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Using RSMs for Computationally Generated Data with Noise

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C E D C

UTP for design

This poster discusses **design of experiments** (DoE's) for Kriging computationally derived data. It turns out that computational noise and expensive evaluation lead naturally to the use of **response surface models** (RSM's) in design space evaluation. Having specified the optimization problem and the need for a DoE (here we compare several), we fit a Krig RSM. This is important, particularly in visualization, as much larger amounts of data are required to produce images than could be evaluated directly. This poster considers noise deriving from data obtained using computational methods and although such computations are of course deterministic, in that they are repeatable, noise is still present. A balance is also required between the number of points in the initial DoE, the total number of evaluations in the DoE after updating and the number of cycles in the CFD.

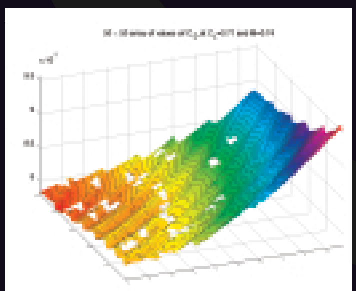

Figure 1: Full factorial 50X50 evaluations in a 2D airfoil trailing edge space.

An airfoil trailing edge design space is given in Figure 1. The ridges show computational noise and the white spaces show the locations of failed evaluations. It is clear that gradient searches in this domain will not find global optima, but local ones, stopping at the bottom of a ridge. Thus the inability to visualize high dimensional spaces and so to see the effects of noise can lead to an inability to fully exploit the additional flexibility in design parameter choice.

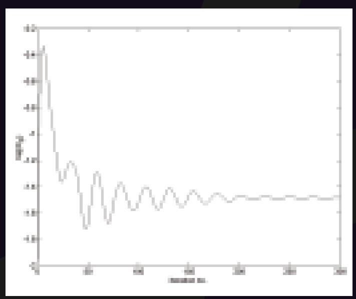

Figure 2: Iteration cycles for C_D – 6 million cell body wing case.

The noise stems from two sources:

- As the design changes different solver meshes are commonly required, as these are altered step changes can arise in any results.
- Secondly, because CFD solvers are iterative, a choice needs to be made as to when to halt a calculation. This can be understood by looking at the cycles of the code, as shown in Figure 2.
- Rounding error will also be present, although probably has less impact.

We explore Kriging sparse data in noisy design spaces further by considering RSMs on a 1D and 2D analytical function, here we use the Branin function in 2D and the y=0.5 line in the Branin function as a 1D function, both with striated noise.

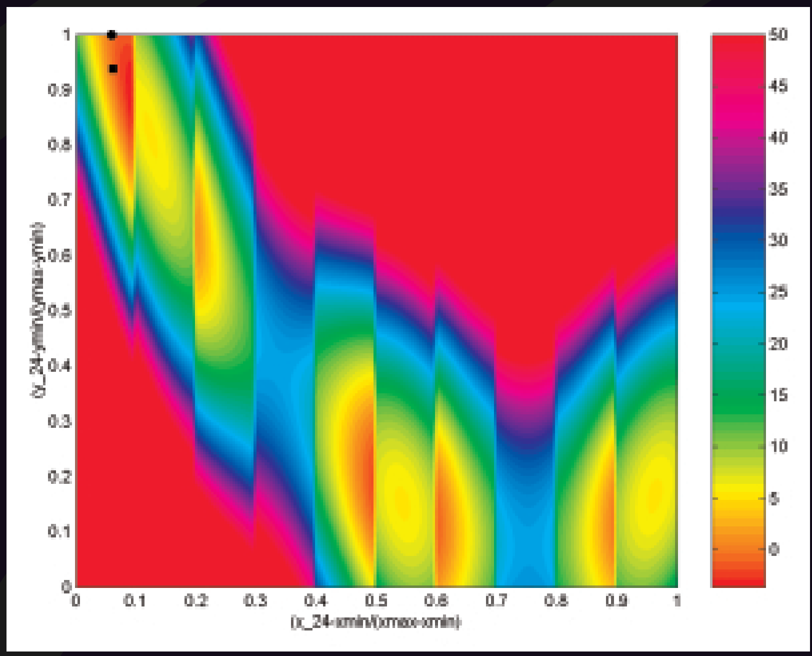

Figure 4: Branin function with striated noise. Optima from Expected Improvement and RMS error update indicated ● ■ .

Figure 3 shows the 1D function, design points from an 11 point DoE, the underlying noise free function and the fitted response. The aim here is to recover the original noise free function from the with noise data. Several techniques exist to effect the interpolation. The first is to add a λ term to the leading diagonal of the matrix to be inverted using **lower/upper** triangular form (LU) **decomposition**. The second is to use **singular value decomposition** (SVD) to provide a least squares fit to the data. In SVD the matrix to be inverted is rewritten as the product of a column orthogonal matrix, a diagonal matrix and a third orthogonal matrix. If w_{max} is the largest element of the diagonal matrix, then the smallest element of the diagonal matrix should not be < *factor X* w_{max}, and if it is then this diagonal element is set to zero. The aim is to choose λ or *factor* such that the underlying trend of the data is identified and the effect of the noise is deleted. Figure 3 shows the effect when such a critical value of *factor* is used.

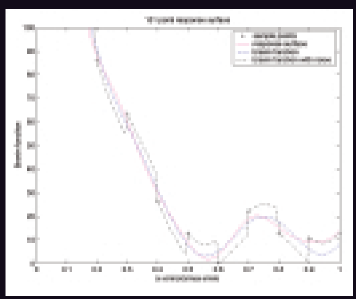

Figure 3: Kriging the Branin function, *factor*=10^{-2}

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Figure 4 shows the Branin function with striated noise, thresholded so that multiple local minima can be identified. The underlying function without noise has 3 local minima where the circular contours can be identified. Empirical rules have been established to determine the number of points for use in a DoE. In Figure 4, the LP_τ DoE is used to give 9 points in an initial DoE. Then, additional points are added incrementally, a few at a time until there have been 24 function evaluations. These additions are made to maximise either **Expected Improvement** (EI) or RMS error. The small filled circle represents the optimum from a DoE updated using EI and the filled square represents the optimum from a DoE updated using RMS error. Both strategies produce a result close to the optimum and, although the EI result is superior, the RMS error update produces by far the better design space map.

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