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One-dimensional Function Extrapolation Using Surrogates

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Abstract

Surrogate modeling is commonly used to estimate function values efficiently and accurately at unsampled points. The estimation procedure is called interpolation when target points are inside the convex hull of sampled points while extrapolation otherwise. This paper explores one-dimensional deterministic function extrapolation using surrogates. We first define a new error metric, relative average error, for quantifying overall performance of extrapolation technique. Ordinary Kriging and Linear Sheppard surrogates proved to be safer on several challenging functions than polynomial response surfaces, support vector regression or radial basis neural functions. This reflected that prediction of these surrogates converge to mean value of samples at points far from samples.

It's commonly recognized that long-range extrapolation is likely to be less accurate than short-range extrapolation. Two kinds of effective extrapolation distance are defined to indicate how far we can extrapolate test functions. We propose using the correlation between the nearest sample and the prediction point given by Ordinary Kriging as indicator of effective extrapolation distance. The relationship between effective extrapolation distance and corresponding correlation over the distance is examined by several test functions. A large value of correlation is associated with effective extrapolation distance.