Balancing Exploration and Exploitation using Kriging Surrogate Models in Electromagnetic Design Optimization

G. I. Hawe[1,2] and J. K. Sykulski[1]
[1]School of Electronics and Computer Science, University of Southampton, Southampton, SO17 1BJ, U.K.
[2]Vector Fields Ltd., 24 Bankside, Kidlington, Oxford, OX5 1JE, U.K.
E-mail: glenn.hawe@vectorfields.co.uk, jks@soton.ac.uk

Abstract— The balance between exploration and exploitation is an important issue when attempting to find the global minimum of an objective function. This paper describes how this balance may be carefully controlled when using Kriging surrogate models to approximate the objective function.

I. Introduction

A common technique for reducing computational cost in electromagnetic optimal design problems is to use surrogate models to approximate the relationship between the design variable space and the objective function space. A range of different methods are available for constructing the surrogate model, one of which is Kriging [1]. Kriging surrogate models have the advantage that useful information regarding their accuracy can be obtained, which may then be exploited when choosing the next points to evaluate during optimization, as 'utility functions' may be constructed which seamlessly balance the predicted value of a point's objective function value with the uncertainty in this prediction, thus providing a useful way to achieve the balance between exploration of unknown regions of objective space and exploitation of attractive areas of objective space. This paper discusses the range of such utility functions now available.

II. Utility Functions

Denote by $y_{\min}$ the minimum objective function value attained in the set of examples used to construct the Kriging surrogate model. At an unevaluated design vector x, denote its objective function value as predicted by the Kriging surrogate model by $\hat{y}$, and the root mean squared error in this prediction by s. Then by writing

$$u = \frac{y_{\min} - \hat{y}}{s}, \qquad (1)$$

the "expected improvement" utility function may be defined as [2]:

$$EIF[I(x)] = (y_{\min} - \hat{y})\Psi(u) + s\,\psi(u) \qquad (2)$$

where Ψ is the standard normal distribution function and ψ is the standard normal density function. This utility function is composed of two terms, the first favoring design vectors with a small predicted objective function value, the second favoring design vectors with large uncertainty in their predicted objective function value. Thus the function is a fixed compromise between exploration and exploitation.

The "generalized expected improvement" utility function is defined as [3]:

$$GEIF\left[I^{g}(x)\right] = s^{g}\sum_{k=0}^{g}(-1)^{k}\left(\frac{g!}{k!(g-k)!}\right)u^{g-k}T_{k}, \qquad (3)$$

where

$$T_{k} = -\phi(u)u^{k-1} + (k-1)T_{k-2}, \qquad (4)$$

with

$$T_{0} = \Phi(u) \qquad (5)$$

$$T_{1} = -\phi(u). \qquad (6)$$

The integer parameter g in (3) controls the balance between local and global search, with larger values of g resulting in more emphasis being placed on searching globally. By varying the integer g during an optimization search the emphasis between searching globally and locally can be controlled.

Recently, the "weighted expected improvement" utility function has been proposed in [4]:

$$WEIF[I(x)] = w(y_{\min} - \hat{y})\Psi(u) + (1-w)s\,\psi(u) \qquad (7)$$

where the real valued parameter w (which is set between 0 and 1) controls the balance between the first and second terms, and thus between searching locally or globally. By varying the value of w during an optimization search, the balance of searching globally and locally can again be controlled.

III. Results

Each of the proposed utility functions are naturally suited for use in electromagnetic design optimization, as they allow the balance of exploration and exploitation to be carefully controlled, whilst computational cost is kept to a minimum. Results on mathematical test functions have shown them to be very efficient in locating global minima. Details of their performance in the optimization of electromagnetic devices will be given in the full paper.

IV. References

[1] L. Lebensztajn, C. A. R. Marretto, M. C. Costa and J-L. Coulomb "Kriging: a useful tool for electromagnetic device optimization", *IEEE Transactions on Magnetics*, Vol. 40, No. 2, pp. 1196-1199, March 2004.

[2] D. R. Jones, M. Schonlau and W. J. Welch "Efficient global optimization of expensive black-box functions," *Journal of Global Optimization*, Vol. 13, pp. 455-492, 1998.

[3] M. J. Sasena, P. Papalambros and P. Goovaerts "Exploration of metamodeling sampling criteria for constrained global optimization", *Engineering Optimization*, Vol. 34, pp. 263-278, 2002.

[4] A. Sobester, S. J. Leary and A. J. Keane "On the design of optimization strategies based on global response surface approximation models", *Journal of Global Optimization*, Vol. 33, pp. 31-59, 2005.

1-4244-0320-0/06/$20.00 ©2006 IEEE