A Bayes–Sard Cubature Method

Toni Karvonen[1], Chris. J. Oates[2,3] & Simo Särkkä[1]

[1]Aalto University, Finland | [2]Newcastle University, UK | [3]Alan Turing Institute, UK

Bayes–Sard Cubature

Problem Statement

Numerical approximation of the integral

$$I(f^\dagger) := \int_D f^\dagger(x) \, \mathrm{d}\nu(x), \quad D \subset \mathbb{R}^d, \quad \nu \text{ a probability measure on } D,$$

of a *deterministic* function $f^\dagger \colon D \to \mathbb{R}$.

Gaussian Process Model and Bayes–Sard Cubature

Model $f^\dagger$ as a Gaussian process

$$f(x) \mid \gamma \sim \mathrm{GP}\big(s(x), k(x,x')\big), \quad s(x) = \sum_{j=1}^{Q} \gamma_j p_j(x), \quad \gamma \sim \mathrm{N}(0, \Sigma).$$

The functions p_j span a Q-dimensional linear function space π (**typically polynomials**). Then

1. obtain *data* $\mathcal{D} = \{(x_i, f^\dagger(x_i))\}_{i=1}^n$ consisting of function evaluations at points $X = \{x_i\}_{i=1}^n \subset D$;
2. marginalise out γ and consider the *flat prior limit* $\Sigma^{-1} \to 0$ [1, Sec. 4.1.2];
3. the posterior for the integral $I(f)$ is Gaussian:

$$I(f) \mid \mathcal{D} \sim \mathrm{N}\big(\mu_X(f^\dagger), \sigma_X^2\big), \quad \mu_X(f^\dagger) = \sum_{i=1}^{n} w_{k,i} f^\dagger(x_i).$$

The posterior mean $\mu_X(f^\dagger)$ is an estimate for the integral $I(f^\dagger)$. We call this **Bayes–Sard cubature** (BSC). The variance σ_X^2 is supposed to quantify associated numerical uncertainty.

Properties of Bayes–Sard Cubature

Property 1. If $f^\dagger \in \pi = \mathrm{span}\{p_1, \ldots, p_Q\}$, then $\mu_X(f^\dagger) = I(f^\dagger)$ (but, in general, $\sigma_X^2 > 0$). *Functions in π are integrated exactly. BSC is thus a mixture of conventional GP-based and classical cubatures.*

Property 2. If $\dim(\pi) = Q = n$, the weights $w_{k,i}$ are completely determined by π. However, σ_X equals the worst-case error (WCE) in $H(k)$. *If π consists of, e.g., polynomials, we recover classical Gaussian cubature rules and can interpret their WCE as a posterior std.*

An Alternative

Related Bayesian cubature methods have been proposed before using improper priors [2,3]. This yields a Student-t posterior over the integral with $n - Q$ degrees of freedom. *Probabilistic interpretation of classical cubature rules is not possible as the posterior does not exist if $Q = n$.*

Summary

- BSC is more robust against improper prior specifications than standard Bayesian cubature.
- Can be easily used in high dimensions even with isotropic kernels.
- Allows for endowing *any* cubature rule with a meaningful probabilistic output.

References

[1] T. J. Santner, B. J. Williams & W. I. Notz, *The Design and Analysis of Computer Experiments*. Springer, 2003.

[2] A. O'Hagan, "Bayes–Hermite quadrature." *Journal of Statistical Planning and Inference*, vol. 29, no. 3, pp. 245–260, 1991.

[3] M. Kennedy, "Bayesian quadrature with non-normal approximating functions." *Statistics and Computing*, vol. 8, no. 4, pp. 365–375, 1998.

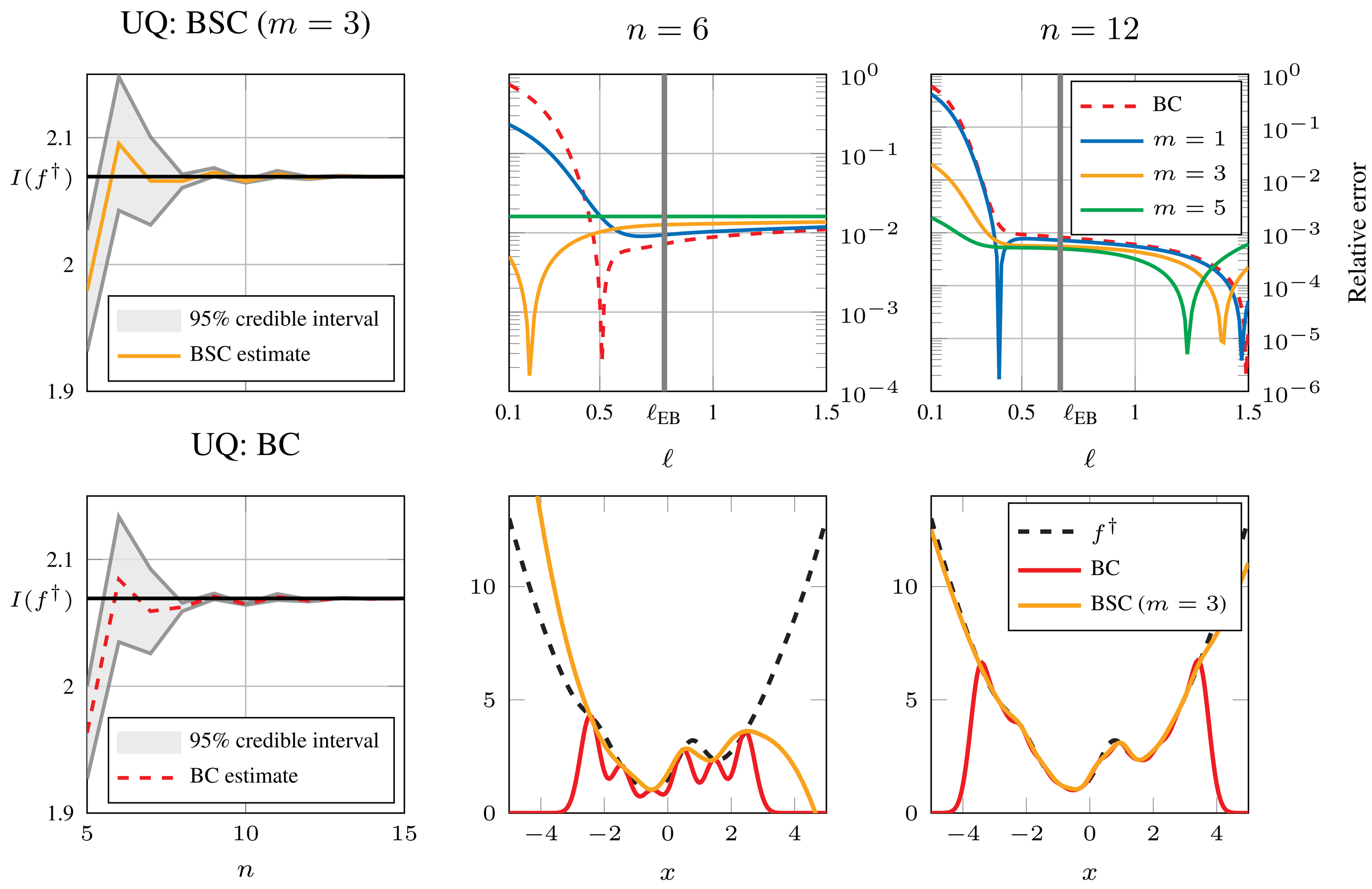
[4] T. Karvonen, S. Särkkä & C. J. Oates, "Symmetry exploits for Bayesian cubature methods." Preprint, arXiv:1809.10227, 2018.

Numerical Examples

In all examples π is, for some $m \in \mathbb{N}_0$, the space of d-variate polynomials of degree at most m.

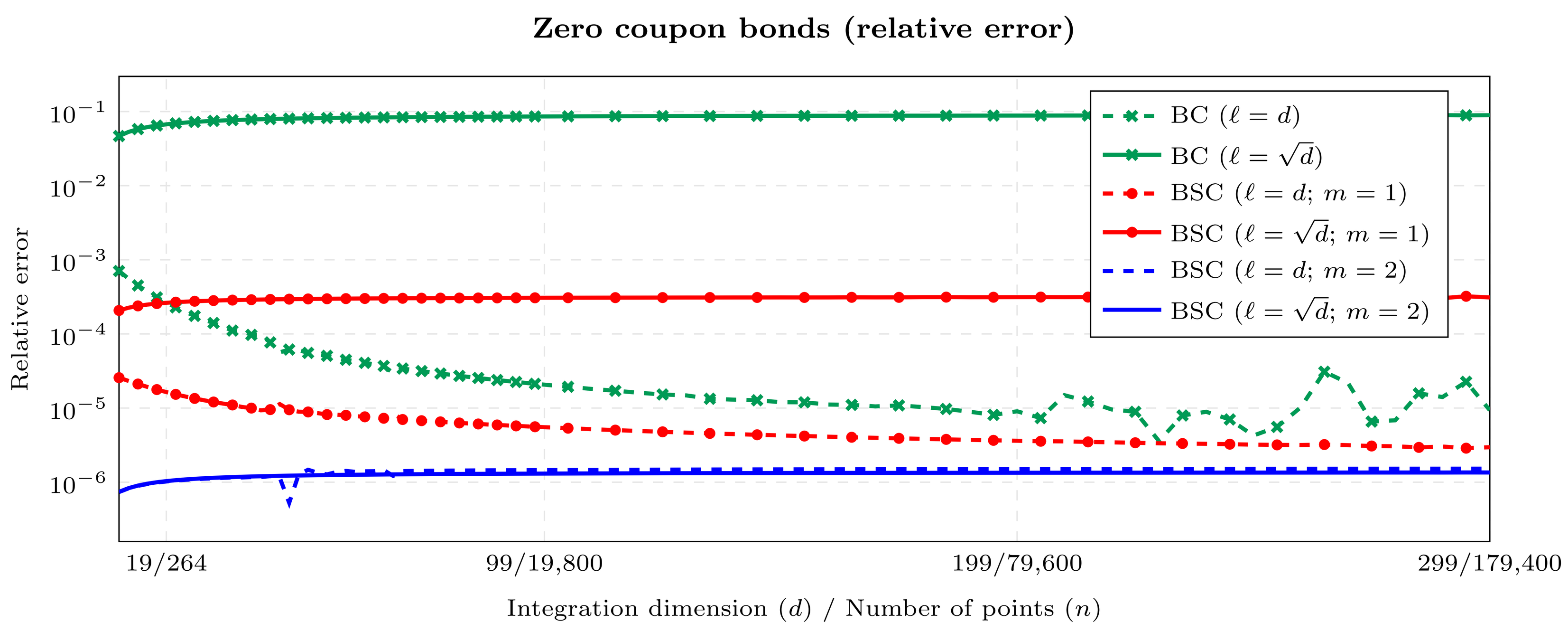
One-Dimensional Toy Example

Computation of Gaussian integral of a one-dimensional toy function.



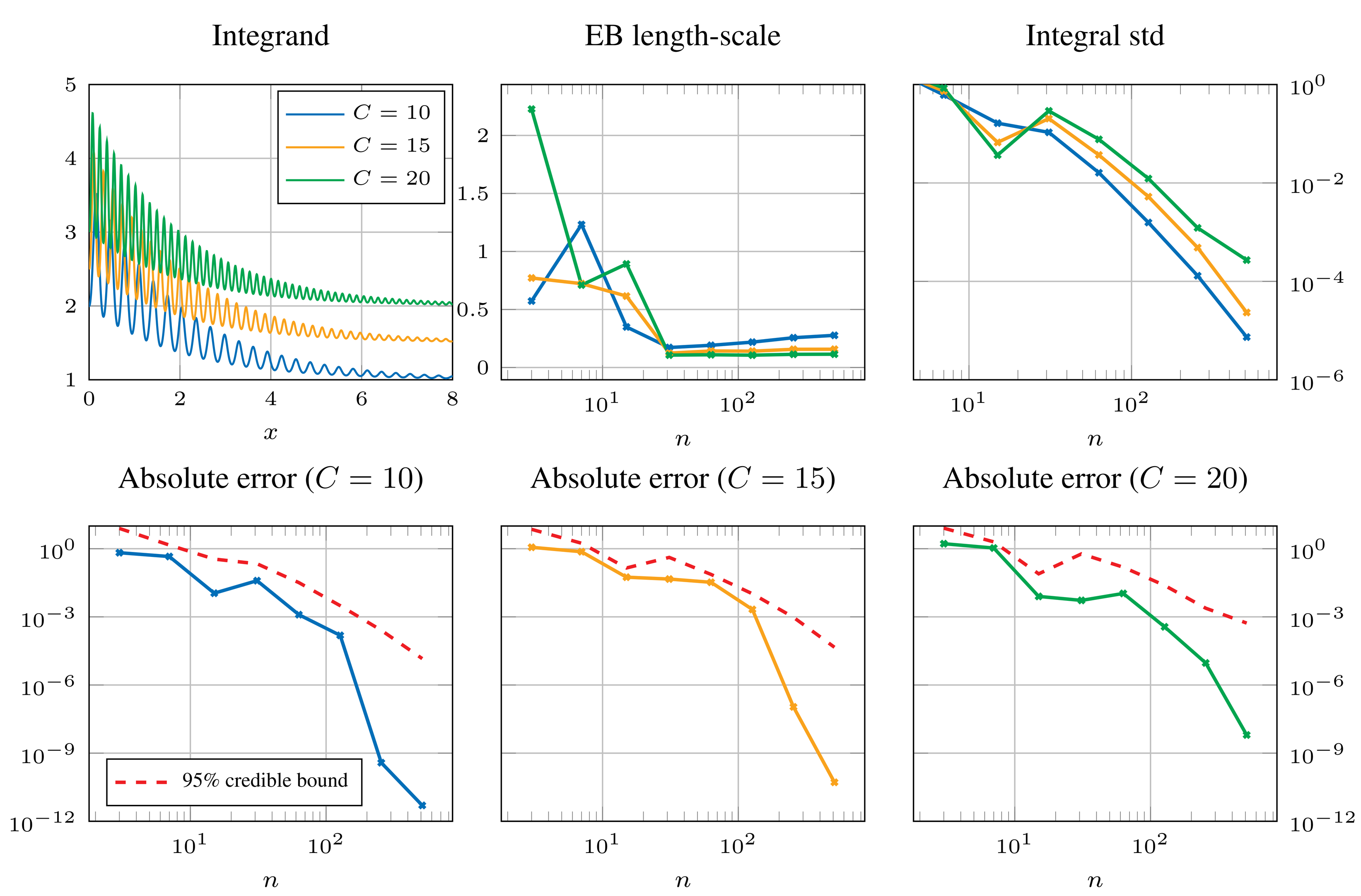
High-Dimensional Financial Example

Computation of the Gaussian integral over $\mathbb{R}^d$ of a high-dimensional financial functions arising from discretisations of an SDE. Symmetric set are used for fast computations [4]. **The integrand varies with d.**



Uncertainty Quantification for Classical Quadrature

Uncertainty quantification for *Gauss–Patterson quadrature* using BSC with the Matérn 5/2 kernel $Q = n$. Kernel length-scale ℓ fitted using empirical Bayes and magnitude λ using the improper prior $p(\lambda) \propto 1/\lambda$.



Contact information for comments and questions:

Toni Karvonen (Aalto University, Finland)
email: toni.karvonen@aalto.fi
web: https://users.aalto.fi/~karvont2/