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17 de setembro de 2019

Outline

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Introduction

Some introduction.

Introduction

Bayesian theory

Building blocks

- Prior probability $p(\theta)$
- Likelihood $p(\mathcal{D}|\theta)$

Posterior probability

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{\int p(\mathcal{D}|\theta')p(\theta')d\theta'}$$

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$$\int_{\Theta} f(\theta)p(\theta|\mathcal{D}, M)d\theta$$

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Bayesian theory requires integration!

Introduction

Approximate inference

Ways to integrate:

- Monte Carlo

$$\int_{\Theta} f(\theta)p(\theta|\mathcal{D})d\theta \approx \frac{1}{N}\sum_{i=1}^{N} f(\theta_i),\ \theta_i \sim p(\theta|\mathcal{D})$$

- Approximate distribution

$$p(\theta|\mathcal{D}) \approx q(\theta), \quad \int_{\Theta} f(\theta)q(\theta)d\theta$$

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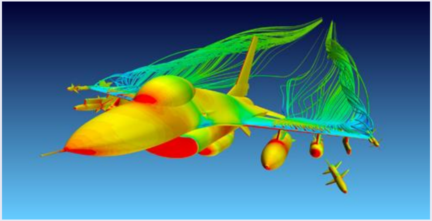
$$p(\theta|\mathcal{D}) \approx q(\theta), \quad \int_{\Theta} f(\theta)q(\theta)d\theta$$

Usual methods demands many evaluations of $p(\mathcal{D}|\theta)p(\theta)$. However, *this is not always feasible.*

In science, there are many cases that $p(\mathcal{D}|\theta)$ demands the computation of a forward model $g(\theta)$, which comes from an expensive simulation.



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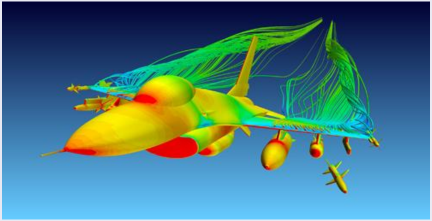

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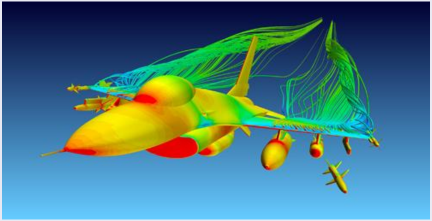
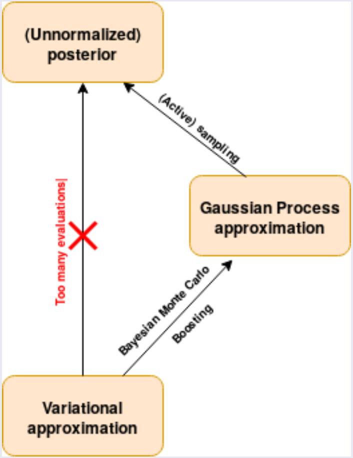


This requires approximate inference methods "on a budget". In this work, one such method is developed, based on preexisting work. We name it

Boosted Variational Bayesian Monte Carlo (BVBMC).

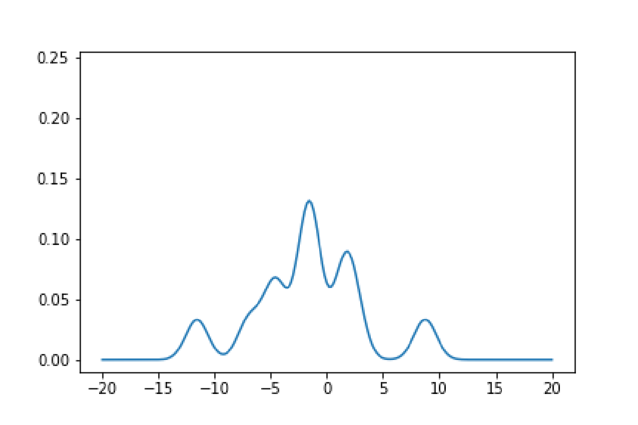
Introduction

BVBMC schema



Introduction

An illustration of BVBMC



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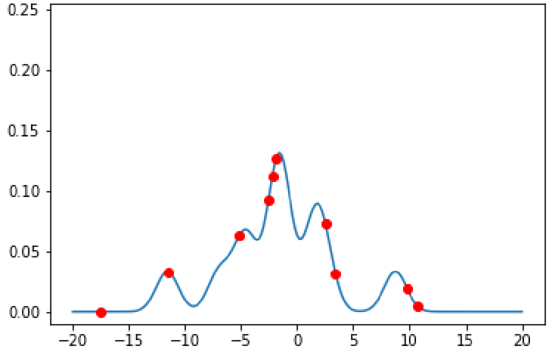

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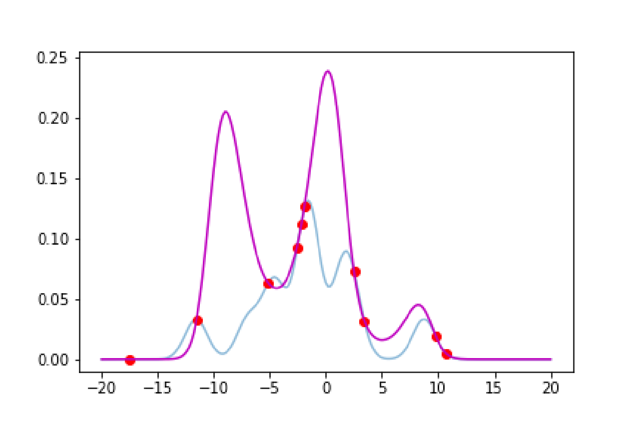

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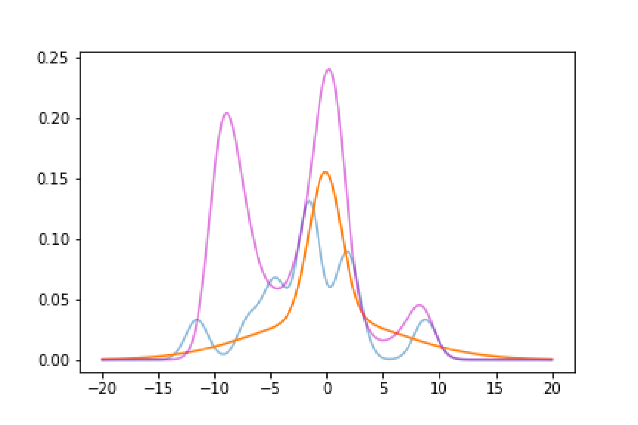

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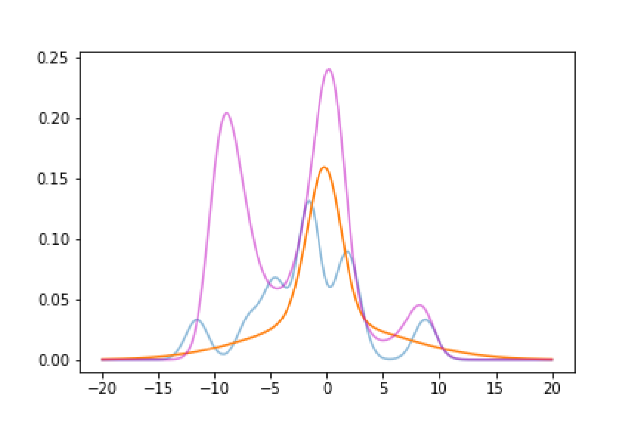

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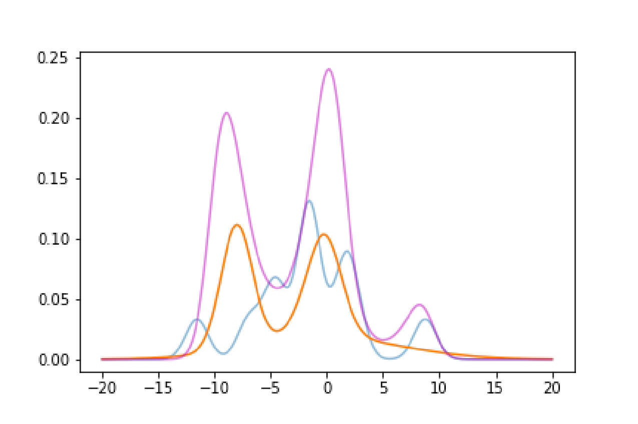

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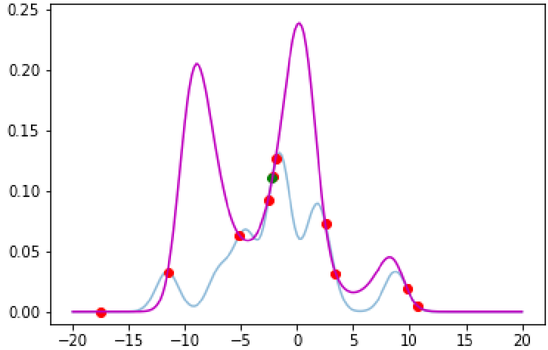

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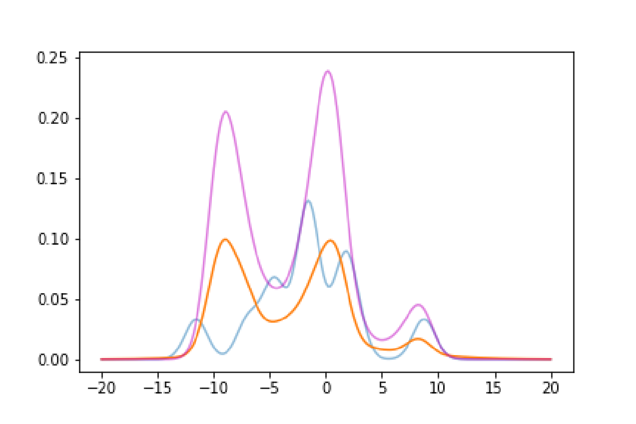

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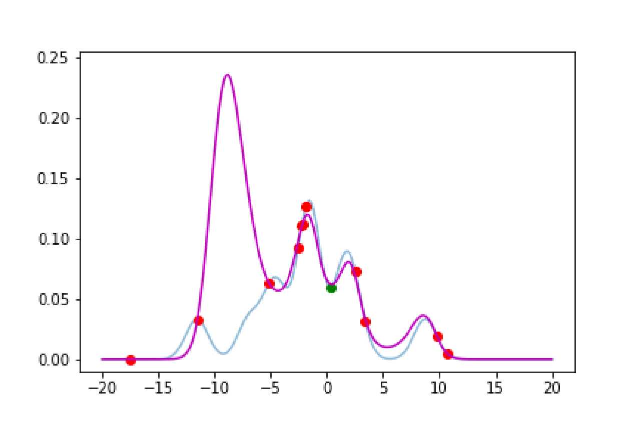

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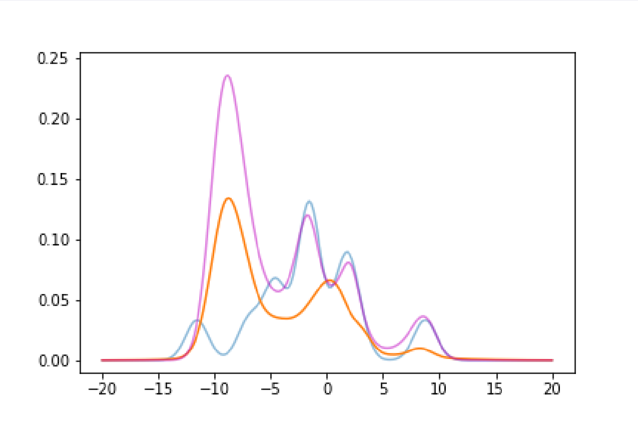

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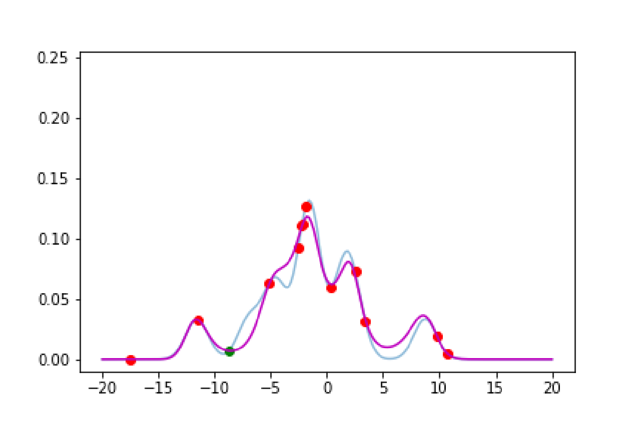

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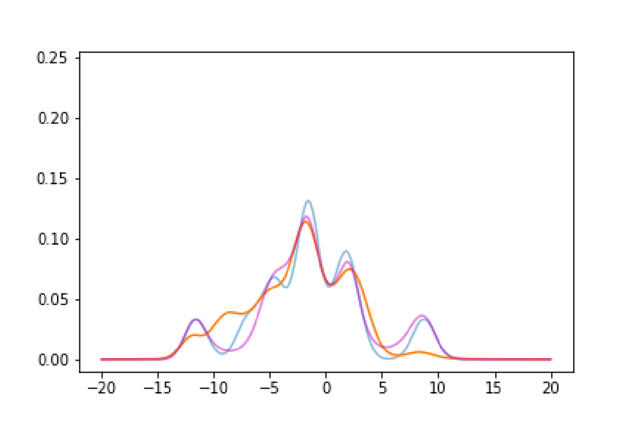

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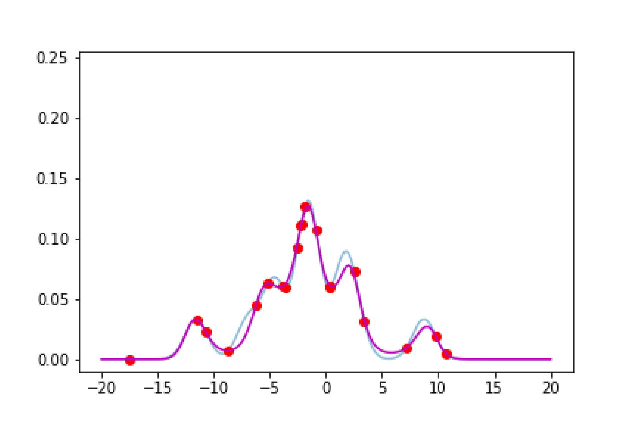

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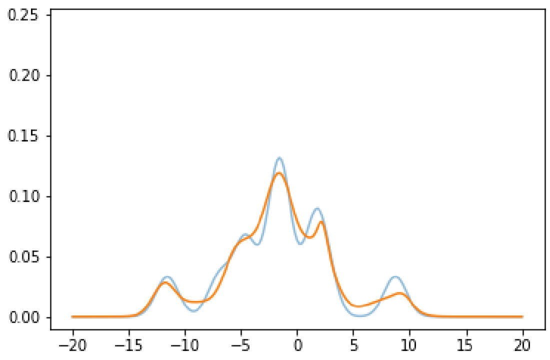

Gaussian Processes

Definition

Gaussian processes (GP): distribution over functions $f : \mathcal{X} \to \mathbb{R}$ such that $f(\mathbf{x}) = (f(x_1), \ldots, f(x_n))$ follows a multivariate normal distribution. A GP is completely defined by:

- $m(x) := \mathbb{E}[f(x)]$, mean function.
- $k(x, x') := \mathbb{E}[f(x), f(x')]$, covariance function or kernel.

such that $f(\mathbf{x}) \sim \mathcal{N}(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}))$.

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Gaussian process regression

Given $\mathcal{D} = (x, y)_{i=1}^{N}$, a Gaussian process regression is made by assuming $p(y|x) = p(y|f(x))$, with f following a prior $GP(m, k)$.

Gaussian Processes

Posterior GP

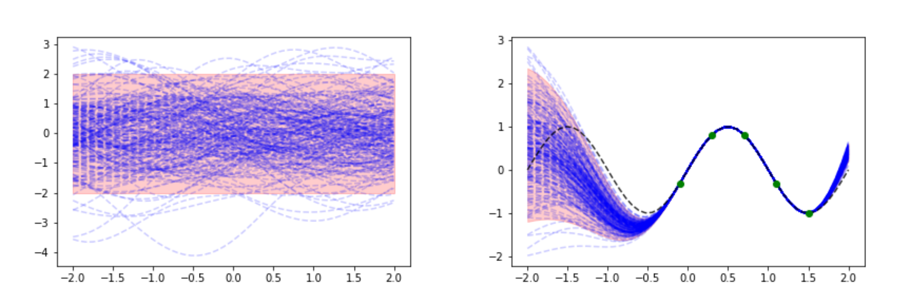
If $p(y|f(x)) = \mathcal{N}(f(x), \sigma_n^2)$, $f|\mathcal{D} \sim GP(m_{\mathcal{D}}, k_{\mathcal{D}})$, where

$$m_{\mathcal{D}}(x) := m(x) + K(x^\star, \mathbf{x})(K(\mathbf{x}, \mathbf{x}) + \sigma_n^2)^{-1}(\mathbf{y} - m(\mathbf{x}))$$
$$k_{\mathcal{D}}(x, x') := k(x, x') - K(x, \mathbf{x})(K(\mathbf{x}, \mathbf{x}) + \sigma_n^2)^{-1} K(\mathbf{x}, x)$$

Reduces to deterministic measurement when $\sigma_n^2 = 0$. More general $p(y|f(x))$ must resort to explicit marginalization.

Gaussian Processes

Example case



(a) GP prior

(b) GP posterior

Gaussian Processes

Kernels

The exigence that $K(\mathbf{x},\mathbf{x})$ limits which functions can be kernels. Some examples of kernels in $\mathbb{R}$ are:

- $k_{SQE}(x,x') = \theta_0 \exp\left(-\frac{1}{2}\frac{(x-x')^2}{l^2}\right)$
- $k_{\text{Matern},3/2}(x,x') = \theta_0 \left(\sqrt{3}\frac{(x-x')}{l}\right) \exp\left(-\sqrt{3}\frac{(x-x')}{l}\right)$

Kernels in $\mathbb{R}^D$ can be constructed by changing $\frac{(x-x')}{l}$ for $\sqrt{\sum_{i=1}^{D} \frac{(x_i-x_i')}{l_i}}$.
If k_1,k_2 are kernels, the following, among others are kernels:
$k_1(x,x') + k_2(x,x')$,$k_1(x,x')k_2(x,x')$,$k_1(x,x')k_2(y,y')$,$k_1(f(y),f(y'))$.

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Mean functions

In general,they are less important than kernels, since the latter determines the structure of the posterior GP. However, *outside the sampling area the GP prediction defaults to the mean*, which may be of importance.

Gaussian processes

Handling hyperparameters

$$\log p(\mathcal{D}|M,\sigma_n) = -\frac{1}{2}(\mathbf{y}-m(\mathbf{x}))^T(K(\mathbf{x},\mathbf{x})+\sigma_n\mathbf{I})^{-1}(\mathbf{y}-m(\mathbf{x}))+ \\ -\frac{1}{2}\log\det(K(\mathbf{x},\mathbf{x})+\sigma_n\mathbf{I})-\frac{1}{2}N\log(2\pi).$$

Inference can be done either by MLE, MAP, or integration techniques.

Scaling

The bottleneck of GP regression: $(K(\mathbf{x},\mathbf{x})+\sigma_n\mathbf{I})^{-1}$. Cost is $\mathcal{O}(N^3)$.
In online learning, each new sample is incorporated in $\mathcal{O}(N^2)$.

Bayesian Monte Carlo

Integrating a GP

$$Z = \int f(x)p(x)dx$$

If $f \sim GP(m, k)$, given $\mathcal{D} = \{(x_i, f(x_i))\}_{i=1}^N$, $Z_{\mathcal{D}} = \int f_{\mathcal{D}}(x)p(x)dx$ is Gaussian:

$$\mathbb{E}[Z_{\mathcal{D}}] = \int m(x)p(x)dx - \mathbf{z}^T K^{-1}(\mathbf{f} - m(\mathbf{x})), \quad \mathrm{Var}[Z_{\mathcal{D}}] = \Gamma - \mathbf{z}^T K^{-1}\mathbf{z},$$

$$z_i = \int k(x, x_i)p(x)dx, \quad \Gamma = \int \int k(x, x')p(x)p(x')dxdx'.$$

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Name Bayesian *Monte Carlo* is misleading.

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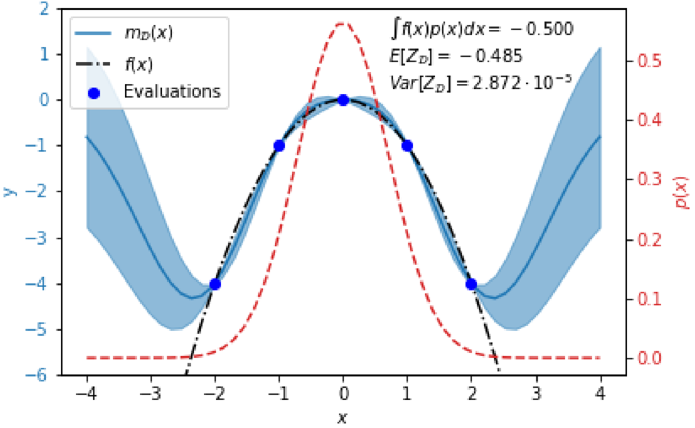
Name Bayesian *Monte Carlo* is misleading.
Treating f as a random variable may be philosophically odd.

Bayesian Monte Carlo



Bayesian Monte Carlo

Kernel integral terms

In the general case, they can be estimated by Monte Carlo. When $p(x)$ is Gaussian or a mixture of Gaussians:

- Analytically tractable when $k(x, x')$ is the SQE kernel.
- Efficiently tractable when $k(x, x') = k(x_1, y_1) \ldots k(x_D, y_D)$.

Active sampling

Given $\{(x_1, f(x_1), \ldots, x_N, f(x_N)\}$, x_{N+1} may be chosen by optimizing acquisition functions.

$$\alpha^N_{\mathrm{MMLT}}(x) = e^{2m_{\mathcal{D}}(x)+k_{\mathcal{D}}(x,x)} \left(e^{k_{\mathcal{D}}(x,x)} - 1\right).$$

Variational Inference

Back to approximating posteriors $p(\theta|\mathcal{D}) \approx q(\theta;\lambda)$

Variational Inference: given $g(\theta)$, seeks minimization of $D_{KL}(q(\cdot;\lambda)||g)$. Given unnormalized $\bar{g}$, this is equivalent to maximizing the evidence lower bound (ELBO)

$$\mathcal{L}(\lambda) = \int \log \bar{g}(\theta) q(\theta) d\theta - \int \log q(\theta) q(\theta) d\theta$$

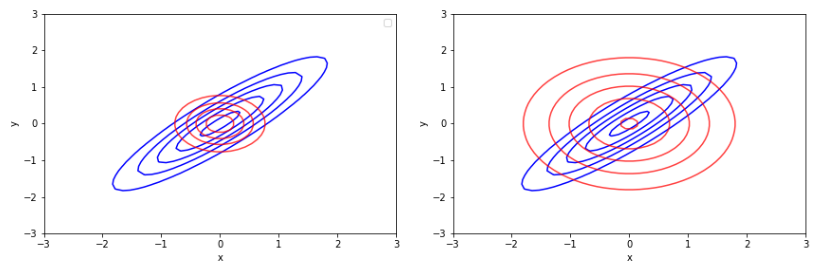
The family of variational posteriors $q(\theta;\lambda)$ must be easy to treat, in order for the approximation to be useful.

$D_{KL}(q(\cdot;\lambda)||g)$ vs $D_{KL}(g||q(\cdot;\lambda))$

$D_{KL}(q(\cdot;\lambda)||g) \neq D_{KL}(g||q(\cdot;\lambda))$: two minimization objectives. Gives two different algorithms (the second one, *expectation propagation*, is not treated here).

Variational Inference

Illustration



(c) $D_{KL}(q||g)$ (d) $D_{KL}(g||q)$

Variational Inference

Mean field variational inference

Consider factorized proposals $q(\theta) = q(\theta_1) \dots q(\theta_D)$.
Training by coordinate descent

$$q_j^*(\theta_j; q_{-j}) \propto \exp \mathbb{E}_{\theta_{-j} \sim q_{-j}}[\log \bar{g}(\theta)].$$

Generic variational inference

Uses stochastic gradient descent to find $q(\theta; \lambda)$.
REINFORCE: $\nabla \mathcal{L}(\lambda) = \mathbb{E}_{q(\theta;\lambda)} \left[\left(\log \left(\frac{\bar{g}(\theta)}{q(\theta;\lambda)} \right) + C \right) \nabla_\lambda \log q(\theta; \lambda) \right]$
Reparametrization:
$\nabla \mathcal{L}(\lambda) = \nabla \left(\mathbb{E}_{r(\epsilon)} \left[\log \frac{\bar{g}(s(\epsilon;\lambda))}{q(s(\epsilon;\lambda);\lambda)} \right] \right) \approx \frac{1}{K} \sum_{i \in [K], \epsilon_i \sim r(\epsilon)} \nabla \left(\log \frac{\bar{g}(s(\epsilon;\lambda))}{q(s(\epsilon;\lambda);\lambda)} \right).$

Variational Inference

Mixture of Gaussians

$q_k(\theta; \lambda) = \sum_{i=1}^k w_i f_i(\theta) = \sum_{i=1}^k w_i \mathcal{N}(\theta; \mu, \Sigma_i)$. Analytical mean and covariance. Samples can be easily generated.

Covariance parameterizations:

- $\Sigma_i = \text{diag}(\sigma_{i,1}^2, \ldots, \sigma_{i,D}^2)$
- $\Sigma_i = \mathbf{u}_i \mathbf{u}_i^T + \text{diag}(\sigma_{i,1}^2, \ldots, \sigma_{i,D}^2)$

Weights parameterizations $w_i(\nu_i) = \frac{\phi(\nu_i)}{\sum_{i=1}^k \phi(\nu_k)}$. ϕ can be:

- $\phi(\nu) = \exp(\nu)$
- $\phi(\nu) = \text{softplus}(\nu) = \log(1 + \exp(\nu))$

$$\mathcal{L}(\lambda) = \sum_{i=1}^k w_i(\nu_i) \mathbb{E}_{\epsilon \sim \mathcal{N}(0,I)} \left[\log \frac{\bar{g}(s(\epsilon; \mu_i, \sigma_i))}{q_k(s(\epsilon; \mu_i, \sigma_i); \lambda)} \right]$$

Variational Inference

Boosting mixtures

Problem: no way to know how many mixtures is needed. Adding mixtures sequentially can become costly. One solution: boosting.

$q_{i-1}(\theta) = \sum_{j=1}^{i-1} w_j f_j(\theta)$

$q_i(\theta) = \sum_{j=1}^{i-1} (1 - w_i) w_j f_j(\theta) + w_i f_i(\theta)$

How to find w_i and $f_i(\theta) = \mathcal{N}(\theta; \mu_i, \Sigma_i)$?

- Optimize jointly $\mathcal{L}_i(w_i, \mu_i, \Sigma_i)$
- Seek good proposal $f_i(\theta)$ and optimize $\mathcal{L}_i(w_i)$ via it's derivative

$$\mathcal{L}_i'(w_i) = \int \log(\bar{g}(\theta))(f_i(\theta) - q_{i-1}(\theta))d\theta - \int \log((1 - w_i)q_{i-1}(\theta) + w_i f_i(\theta))(f_i(\theta) - q_{i-1}(\theta))d\theta.$$

Variational Inference

Gradient boosting of mixtures

$$f_i = \arg\min_f \nabla D_{KL}(q_{i-1}||g) \cdot f = \arg\min_f \int \log \frac{q_{i-1}(\theta)}{g(\theta)} f(\theta) d\theta.$$

Problem: degenerate solution. Needs regularization.
Maximization objective for mixture of Gaussians:

$$\begin{aligned} \text{RELBO}(\mu_i, \Sigma_i) = & \int \log(\bar{g}(\theta))\mathcal{N}(\theta|\mu_i, \Sigma_i)d\theta - \\ & \int \log(q_{i-1}(\theta))\mathcal{N}(\theta|\mu_i, \Sigma_i)d\theta + \frac{\lambda}{4}\log|\Sigma|, \end{aligned}$$

Estimated by the reparameterization trick.

Variational Inference

```
procedure VariationalBoosting(log ḡ, μ_0, Σ_0)
    ▷ μ_0, Σ_0 the are initial boosting values
    w_0 := 1.0
    for t = 1, ..., T do
        μ_t, Σ_t := arg max RELBO(μ_t, Σ_t)      ▷ Using reparameterization
        w_t := arg max L_i(w_i)        ▷ Using L'_t(w_t) for gradient descent
        for j = 0, ..., t − 1 do
            w_j ← (1 − w_t) w_j
        end for
    end for
    return {(μ_t, Σ_t, w_t)}_{t=1}^T
end procedure
```

Variational Inference

Variational Bayesian Monte Carlo (VBMC)

$\mathcal{L}(\lambda) = \int \log \bar{g}(\theta) q(\theta;\lambda) d\theta - \int \log q(\theta;\lambda) q(\theta;\lambda) d\theta$

Use Bayesian Monte Carlo:

$\mathcal{L}_{\mathcal{D}}(\lambda) = \int \log \bar{g}_{\mathcal{D}}(\theta) q(\theta;\lambda) d\theta - \int \log q(\theta;\lambda) q(\theta;\lambda) d\theta$

$$\text{Maximize } \mathbb{E}[\mathcal{L}_{\mathcal{D}}(\lambda)] = M(\lambda) + \mathbf{z}^T \mathbf{w} - \int \log q(\theta;\lambda) q(\theta;\lambda) d\theta$$

$$\mathbf{w} = K^{-1} \mathbf{y}$$

$$M(\lambda) = \int m(\theta) q(\theta;\lambda) d\theta$$

$$\mathbf{z}_i = \int k(x, x_i) q(\theta;\lambda) dx.$$

Variational Inference

Mean function

$m(\theta) = 0$: $\log \bar{g}_{\mathcal{D}}(\theta)$ is not a log probability
Principled solution: $m(\theta) = -\frac{1}{2}\sum_{i=1}^{D} \frac{(\theta_i - c_i)^2}{l_i^2}$. Lends analytical $M(\lambda)$.
Ad-hoc solution: $m(\theta) = C$, with C being a large negative constant.

Active evaluation

Just as in BMC, it is possible to do active evaluation. Some options:

- $\alpha_{\text{US}}^{\mathcal{D}}(\theta_{N+1}) = k_{\mathcal{D}}(\theta_{N+1}, \theta_{N+1}) q_k(\theta_{N+1}; \lambda)^2$.
- $\alpha_{\text{PROP}}^{\mathcal{D}}(\theta_{N+1}) = k_{\mathcal{D}}(\theta_{N+1}, \theta_{N+1}) \exp(m_{\mathcal{D}}(\theta_{N+1})) q_k(\theta_{N+1}; \lambda)^2$

Boosted Variational Bayesian Monte Carlo

BVBMC

BVBMC = VBMC + boosting + small changes

BMC in boosted variational inference

$$\text{RELBO}_{\mathcal{D}}(\mu_i, \Sigma_i) = \int \mathbb{E}[\log \bar{g}_{\mathcal{D}}(\theta)] \mathcal{N}(\theta|\mu_i, \Sigma_i) d\theta - \int \log(q_{i-1}(\theta)) \mathcal{N}(\theta|\mu_i, \Sigma_i) d\theta + \frac{\lambda}{4} \log |\Sigma_i|$$

$$\mathcal{L}_{i,\mathcal{D}}(w) = \int \log \bar{g}_{\mathcal{D}}(\theta)((1 - w_i) q_{i-1}(\theta) + w_i f_i(\theta)) d\theta - \int \log((1 - w_i) q_{i-1}(\theta) + w_i f_i(\theta))((1 - w_i) q_{i-1}(\theta) + w_i f_i(\theta)) d\theta$$

Boosted Variational Bayesian Monte Carlo

Practical considerations

- RELBO stabilization

$$\mathrm{RELBO}_{\mathcal{D}}^{\delta_D}(\mu_i, \Sigma_i) = \int \log\left(\frac{r_{\mathcal{D}}(\theta)}{q_{i-1}(\theta) + \delta_D}\right) \mathcal{N}(\theta; \mu_i, \Sigma_i) d\theta + \log|\Sigma_i|.$$

- Output scaling

$$\tilde{y}_i = (y_i - m_y)/\sigma_y,\ \tilde{\mathcal{D}} = \{x_i, \tilde{y}_i\},\ \sigma_y \log g_{\tilde{\mathcal{D}}}(x) + \mu_y$$

- Component pruning: discard negligible components
- Initialization: either large covariance or maximize ELBO for first Gaussian component.
- Mean function: $m(\theta) = C$ found to be more stable.

Practical considerations

- Periodic joint parameter updating: sometimes maximize $\mathbb{E}[\mathcal{L}_{\mathcal{D}}(\lambda)]$ for all parameters in $\sum_{i=1}^{k} w_k \mathcal{N}(\theta; \mu_k, \Sigma_k)$.
- Product of Matern kernels:

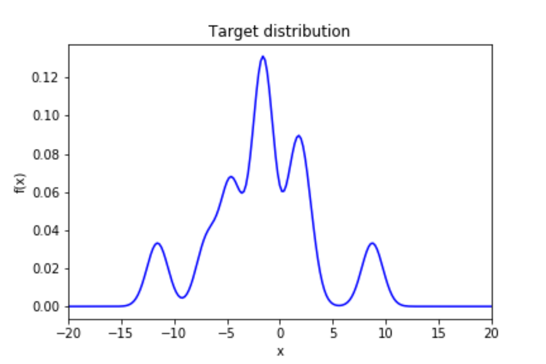
$$k_{\text{PMat},\nu}(x, x'; \theta, l) = \theta \prod_{d=1}^{D} k_{\text{Matern},\nu}(|x_i - x_i'|; l_d).$$

  Is integrated in BVBMC by Gauss-Hermite quadrature. Found to be more stable than the SQE kernel.
- More acquisition functions:

$$\alpha^{\mathcal{D}}_{MMLT}(x_{m+1}) = e^{2m_{\mathcal{D}}(x) + k_{\mathcal{D}}(x,x)} \left(e^{k_{\mathcal{D}}(x,x')} - 1 \right).$$

$$\alpha^{\mathcal{D}}_{MMLT_P}(x_{m+1}) = e^{2m_{\mathcal{D}}(x) + k_{\mathcal{D}}(x,x)} \left(e^{k_{\mathcal{D}}(x,x')} - 1 \right) q_k(\theta_{N+1}; \lambda)^2.$$

1-d mixture of Gaussians



$$f(x) = \sum_{i=1}^{12} w_i \mathcal{N}(x; \mu_i, \sigma_i^2),$$

$$w_i = \tfrac{1}{12},\ \mu_i \sim \mathcal{N}(0, \sqrt{5}),\ \sigma_i^2 = 1.$$