Methods for large-scale and high-dimensional kernel cubature

Author and Presenter: Toni **Karvonen** (Aalto University, Finland)

Co-authors: Chris **Oates** (Newcastle University & Alan Turing Inst., UK)
Simo **Särkkä** (Aalto University, Finland)

Abstract

Kernel cubature rules, worst-case optimal numerical integration methods in reproducing kernel Hilbert spaces, can be interpreted as *probabilistic numerical methods* [1] and used for statistical quantification of uncertainty due to incomplete knowledge of the integrand. Motivated by this equivalence, we develop computational methods for efficient construction of large-scale and potentially high-dimensional kernel cubature rules. For N data points, the naive implementation of kernel cubature rules is based on solving a linear system of N equations. The resulting cubic time and quadratic memory cost in N are serious computational bottlenecks. We show how relatively flexible *fully symmetric sets*, obtained from given vectors via coordinate permutations and sign-changes, can be exploited for efficient computation of the weights of kernel cubature rules for up to millions of points. If the point set is a union of J fully symmetric sets, time complexity is reduced from $\mathcal{O}(N^3)$ to $\mathcal{O}(J^3 + JN)$ and memory complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(J^2)$. This talk is mainly based on the articles [2, 3], but we also discuss some other recent approaches based on *sparse grids* [4] and a combination of *low discrepancy points and shift-invariant kernels* [5].

References

[1] F.-X. Briol, C. J. Oates, M. Girolami, M. A. Osborne and D. Sejdinovic: *Probabilistic integration: A role in statistical computation?* Statistical Science, 34(1):1-22, 2019.

[2] T. Karvonen and S. Särkkä: *Fully symmetric kernel quadrature*, SIAM Journal on Scientific Computing, 40(2):A697-A720, 2018.

[3] T. Karvonen, S. Särkkä and C. J. Oates: *Symmetry exploits for Bayesian cubature methods*, To appear in Statistics and Computing, 2019.

[4] J. Oettershagen: *Construction of Optimal Cubature Algorithms with Applications to Econometrics and Uncertainty Quantification*, PhD thesis, Institut für Numerische Simulation, Universität Bonn, 2017.

[5] J. Rathinavel and F. Hickernell: *Fast automatic Bayesian cubature using lattice sampling*, Preprint, arXiv:1809.09803v1, 2018.