Gaussian Processes in the Flat Limit

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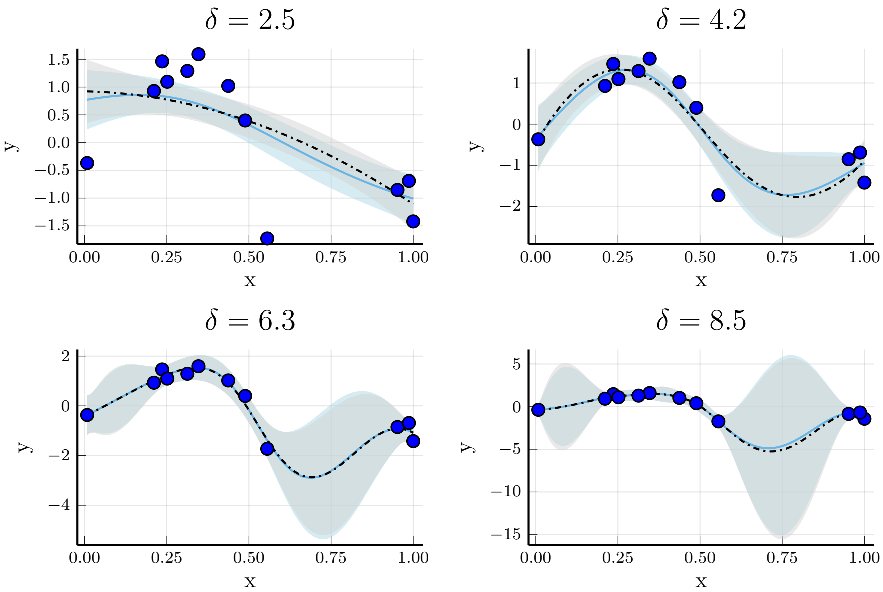
Gaussian processes (GPs) are a cornerstone of modern Bayesian methods, used almost wherever one may require nonparametric priors. The most typical use of GPs is in Gaussian process regression, also known as kriging. Quite naturally, the theory of Gaussian Process methods is well-developed. Aside from limited special cases in which Fourier analysis is applicable, GP-based methods have mostly been studied under large-n asymptotics , which involve treating measurement locations as random and letting their number go to infinity. In this paper we report intriguing theoretical results obtained under a different asymptotic, one that treats the data as fixed, rather than random, with fixed sample size. The limit we look at is the so-called "flat limit", pioneered by Driscoll & Fornberg in 2002. The flat limit consists in letting the spatial width of the kernel function go to infinity, which results in the covariance function becoming flat over the range of the data.

Studying Gaussian processes under the flat limit may seem at first sight to be entirely pointless - does that not correspond to a prior that contains only flat functions? Surprisingly, we show that the answer is no. This occurs because covariance functions have a second hyperparameter that sets the vertical scale (pointwise variance). When one lets pointwise variance grow as the covariance becomes wider, the actual function space spanned by Gaussian processes remains interesting and useful. In the cases studied here, they are (multivariate) polynomials and (polyharmonic) splines.



The figure shows GP regression compared to its flat limit approximation. In each panel, the solid black line represents the fit of a GP to the datapoints shown in blue kernel. We use a stationary Matèrn kernel with a fixed spatial scale, but vary its vertical scale parameter across the four panels, so that the resulting fit has different degrees of freedom δ. With more degrees of freedom, the fit becomes closer to the measurements. In light blue, the confidence bands of the fit. Superimposed, we show a "flat limit" approximation to the GP, which corresponds to fitting a smoothing spline model that would be equivalent with the spatial scale parameter going to infinity. The good quality of the approximation in such cases shows that our results could have interesting practical applications.

A technical report is available at `https://arxiv.org/abs/2201.01074`.

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Tobin A Driscoll and Bengt Fornberg. Interpolation in the limit of increasingly flat radial basis. *Computers & Mathematics with Applications*, 43(3-5):413–422,2002.