Uniformly distributed sequences and space-filling

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Keywords. Computer experiments; space covering; global optimization; kernel methods; discrepancy; dispersion

Let X be a compact subset of R^d and f be a black-box function on X. A standard objective in global optimization, computer experiments as well as in diverse applications is to approximate the behaviour of f on X from only a few evaluations in X. When little is known about the function, space-filling design is advisable: typically, points of evaluation spread out across the available space are obtained by minimizing a certain criterion measuring distance to uniformity.

In this talk, we follow [1, 2] and review several classes of uniformity criteria including dispersion (or covering radius) and various discrepancies and establish connections between some of these criteria. We also investigates connections between design for integration (quadrature design), construction of the (continuous) best linear unbiased estimators for the location model, and minimization of energy (kernel discrepancy) for signed measures. Integrally strictly positive definite kernels define strictly convex energy functionals, with an equivalence between the notions of potential and directional derivative, showing the strong relation between discrepancy minimization and more traditional design of optimal experiments. In particular, kernel herding algorithms, which are special instances of vertex-direction methods used in optimal design, can be applied to the construction of point sequences with suitable space-filling properties.

We will pay special attention to kernels with singularities where the space-filling sequences have some very attractive properties of but the machinery of the reproducing kernel Hilbert spaces is not applicable. Various regularization techniques should be used in practise for solving arising optimization problems. In doing this we have to work with infinitesimals; in doing so we would advocate the use of the infinity computer of Ya.Sergeyev [3]. We will also observe big differences between the cases when the dimension d is small and when d is large.

References

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