# Variational Bayesian Monte Carlo


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Bayesian inference with expensive black-box statistical models

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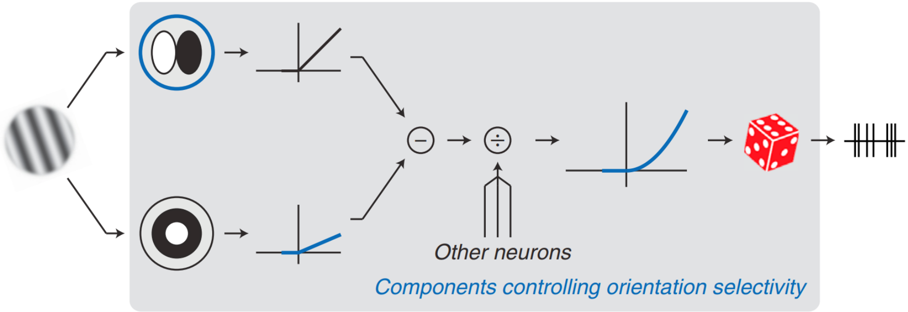
(Why Bayesian inference?)

# Example: LN-LN neuronal model




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

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

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

# What do we need?

- An *approximate inference* framework
- A *surrogate model*
- A method to combine the two

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- An *approximate inference* framework: variational inference
- A *surrogate model*: Gaussian processes
- A method to combine the two: Bayesian quadrature

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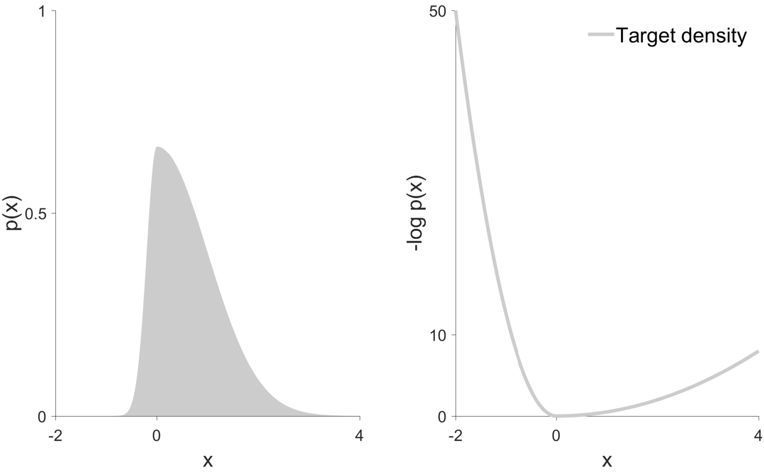
VI casts Bayesian inference into optimization + integration

# Variational inference: example



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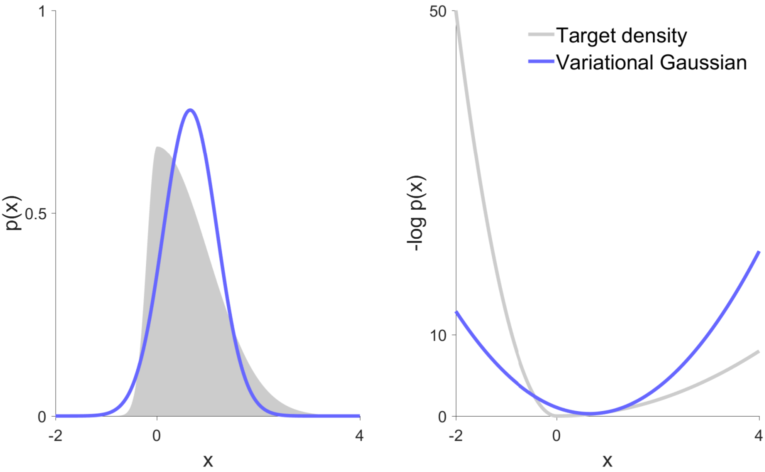


$$q_\phi(x) = \mathcal{N}\left(x, \mu, \sigma^2\right) \qquad \phi = \left(\mu, \sigma^2\right)$$

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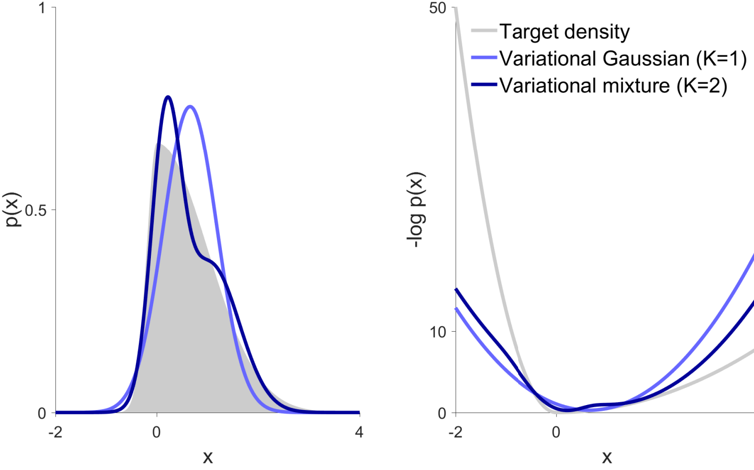


$$q_\phi(x) = \sum_{k=1}^{K} w_k \mathcal{N}\left(x, \mu_k, \sigma_k^2\right) \qquad \phi = \left(w_k, \mu_k, \sigma_k^2\right)_{k=1}^{K}$$

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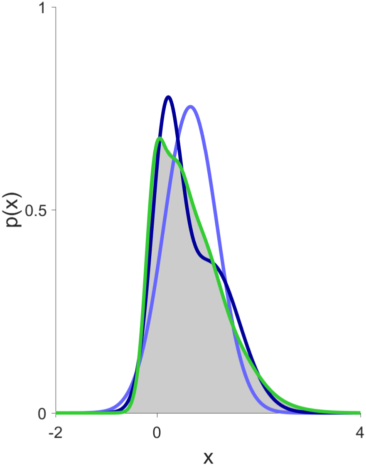


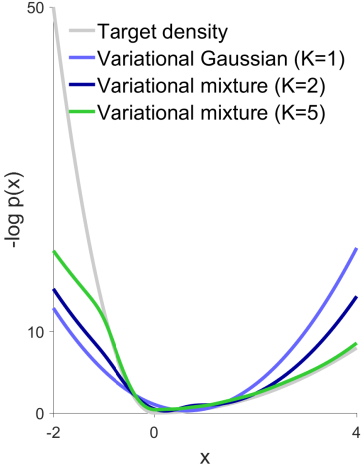


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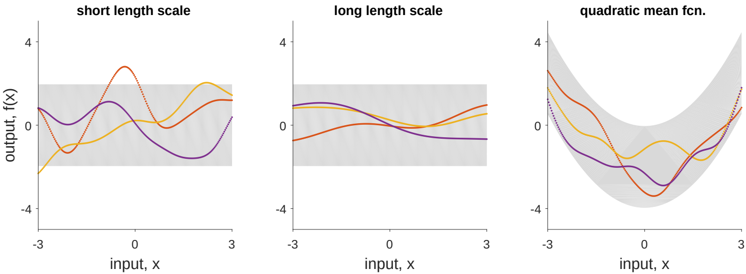

# Posterior GPs

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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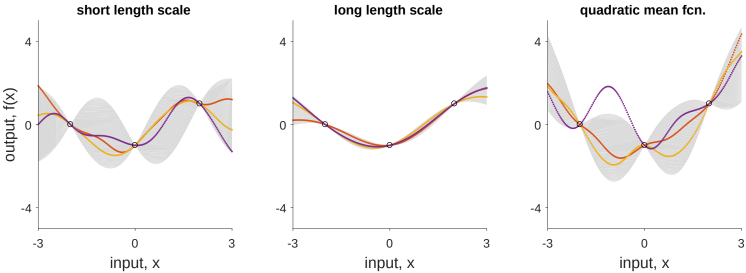

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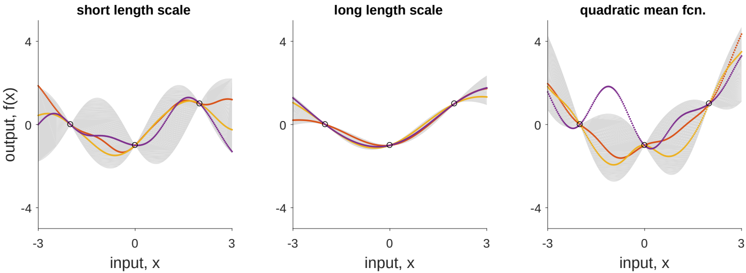


GP marginal likelihood $p(\boldsymbol{y}|\mathbf{X}, \psi)$

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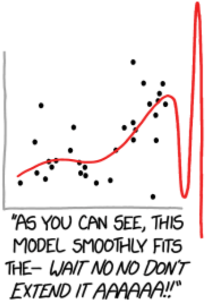


from `xkcd.com/2048`

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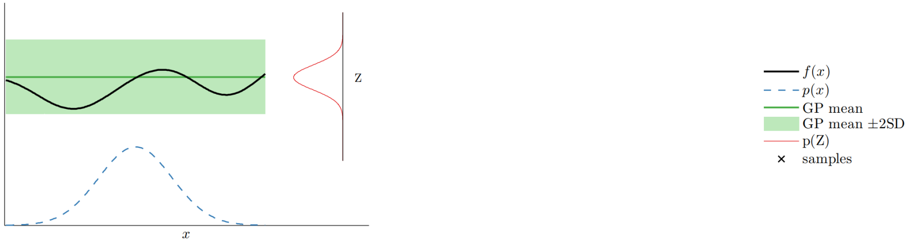


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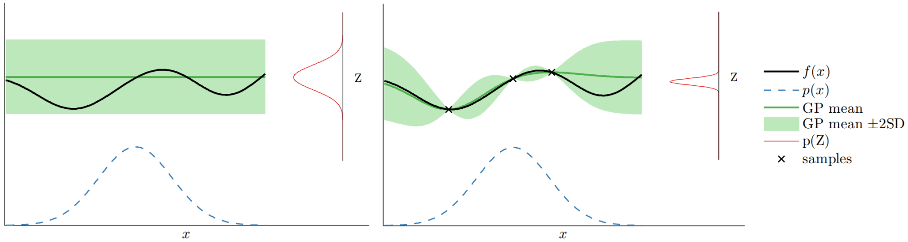


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- *Uncertainty sampling*: Maximize variance of integrand $p(\boldsymbol{x})f(\boldsymbol{x})$

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VI + BQ $\Rightarrow$ VBMC

# VBMC in an nutshell

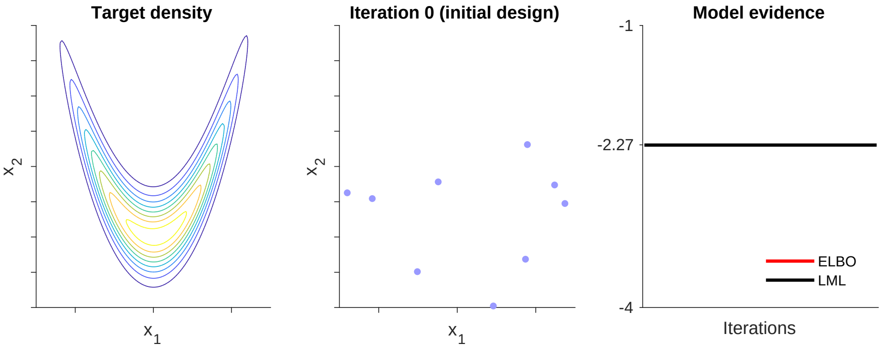
In each iteration $t$:

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 $q_{\phi_t}$ by optimizing the ELBO

Loop until reaching termination criterion

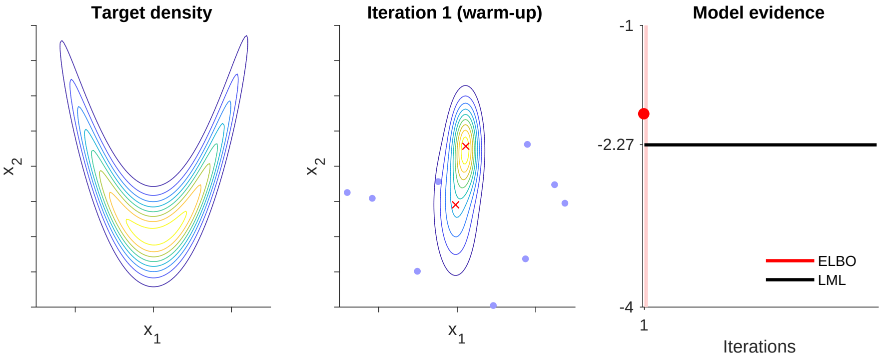
Acerbi, *NeurIPS* (2018)

# VBMC demo

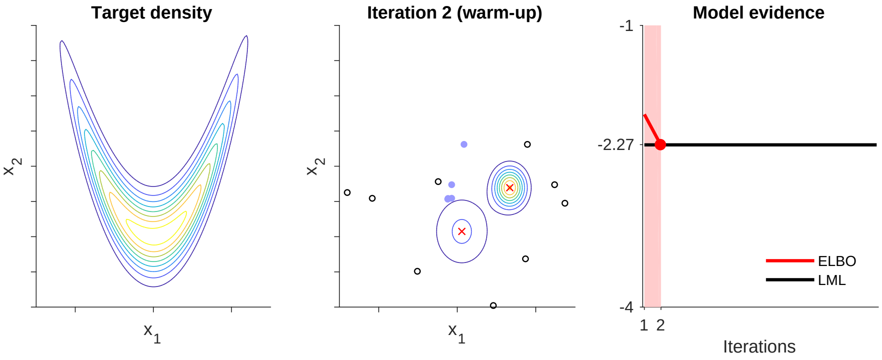


Target density
$x_2$
$x_1$
Iteration 0 (initial design)
$x_2$
$x_1$
Model evidence
-1
-2.27
-4
ELBO
LML
Iterations

# VBMC demo

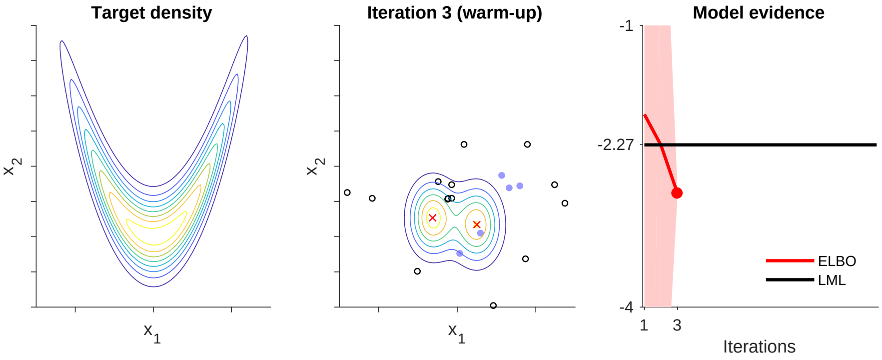

Target density
Iteration 1 (warm-up)
Model evidence
x2
x1
-1
-2.27
-4
1
Iterations
ELBO
LML

# VBMC demo



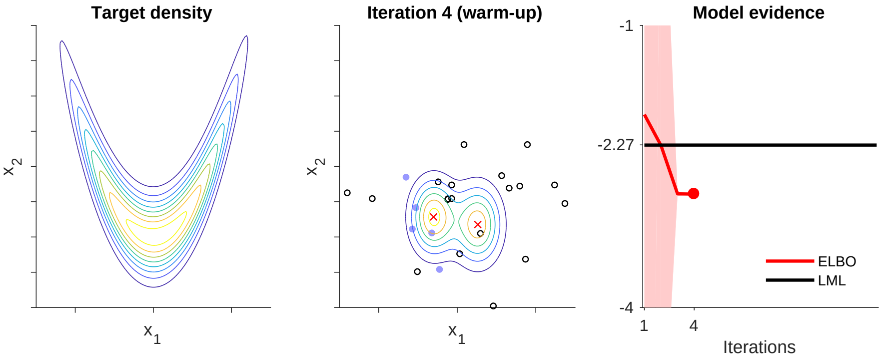
Target density
x2
x1
Iteration 2 (warm-up)
x2
x1
Model evidence
-1
-2.27
-4
1 2
Iterations
ELBO
LML

# VBMC demo



Target density
x2
x1
Iteration 3 (warm-up)
x2
x1
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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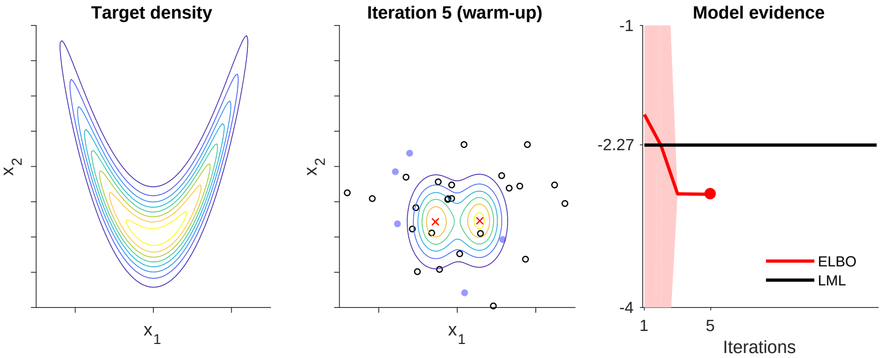

Target density
x_2
x_1
Iteration 5 (warm-up)
x_2
x_1
Model evidence
-1
-2.27
-4
1
5
Iterations
ELBO
LML

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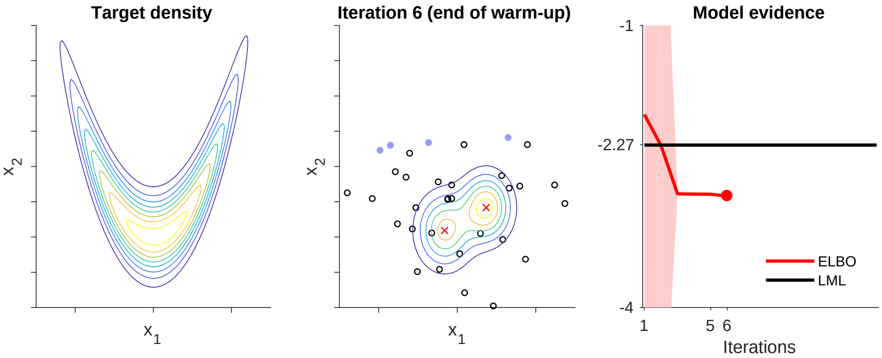
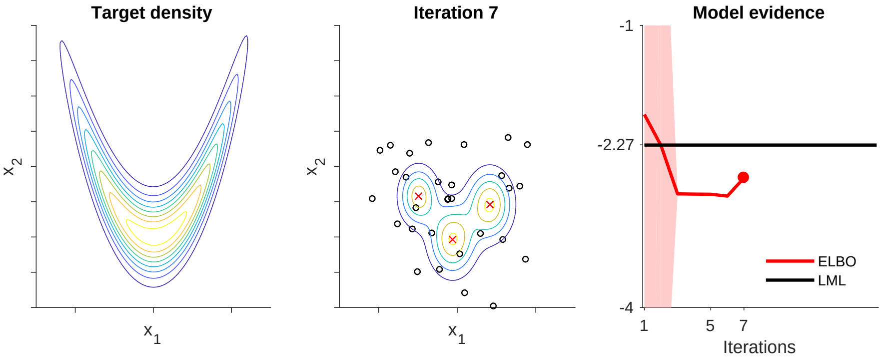


Target density
x2
x1
Iteration 6 (end of warm-up)
x2
x1
Model evidence
-1
-2.27
-4
1
5
6
Iterations
ELBO
LML

# 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

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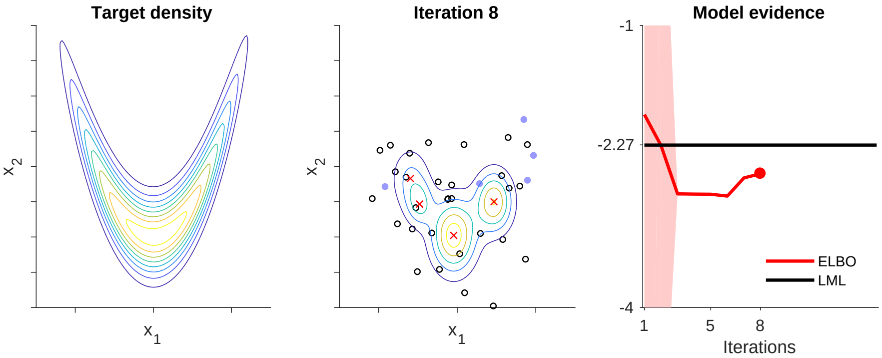
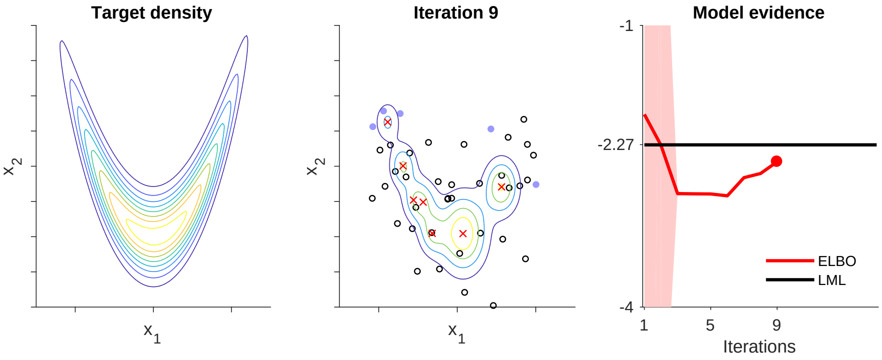

Target density
$x_2$
$x_1$
Iteration 8
$x_2$
$x_1$
Model evidence
-1
-2.27
-4
1
5
8
Iterations
ELBO
LML

# VBMC demo



Target density
x_1
x_2
Iteration 9
x_1
x_2
Model evidence
-1
-2.27
-4
1
5
9
Iterations
ELBO
LML

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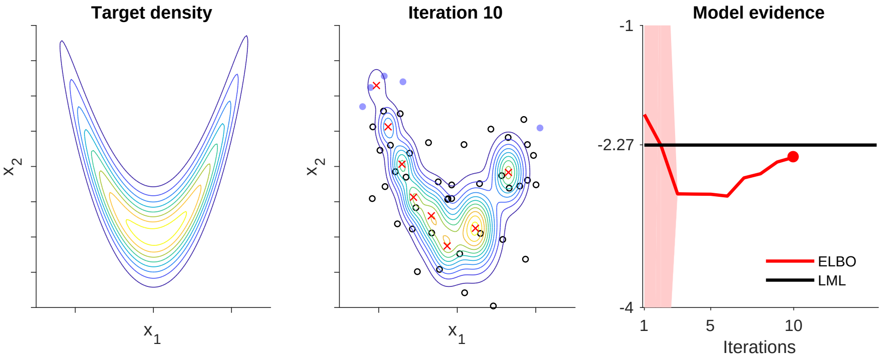

Target density
Iteration 10
Model evidence
x 2
x 1
-1
-2.27
-4
1
5
10
Iterations
ELBO
LML

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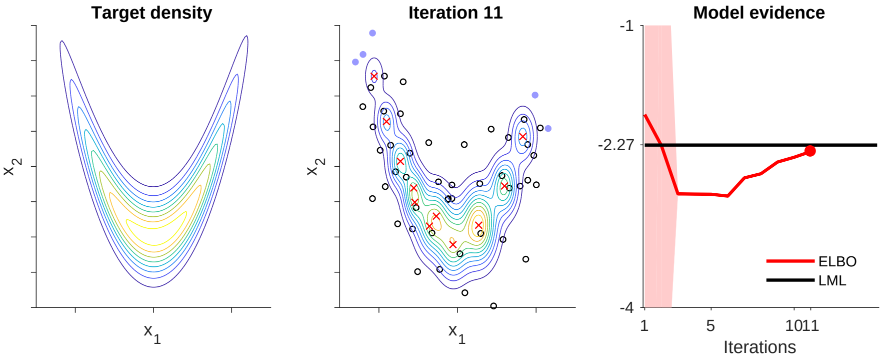
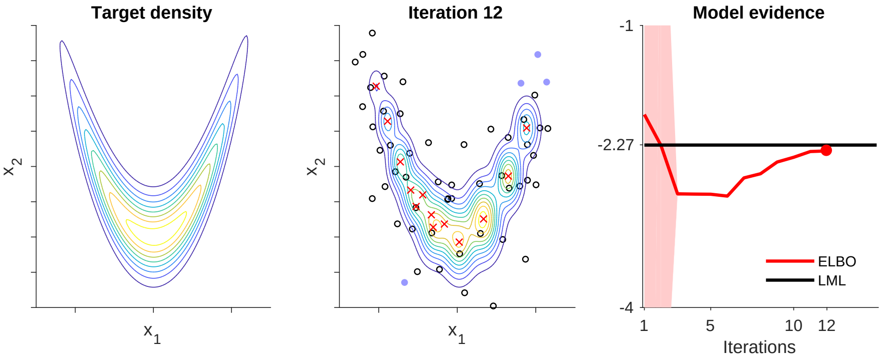


Target density
x 2
x 1
Iteration 11
x 2
x 1
Model evidence
-1
-2.27
-4
1
5
1011
Iterations
ELBO
LML

# VBMC demo



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

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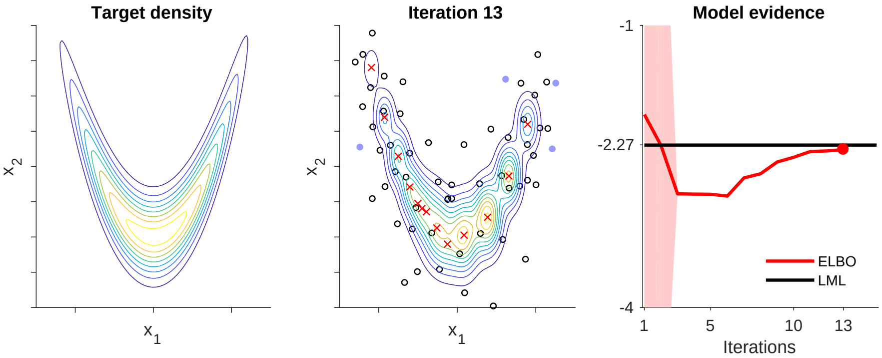

Target density
$x_2$
$x_1$
Iteration 13
$x_2$
$x_1$
Model evidence
-1
-2.27
-4
1
5
10
13
Iterations
ELBO
LML

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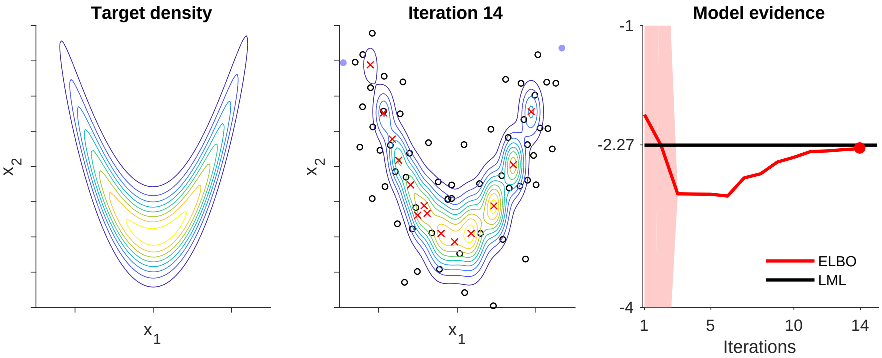

Target density
$x_2$
$x_1$
Iteration 14
$x_2$
$x_1$
Model evidence
-1
-2.27
-4
1
5
10
14
Iterations
ELBO
LML

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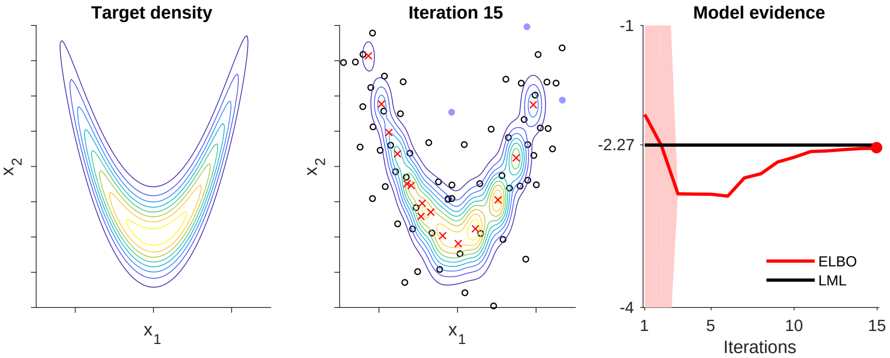
Target density
$x_2$
$x_1$
Iteration 15
$x_2$
$x_1$
Model evidence
-1
-2.27
-4
1
5
10
15
Iterations
ELBO
LML

# Variational posterior

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

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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

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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)

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

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$\implies$ 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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### Evidence Lower Confidence Bound (ELCBO)

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

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

# Experiment setup

Benchmark sets:

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- Three families of synthetic functions ($D \in \{2, 4, 6, 8, 10\}$)
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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 ($a_{\text{us}}$) and VBMC-P ($a_{\text{pro}}$)
- 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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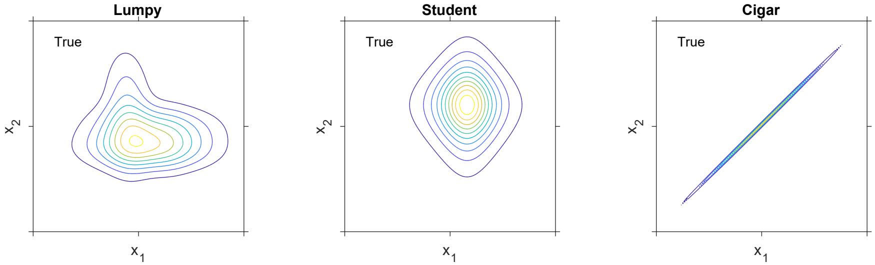
Three families: *Lumpy*, *Student*, *Cigar* $\quad D \in \{2, 4, 6, 8, 10\}$



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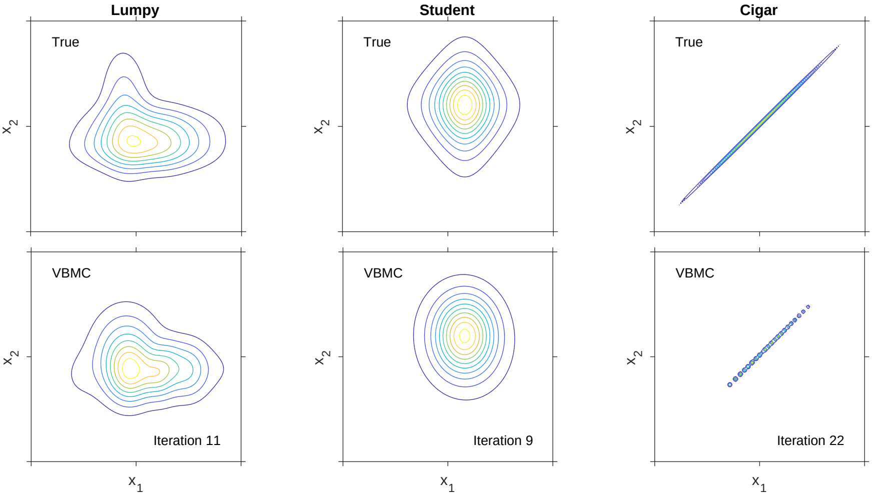

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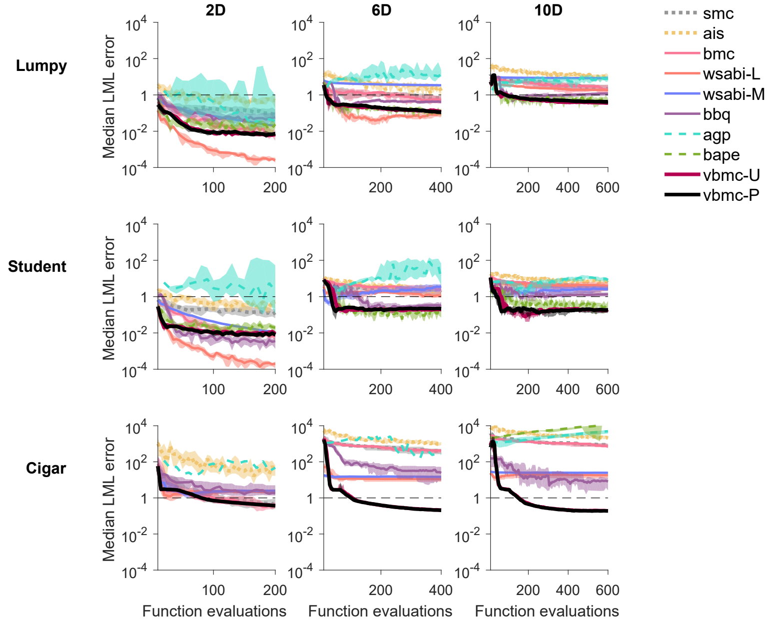

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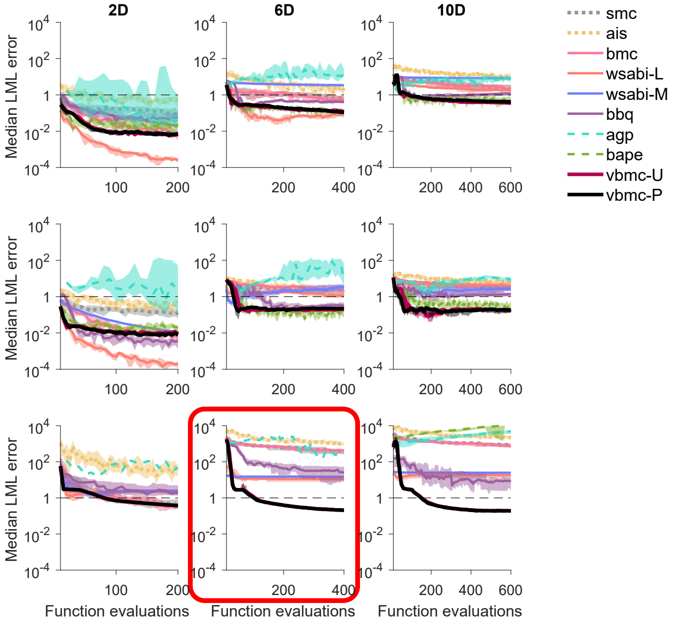

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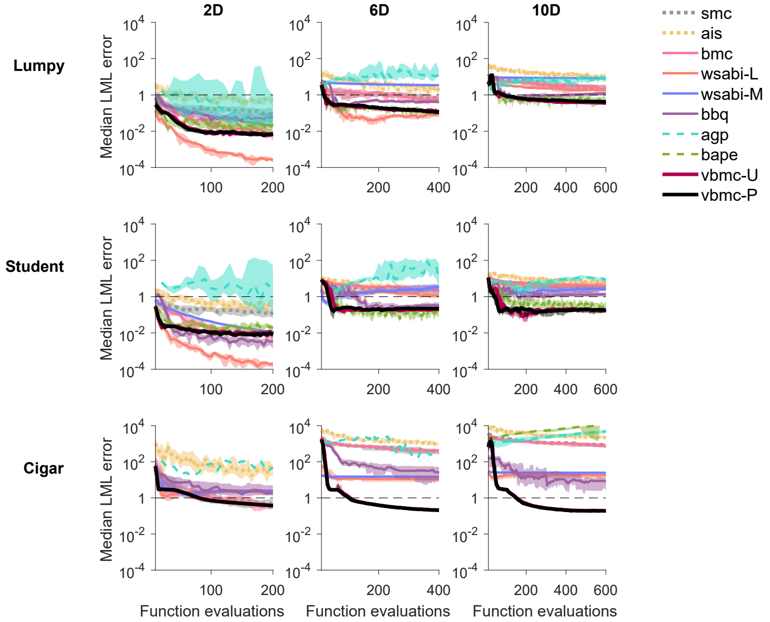

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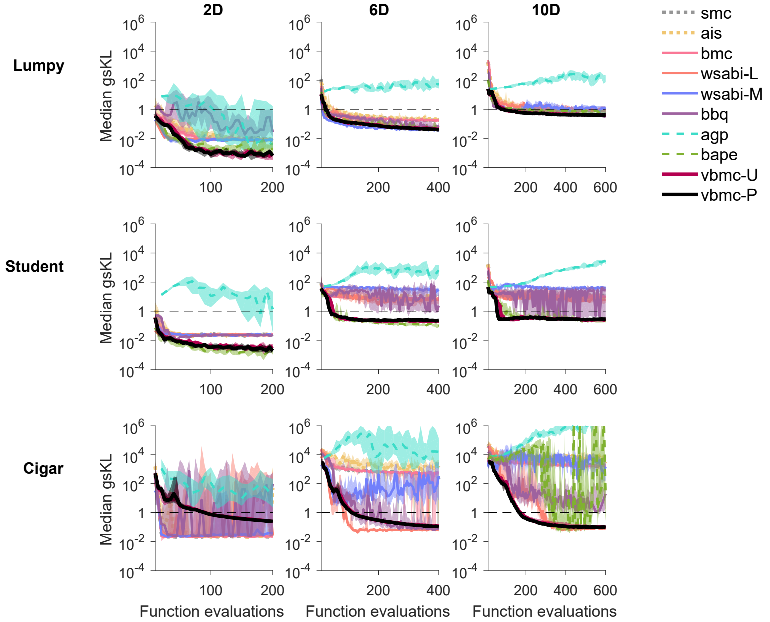
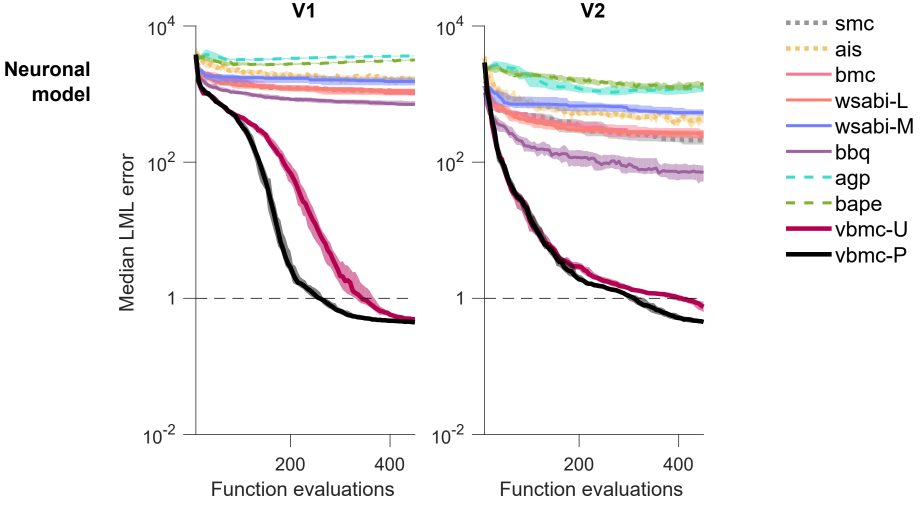


# Neuronal model: Results

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



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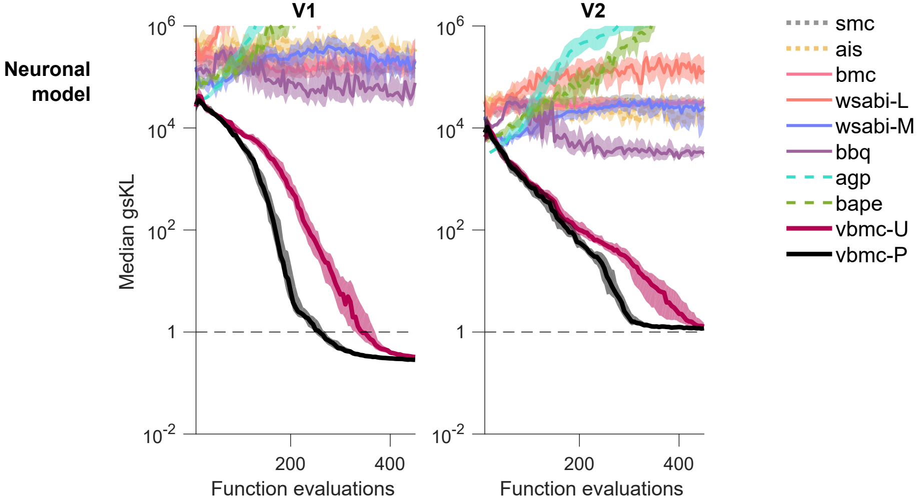
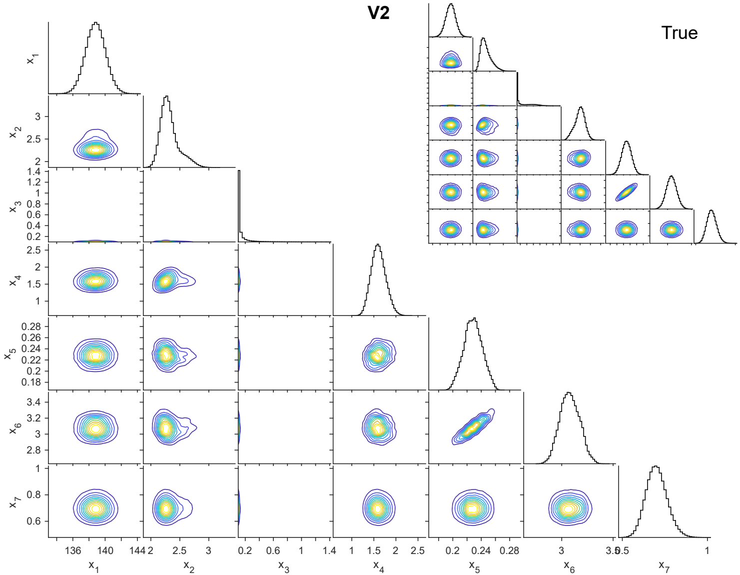
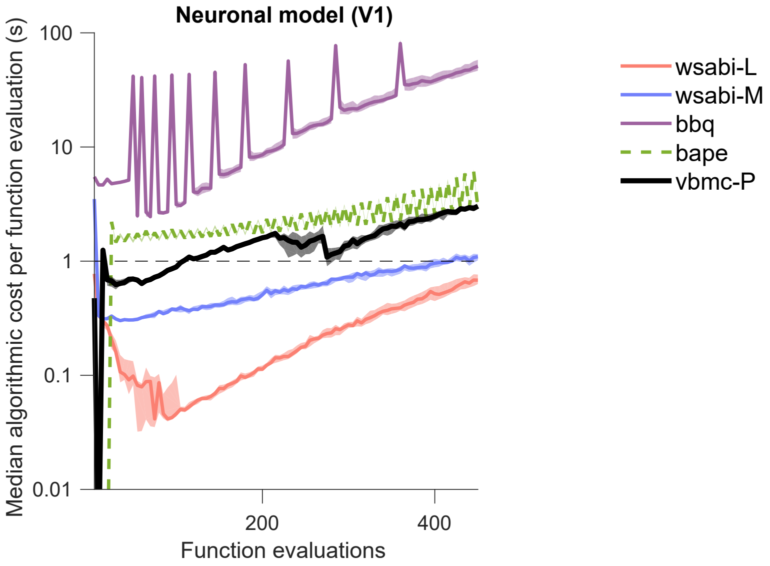


# Neuronal model: VBMC




VBMC (iteration 52)

# Computational cost



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Other quadrature methods: (BMC, BBQ, WSABI)

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- GP representation
- Integration scope

# Discussion and future directions

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- Model mismatch and robustness (e.g., nonstationarity)
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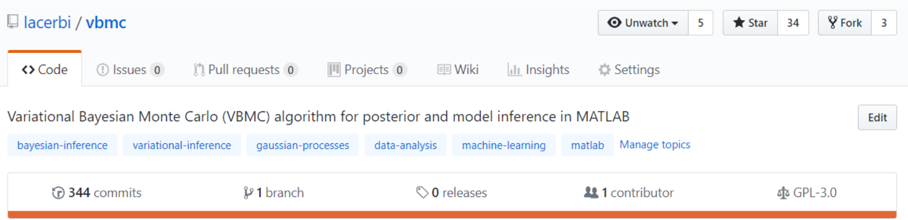
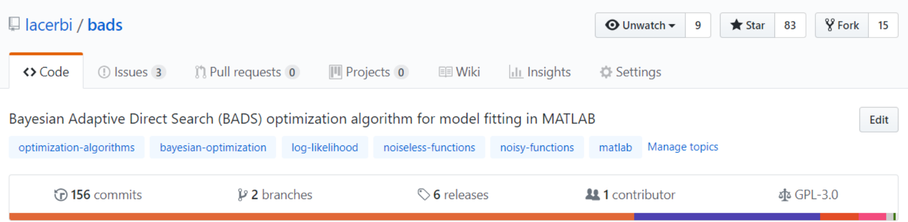
- Killer application in machine learning

# Toolboxes




Acerbi & Ma, *NIPS* (2017)

# Final slide

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

# References


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# Control experiment

LML computed with WSABI-L on VBMC samples