Bayesian Quadrature for Multiple Related Integrals

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Bayesian Numerical Methods
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- **Standard Numerical Analysis**: Study of how to best project continuous mathematical problems into discrete scales. (also thought of as the study of numerical errors).

- **Statistics**: Infer some quantity of interest (usually the parameter of a model) from data samples. Sounds familiar?

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F-X Briol (Warwick & Imperial)
BQ for Multiple Related Integrals
May 2018
What is the Point?

Quantification of the **epistemic uncertainty** associated with the numerical problem using **probability measures**, rather than worst-case bounds (not always representative of the actual error).

Propagation of uncertainty through pipelines.

Bayesian Numerical Methods can be framed as Bayesian Inverse Problems for the solution of the numerical problem.

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The Problem

- Let's come back to our problem of computing integrals! Consider a function $f : \mathcal{X} \rightarrow \mathbb{R}$ ($\mathcal{X} \subseteq \mathbb{R}^p$) assumed to be square-integrable and a probability measure $\Pi$.

$$\Pi[f] = \int_{\mathcal{X}} f(x) d\Pi(x) \approx \sum_{i=1}^{n} w_i f(x_i) = \hat{\Pi}[f]$$

where $\{x_i\}_{i=1}^{n} \in \mathcal{X}$ & $\{w_i\}_{i=1}^{n} \in \mathbb{R}$.

- Examples include:
  1. **Monte Carlo (MC):** Sample $\{x_i\}_{i=1}^{n} \sim \Pi$ and let $w_i = 1/n \ \forall i$.
  2. **Markov Chain Monte Carlo (MCMC):** Sample states $\{x_i\}_{i=1}^{n}$ from a Markov Chain with invariant distribution $\Pi$ and let $w_i = 1/n \ \forall i$.
  3. **Gaussian quadrature, importance sampling, QMC, SMC, etc...**
Bayesian Numerical Integration

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Sketch of Bayesian Quadrature

- For $n=0$, the integrand is a simple curve with a broad posterior distribution.
- As $n$ increases from 3 to 8, the integrand becomes more complex, and the posterior distribution narrows and becomes more concentrated around the solution of the integral.

The solution of the integral is shown as a vertical dashed line, with the posterior distribution indicating the uncertainty in the estimate of the integral value.
Bayesian Quadrature

1. Place a Gaussian Process prior (assumed w.l.o.g. to have zero mean).
2. Evaluate the integrand \( f \) at several locations \( \{x_i\}_{i=1}^n \) on \( X \). We get a Gaussian Process with mean and covariance function:

\[
\begin{align*}
m_n(x) &= k(x, X)k(X, X)^{-1}f(X) \\
k_n(x, x') &= k(x, x') - k(x, X)k(X, X)^{-1}k(X, x')
\end{align*}
\]

3. Taking the pushforward through the integral operator, we get:

\[
\begin{align*}
\mathbb{E}_n[\Pi[f]] &= \hat{\Pi}_{BQ}[f] := \Pi[k(\cdot, X)]k(X, X)^{-1}f(X) \\
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Important Points

- The probability measure represents our uncertainty about the value of $\Pi[f]$ due to the fact that we can’t evaluate the integrand $f$ everywhere.

- We have chosen to model $f$ (and hence $\Pi[f]$) using a Gaussian measure. This is mostly for computational tractability, but isn’t necessarily the right thing to do!

- Notice that the formulae below do not specify where to evaluate $f$, but provide a posterior given the points at which we have evaluated.

\[
E_n[\Pi[f]] = \hat{\Pi}_B[f] := \Pi[k(\cdot, X)]k(X, X)^{-1}f(X)
\]
\[
\nabla_n[\Pi[f]] = \Pi\bar{\Pi}[k] - \Pi[k(\cdot, X)]k(X, X)^{-1}\Pi[k(X, \cdot)].
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We have the freedom to combine these with MC, MCMC, QMC, etc...
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Toy example

**Toy problem:** $f(x) = \sin(x) + 1$ & $\mathcal{N}$ is $\mathcal{N}(0, 1)$. We use the kernel $k(x, y) = \exp(-\frac{(x - y)^2}{l^2})$ (with $l = 1$) and sample $\{x_i\}_{i=1}^n \sim \mathcal{N}$. 

![Graph showing MSE vs. number of function evaluations]
**Toy example: The effect of sampling**

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**Toy example: The effect of sampling and kernel choice**

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**Number of samples:** 25
Toy example: The effect of sampling and kernel choice

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Number of samples: 50
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Number of samples: 75
Calibration

Clearly, from the previous slide we can tell that hyperparameters will be of great importance. To do this we have several alternatives:

- Go full Bayesian and put a prior on the parameter, then look at the posterior predictive. **Problem:** We lose the conjugacy property and this becomes very expensive to do!

- Do some sort of cross validation. **Problem:** This is still expensive as requires solving many linear systems.

- Do some empirical Bayes, i.e. maximise the marginal likelihood of the data. **Problem:** Not very Bayesian.

In practice, we tend to use empirical Bayes for speed reason...
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Convergence Results

So why does it converge fast?

- For integration in an RKHS $\mathcal{H}$ (associated to the GP kernel $k$), the standard quantity to consider is the worst-case error:

$$e(\hat{\Pi}; \Pi, \mathcal{H}) := \sup_{\|f\|_{\mathcal{H}} \leq 1} \left| \Pi[f] - \hat{\Pi}[f] \right|$$

- One can show that BQ attains optimal rates of convergence for certain classes of smooth functions. In particular, with i.i.d points, one can get $\mathcal{O}(n^{-\alpha/d} + \epsilon)$ for spaces of smoothness $\alpha$ and $\mathcal{O}(\exp(-Cn^{1/d} - \epsilon))$ for infinitely smooth functions.

We need to compute three integrals at each pixel:

\[
L_o(\omega_o) = L_e(w_o) + \int_{S^2} L_i(\omega_i) \rho(\omega_i, \omega_o)[\omega_i \cdot n] + d\sigma(\omega_i)
\]

Application: Global Illumination

- The kernel used gives an RKHS norm-equivalent to a Sobolev space of smoothness $\frac{3}{2}$:
  \[
k(x, x') = \frac{8}{3} - \|x - x'\|_2 \text{ for all } x, x' \in S^2.
\]

- We can show a convergence rate of $e(\hat{\Pi}_{BMC}; \Pi, \mathcal{H}) = \mathcal{O}_P(n^{-\frac{3}{4}})$ which is optimal for this space!
Application: Global Illumination

Spreading the points and re-weighting can help significantly!


Bayesian Quadrature for Multiple Integrals
What About Multiple Integrals?

- In the example, we actually need to approximate thousands of integrals for each frame of a virtual environment... **This is slow and expensive!**

- We can formalise the process above as that of finding the integral of a set of functions $f_1, \ldots, f_D$ against some measure $\Pi$. But what if we know something about how $f_1$ relates to $f_2$, etc...?

- It might make more sense to approximate the integral with a quadrature rule of the form:

$$\hat{\Pi}[f_d] = \sum_{d'=1}^{D} \sum_{i=1}^{n} (W_i)_{dd'} f_{d'}(x_{d'i})$$

where the weights would encode the correlation across functions.
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where the weights would encode the correlation across functions.
We can use the same type of results for Gaussian Processes on the extended space of vector-valued functions $f : \mathcal{X} \rightarrow \mathbb{R}^D$ (rather than $f : \mathcal{X} \rightarrow \mathbb{R}$) where $f(x) = (f_1(x), \ldots, f_D(x))$.

This approach allows us to directly encode the relation between each function $f_i$ by specifying the kernel $K$.

In this case the posterior distribution is a $\mathcal{GP}(m_n, K_n)$ with vector-valued mean $m_n : \mathcal{X} \rightarrow \mathbb{R}^D$ and matrix-valued covariance $K_n : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^{D \times D}$:

$$m_n(x) = K(x, X)K(X, X)^{-1}f(X)$$

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The overall cost for computing this is $O(n^3D^3)$.

Bayesian Quadrature for Multiple Related Functions

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  \]

  \[
  K_n(x, x') = K(x, x') - K(x, X)K(X, X)^{-1}K(X, x').
  \]

  The overall cost for computing this is $O(n^3D^3)$.

Consider multi-output Bayesian Quadrature with a $\mathcal{GP}(\mathbf{0}, \mathbf{K})$ prior on $\mathbf{f} = (f_1, \ldots, f_D)^\top$. The posterior distribution on $\Pi[\mathbf{f}]$ is a $D$-dimensional Gaussian with mean and covariance matrix:

$$
\mathbb{E}_N[\Pi[\mathbf{f}]] = \Pi[\mathbf{K}(\cdot, \mathbf{X})] \mathbf{K}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{f}(\mathbf{X})
$$

$$
\mathbb{V}_N[\Pi[\mathbf{f}]] = \Pi[\mathbf{K}] - \Pi[\mathbf{K}(\cdot, \mathbf{X})] \mathbf{K}(\mathbf{X}, \mathbf{X})^{-1} \Pi[\mathbf{K}(\mathbf{X}, \cdot)]
$$

Kernel evaluations are now matrix-valued (i.e. in $\mathbb{R}^{D \times D}$) as opposed to scalar-valued. A simple example is the following separable kernel:

$$
\mathbf{K}(\mathbf{x}, \mathbf{x}') = B \mathbf{k}(\mathbf{x}, \mathbf{x}')
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$B$ encodes the covariance between function, and $k$ the type of function in each of the components.

In this case, we can reduce the cost to $\mathcal{O}(n^3 + D^3)$. 
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Some Theory for Multi-output BQ

Define the individual worst-case errors:

\[ e(\hat{\Pi}; \Pi, \mathcal{H}_K, d) = \sup_{\|f\|_K \leq 1} \left| \Pi[f_d] - \hat{\Pi}[f_d] \right| \]

**Theorem (Convergence rate for BQ with separable kernel)**

Suppose we want to approximate \( \Pi[f] \) for some \( f : X \to \mathbb{R}^D \) and \( \hat{\Pi}_{BQ}[f] \) is the multi-output BQ rule with the kernel \( K(x, x') = B k(x, x') \) for some positive definite \( B \in \mathbb{R}^{D \times D} \) and scalar-valued kernel \( k : X \times X \to \mathbb{R} \) where all functions are evaluated on a point set \( \{x_i\}_{i=1}^n \).

Then, \( \forall d = 1, \ldots, D \), we have:

\[ e(\hat{\Pi}_{BQ}; \Pi, \mathcal{H}_K, d) = O \left( e(\hat{\Pi}_{BQ}; \Pi, \mathcal{H}_k) \right) \]
Some Theory for Multi-output BQ

Assume that $\mathcal{X} \subset \mathbb{R}^p$ is a domain with Lipschitz boundary and satisfying an interior cone condition. Furthermore, assume the $\{x_i\}_{i=1}^n$ are either:

(A1) IID samples from some distribution $\Pi'$ with density $\pi' > 0$ on $\mathcal{X}$, or

(A2) obtained from a quasi-uniform grid on $\mathcal{X}$.

- If $\mathcal{H}_k$ is norm-equivalent to an RKHS with Matérn kernel of smoothness $\alpha > \frac{p}{2}$, we have $\forall d = 1, \ldots, D$:

$$e(\mathcal{H}_K, \hat{\Pi}_{BQ}, \mathcal{X}, d) = \mathcal{O}\left(n^{-\frac{\alpha}{p} + \epsilon}\right).$$

for $\epsilon > 0$ arbitrarily small.

- If $\mathcal{H}_k$ is norm-equivalent to the RKHS with squared-exponential, multiquadric or inverse multiquadric kernel, we have $\forall d = 1, \ldots, D$:

$$e(\mathcal{H}_K, \hat{\Pi}_{BQ}, \mathcal{X}, d) = \mathcal{O}\left(\exp\left(-C_1 n_{\frac{1}{p}} - \epsilon\right)\right).$$

for some $C_1 > 0$ and $\epsilon > 0$ arbitrarily small.
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e(\mathcal{H}_k, \hat{\Pi}_{BQ}, X, d) = O \left( \exp \left( -C_1 n_p^{\frac{1}{p} - \epsilon} \right) \right).
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  for some $C_1 > 0$ and $\epsilon > 0$ arbitrarily small.
Theory in the Misspecified Case

**Theorem (Misspecified Convergence Result for Separable Kernel)**

Let $k_\alpha$ be a kernel norm-equivalent to a Matérn kernel on some domain $\mathcal{X}$ with Lipschitz boundary and interior cone condition and consider the BQ rule $\hat{\Pi}_{BQ}[f]$ corresponding to a separable kernel $K_\alpha(x, x') = B k_\alpha(x, x')$.

Suppose $\{x_i\}_{i=1}^n$ satisfies $(A_2)$, and $f \in \mathcal{H}_{C_\beta}$ where $\frac{p}{2} \leq \beta \leq \alpha$.

Then, $\forall d = 1, \ldots, D$:

$$\left| \Pi[f_d] - \hat{\Pi}_{BQ}[f_d] \right| = \mathcal{O} \left( n^{-\frac{\beta}{p}} + \epsilon \right)$$

for some $\epsilon > 0$. 
We compute integrals for different integrands based on various angles $\omega_0$ (akin to a camera moving).

- We pick a separable kernel $K(x, x') = Bk(x, x')$ where $B$ is chosen to represent the angle between integrands and $k(x, x') = \frac{8}{3} - \|x - x'\|_2$.

- We can prove that the worst-case integration error converges at a rate $O(n^{-\frac{3}{4}})$ for each integrand. This is the same rate as uni-output BQ (but we usually improve on constants).
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We compute integrals for different integrands based on various angles $\omega_0$ (akin to a camera moving).

We pick a separable kernel $K(x, x') = Bk(x, x')$ where $B$ is chosen to represent the angle between integrands and $k(x, x') = \frac{8}{3} - \|x - x'|_2$.

We can prove that the worst-case integration error converges at a rate $O(n^{-\frac{3}{4}})$ for each integrand. This is the same rate as uni-output BQ (but we usually improve on constants).
Multi-output BQ for the Computer Graphics Example
Application: Multifidelity Modelling

In each case, we have access to a cheap simulator/function (left) and an expensive simulator/function (right).

blue = truth, red = uni-output, yellow & purple = two outputs

Application: Multifidelity Modelling

- In multifidelity modelling, multi-output Gaussian processes are already being used as efficient surrogate models.

- Furthermore, we are in general interested in some statistic of the expensive surrogate model. We therefore might as well re-use this multi-output GP approximate the integral.

- Results:

<table>
<thead>
<tr>
<th>Model</th>
<th>1-output BQ</th>
<th>2-output BQ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step function (l)</td>
<td>0.024 (0.223)</td>
<td>0.021 (0.213)</td>
</tr>
<tr>
<td>Step function (h)</td>
<td>0.405 (0.03)</td>
<td>0.09 (0.091)</td>
</tr>
<tr>
<td>Forrester function (l)</td>
<td>0.076 (4.913)</td>
<td>0.076 (4.951)</td>
</tr>
<tr>
<td>Forrester function (h)</td>
<td>3.962 (3.984)</td>
<td>2.856 (27.01)</td>
</tr>
</tbody>
</table>
References


