boldsymbol{x}$$

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- GP representation

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- GP representation
- Integration scope

Discussion and future directions

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Discussion and future directions

- Nonstationarity
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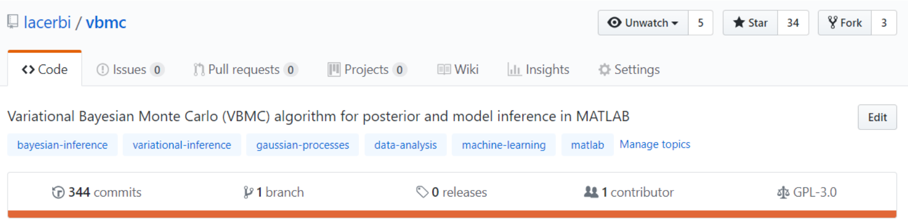
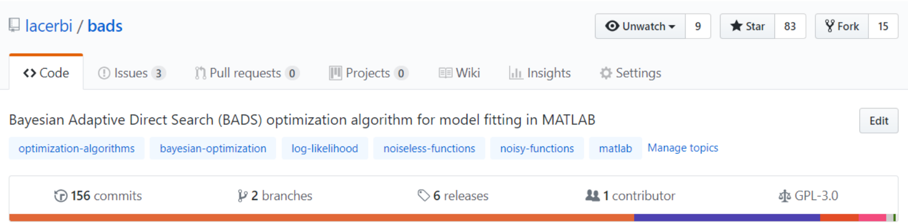
- More principled algorithmic solutions
- Killer application in machine learning

Toolboxes


lacerbi / vbmc
Unwatch 5
Star 34
Fork 3
Code
Issues 0
Pull requests 0
Projects 0
Wiki
Insights
Settings
Variational Bayesian Monte Carlo (VBMC) algorithm for posterior and model inference in MATLAB
Edit
bayesian-inference
variational-inference
gaussian-processes
data-analysis
machine-learning
matlab
Manage topics
344 commits
1 branch
0 releases
1 contributor
GPL-3.0


lacerbi / bads
Unwatch 9
Star 83
Fork 15
Code
Issues 3
Pull requests 0
Projects 0
Wiki
Insights
Settings
Bayesian Adaptive Direct Search (BADS) optimization algorithm for model fitting in MATLAB
Edit
optimization-algorithms
bayesian-optimization
log-likelihood
noiseless-functions
noisy-functions
matlab
Manage topics
156 commits
2 branches
6 releases
1 contributor
GPL-3.0

Final slide

- VBMC paper: `https://arxiv.org/abs/1810.05558`
- VBMC toolbox at: `github.com/lacerbi/vbmc`
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