Bayesian Quadrature for Multiple Related Integrals

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arXiv:1801.04153

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Bayesian Numerical Methods

Bayesian Numerical Methods

- **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?

- **Bayesian Numerical Methods:** Perform Bayesian statistical inference on the solution of numerical problems.

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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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Bayesian Numerical Integration

The Problem

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

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

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

- 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 Π and let $w_i = 1/n \; \forall i$.
    3. **Gaussian quadrature, importance sampling, QMC, SMC, etc...**

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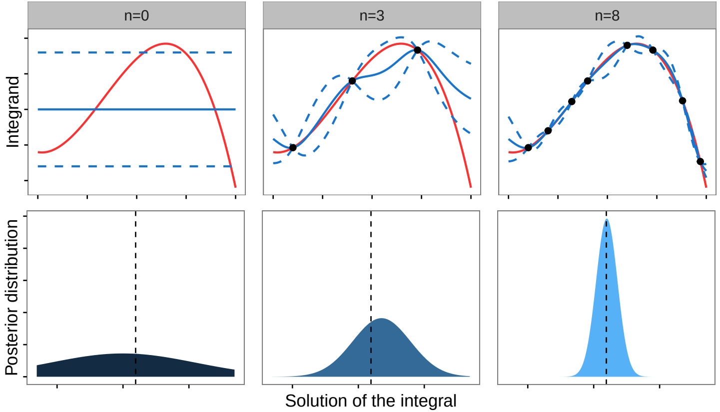
Sketch of Bayesian Quadrature



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 $\mathcal{X}$. We get a Gaussian Process with mean and covariance function:

$$\begin{aligned} m_n(\boldsymbol{x}) &= k(\boldsymbol{x},\boldsymbol{X})k(\boldsymbol{X},\boldsymbol{X})^{-1}f(\boldsymbol{X}) \\ k_n(\boldsymbol{x},\boldsymbol{x}') &= k(\boldsymbol{x},\boldsymbol{x}') - k(\boldsymbol{x},\boldsymbol{X})k(\boldsymbol{X},\boldsymbol{X})^{-1}k(\boldsymbol{X},\boldsymbol{x}') \end{aligned}$$

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

$$\begin{aligned} \mathbb{E}_n[\Pi[f]] &= \hat{\Pi}_{\mathrm{BQ}}[f] := \Pi[k(\cdot,\boldsymbol{X})]k(\boldsymbol{X},\boldsymbol{X})^{-1}f(\boldsymbol{X}) \\ \mathbb{V}_n[\Pi[f]] &= \Pi\bar{\Pi}[k] - \Pi[k(\cdot,\boldsymbol{X})]k(\boldsymbol{X},\boldsymbol{X})^{-1}\Pi[k(\boldsymbol{X},\cdot)]. \end{aligned}$$

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Important Points

- The probability measure represents our uncertainty about the value of $\Pi[f]$ due to the fact that we cant 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.

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We have the freedom to combine these with MC, MCMC, QMC, etc...

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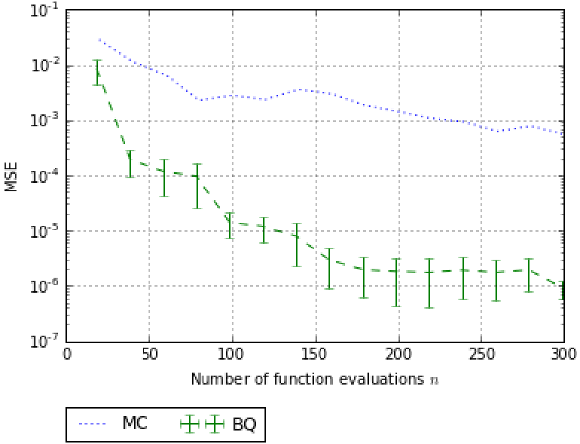
Toy example

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



Toy example: The effect of sampling

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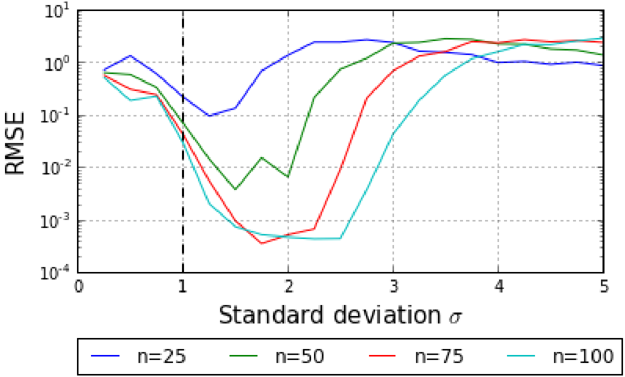

Toy example: The effect of sampling and kernel choice

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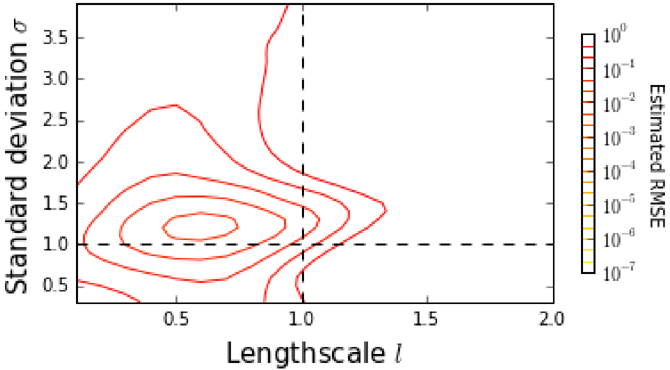
Number of samples: 25



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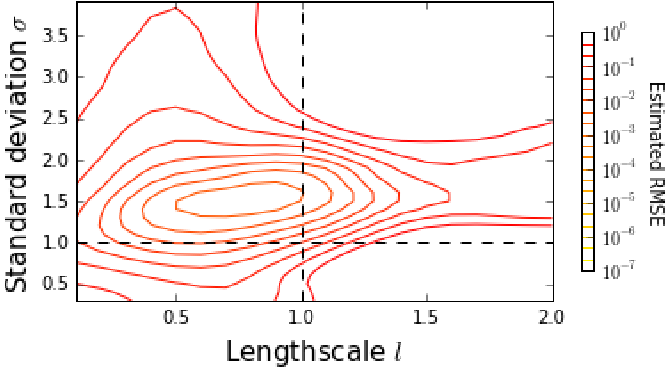
Number of samples: 50



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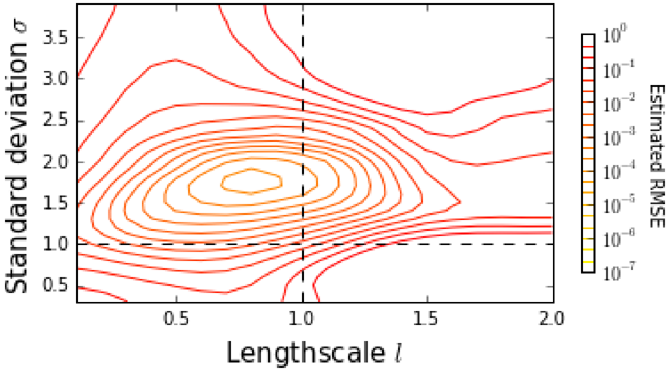
Number of samples: 75



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?

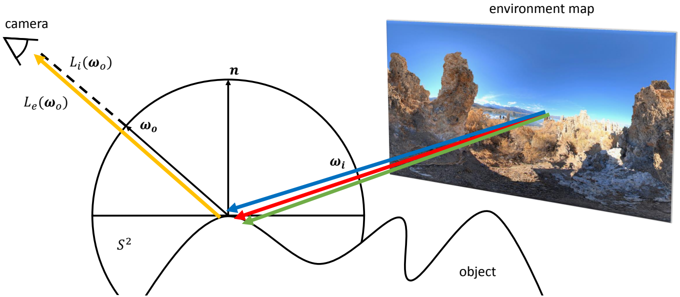
- For integration in an RKHS $\mathcal{H}$ (associated to the GP kernel k), the standard quantity to consider is the worst-case error:

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

- 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 $\mathcal{O}(n^{-\frac{\alpha}{d}+\epsilon})$ for spaces of smoothness α and $\mathcal{O}(\exp(-Cn^{\frac{1}{d}-\epsilon}))$ for infinitely smooth functions.

Briol, F.-X., Oates, C. J., Girolami, M., Osborne, M. A., & Sejdinovic, D. (2015). Probabilistic Integration: A Role for Statisticians in Numerical Analysis?, *arXiv:1512.00933*.

Application: Global Illumination



We need to compute three integrals at each pixel:

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

[1] Marques, R., Bouville, C., Ribardiere, M., Santos, P., & Bouatouch, K. (2013). A spherical Gaussian framework for Bayesian Monte Carlo rendering of glossy surfaces. IEEE Transactions on Visualization and Computer Graphics, 19(10), 1619-1632.

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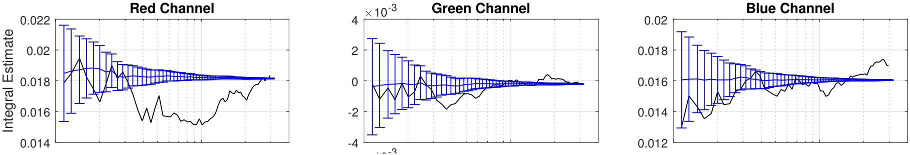
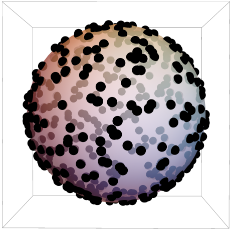


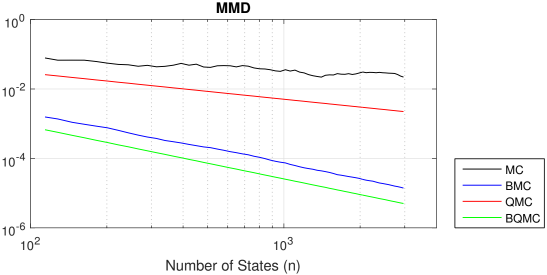
- The kernel used gives an RKHS norm-equivalent to a Sobolev space of smoothness $\frac{3}{2}$:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \frac{8}{3} - \|\boldsymbol{x} - \boldsymbol{x}'\|_2 \text{ for all } \boldsymbol{x}, \boldsymbol{x}' \in \mathbb{S}^2.$$

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

Application: Global Illumination





Spreading the points **and** re-weighting can help significantly!

[1] Briol, F.-X., Oates, C. J., Girolami, M., & Osborne, M. A. (2015). Frank-Wolfe Bayesian Quadrature: Probabilistic Integration with Theoretical Guarantees. In Advances In Neural Information Processing Systems 28 (pp. 1162–1170).
[2] Briol, F.-X., Oates, C. J., Cockayne, J., Chen, W. Y., & Girolami, M. (2017). On the Sampling Problem for Kernel Quadrature. In Proceedings of the 34th International Conference on Machine Learning (pp. 586–595).

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 $f_1, \dots, f_D$ against some measure Π. 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:

$$\hat{\Pi}[f_d] = \sum_{d'=1}^{D} \sum_{i=1}^{n} (\boldsymbol{W}_i)_{dd'} f_{d'}(\boldsymbol{x}_{d'i})$$

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Bayesian Quadrature for Multiple Related Functions

- We can use the same type of results for Gaussian Processes on the extended space of vector-valued functions $\boldsymbol{f} : \mathcal{X} \to \mathbb{R}^D$ (rather than $\boldsymbol{f} : \mathcal{X} \to \mathbb{R}$) where $\boldsymbol{f}(x) = (f_1(x), \ldots, f_D(x))$.
- This approach allow us to directly encode the relation between each function f_i by specifying the kernel K.
- In this case the posterior distribution is a $\mathcal{GP}(\boldsymbol{m}_n, \boldsymbol{K}_n)$ with vector-valued mean $\boldsymbol{m}_n : \mathcal{X} \to \mathbb{R}^D$ and matrix-valued covariance $\boldsymbol{K}_n : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^{D \times D}$:

$$\begin{aligned} \boldsymbol{m}_n(\boldsymbol{x}) &= \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\boldsymbol{f}(\boldsymbol{X}) \\ \boldsymbol{K}_n(\boldsymbol{x}, \boldsymbol{x}') &= \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{x}') - \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{x}'). \end{aligned}$$

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

Alvarez, M. A., Rosasco, L., & Lawrence, N. D. (2012). Kernels for vector-valued functions: A review. Foundations and Trends in Machine Learning, 4(3), 195-266.

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

$$\begin{aligned}\boldsymbol{m}_n(\boldsymbol{x}) &= \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\boldsymbol{f}(\boldsymbol{X}) \\ \boldsymbol{K}_n(\boldsymbol{x}, \boldsymbol{x}') &= \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{x}') - \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{x}').\end{aligned}$$

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

Alvarez, M. A., Rosasco, L., & Lawrence, N. D. (2012). Kernels for vector-valued functions: A review. Foundations and Trends in Machine Learning, 4(3), 195-266.

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

$$
\begin{aligned}
\mathbb{E}_N\left[\Pi[\boldsymbol{f}]\right] &= \Pi[\boldsymbol{K}(\cdot, \boldsymbol{X})]\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\boldsymbol{f}(\boldsymbol{X}) \\
\mathbb{V}_N\left[\Pi[\boldsymbol{f}]\right] &= \Pi\bar{\Pi}\left[\boldsymbol{K}\right] - \Pi[\boldsymbol{K}(\cdot, \boldsymbol{X})]\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}\bar{\Pi}[\boldsymbol{K}(\boldsymbol{X}, \cdot)]
\end{aligned}
$$

- 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:

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\boldsymbol{K}(x, x') = \boldsymbol{B}k(x, 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:

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

Theorem (Convergence rate for BQ with separable kernel)

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

$$e(\hat{\Pi}_{BQ}; \Pi, \mathcal{H}_{\boldsymbol{K}}, d) \quad = \quad \mathcal{O}\left(e(\hat{\Pi}_{BQ}; \Pi, \mathcal{H}_k) \right)$$

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 Π' 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 $\forall d = 1, \ldots, D$:

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

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

$$e(\mathcal{H}_{\boldsymbol{K}}, \hat{\Pi}_{\mathrm{BQ}}, \boldsymbol{X}, d) \quad = \quad \mathcal{O}\left(\exp\left(-C_1 n^{\frac{1}{p}-\epsilon}\right)\right).$$

  for some $C_1 > 0$ and $\epsilon > 0$ arbitrarily small.

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Theory in the Misspecified Case

Theorem (Misspecified Convergence Result for Separable Kernel)

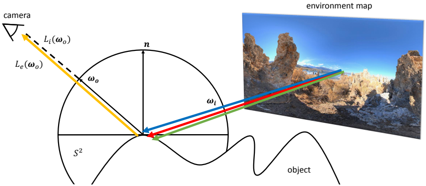
Let k_α be a kernel norm-equivalent to a Matérn kernel on some domain $\mathcal{X}$ with Lipschitz boundary and interior cone condition and consider the BQ rule $\hat{\Pi}_{BQ}[\boldsymbol{f}]$ corresponding to a separable kernel $\boldsymbol{K}_\alpha(x,x') = \boldsymbol{B} k_\alpha(x,x')$.

Suppose $\{x_i\}_{i=1}^n$ satisfies (A_2), and $\boldsymbol{f} \in \mathcal{H}_{\boldsymbol{C}_\beta}$ 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 $\epsilon > 0$.

Multi-output BQ for the Computer Graphics Example



- We compute integrals for different integrands based on various angles ω_0 (akin to a camera moving).
- We pick a separable kernel $\boldsymbol{K}(x, x') = \boldsymbol{B}k(x, x')$ where $\boldsymbol{B}$ is chosen to represent the angle between integrands and $k(\boldsymbol{x}, \boldsymbol{x}') = \frac{8}{3} - \|\boldsymbol{x} - \boldsymbol{x}'\|_2$.
- We can prove that the worst-case integration error converges at a rate $\mathcal{O}(n^{-\frac{3}{4}})$ for each integrand. This is the same rate as uni-output BQ (but we usually improve on constants).

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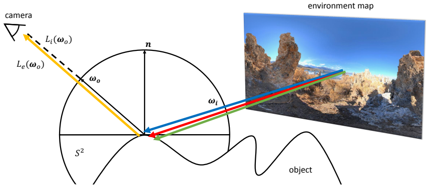

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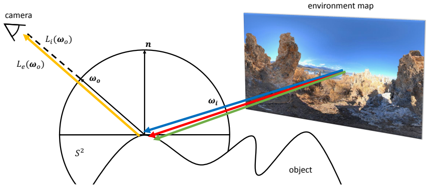

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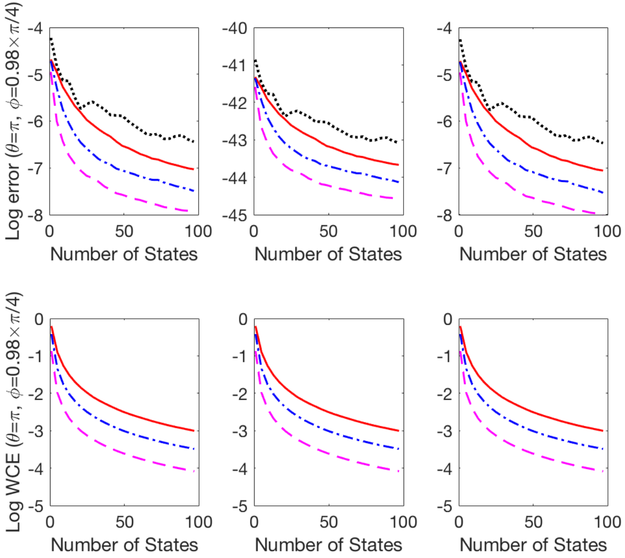
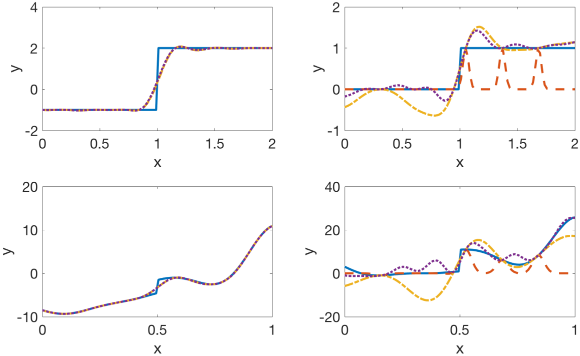


Application: Multifidelity Modelling

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

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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:

Model	1-output BQ	2-output BQ
Step function (l)	0.024 (0.223)	0.021 (0.213)
Step function (h)	0.405 (0.03)	0.09 (0.091)
Forrester function (l)	0.076 (4.913)	0.076 (4.951)
Forrester function (h)	3.962 (3.984)	2.856 (27.01)

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