

\* . \*\* . †

## Design of Experiment for kriging

JaeJoon Jung, Changseob Lee and TaeHee Lee

**Key Words :** Approximate Model( ), DOE ( ), Kriging ( ), Maximin Distance Experiment Design( ), Maximum Entropy Experiment Design ( ), Space Filling Experiment Design ( )

### Abstract

Approximate optimization has become popular in engineering field such as MDO and Crash analysis which is time consuming. To accomplish efficient approximate optimization, accuracy of approximate model is very important. As surrogate model, Kriging have been widely used approximating highly nonlinear system . Because Kriging employs interpolation method, it is adequate for deterministic computer simulation. Because there are no random errors and measurement errors in deterministic computer simulation, instead of classical DOE ,space filling experiment design which fills uniformly design space should be applied. In this work, various space filling designs such as maximin distance design, maximum entropy design are reviewed. And new design improving maximum entropy design is suggested and compared.

$\hat{y}(\mathbf{x})$  : 가  
 $y(\mathbf{x})$  :  
 $\mathbf{R}$  : (approximate model)  
 $\ln L$  : 가  
 $Ent(\mathbf{x})$  : (Response Surface Model: RSM)  
 $\lambda$  : (Kriging)  
 1. (least square method)  
 (regression model)  
 (Design and Analysis of Computer Experiment : DACE)

Schmit Farshi 가

†

E-mail : thlee@hanyang.ac.kr  
TEL: (02)2290-0449 FAX (02)298-4634

\*

Metheron

\*\*

(kriging)

(Krige, 1951; Matheron, 1963). Sacks

(Sacks, 1989),

Simpson Giunta

(Simpson, 1998; Giunta

et al., 1998). Chen

RBF(Radial Basis Function), MARS(Multivariate Adaptive Regression Spline)

가

RBF 가

(Chen et al, 2000).

가

(measurement error)

(random error)가

(Design of

Experiment: DOE)

(space-filling)

(Sacks et al., 1989).

(Latin hypercube), Sacks

(Maximum entropy sampling),

(Maximin distance design)

Sacks

2.

2.1

가

$$f(\mathbf{x})^T \beta$$

$$z(\mathbf{x})$$

(deviation)

가

$$y(\mathbf{x}) = f(\mathbf{x})^T \beta + z(\mathbf{x})$$

(1)

$$f(\mathbf{x})$$

$p$

$$\beta$$

(regression coefficient)

$$z(\mathbf{x})$$

$$0$$

(stochastic process)

$$\text{Cov}[z(l), z(m)] = \sigma^2 \mathbf{R}(l, m, \boldsymbol{\theta})$$

(2)

$$z(\mathbf{x})$$

$$y(\mathbf{x})$$

$$\sigma^2 \boldsymbol{\theta}$$

$$R(\mathbf{x}^i, \mathbf{x}^j)$$

$$\mathbf{x}^i \quad \mathbf{x}^j$$

$$R(\mathbf{x}^i, \mathbf{x}^j, \boldsymbol{\theta}) = \exp \left[ - \sum_{k=1}^{n_d} \theta_k |\mathbf{x}^i - \mathbf{x}^j|^2 \right] \quad (3)$$

$n_d$

(correlation parameter)  $\boldsymbol{\theta} = [\theta_1, \theta_2, \dots, \theta_{n_d}]^T$

2.2

(Best linear unbiased predictor: BLUP)

$$n \quad \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$$

$$y(\mathbf{x}_1), y(\mathbf{x}_2), \dots, y(\mathbf{x}_n)$$

$$\mathbf{Y}$$

$$\mathbf{Y} \equiv [y(\mathbf{x}_1) \ y(\mathbf{x}_2) \ \dots \ y(\mathbf{x}_n)]^T$$

(4)

$$= \mathbf{F}\beta + \mathbf{Z}$$

$$\mathbf{Z} \quad \mathbf{Z} = [z(\mathbf{x}_1) \ z(\mathbf{x}_2) \ \dots \ z(\mathbf{x}_n)]^T$$

$\mathbf{F}$

(expanded design matrix)

$$\mathbf{F}_{n \times p} \equiv \begin{bmatrix} f_1(\mathbf{x}_1) & \dots & f_p(\mathbf{x}_1) \\ \vdots & \vdots & \vdots \\ f_1(\mathbf{x}_n) & \dots & f_p(\mathbf{x}_n) \end{bmatrix} \quad (5)$$

$n$

$$y(\mathbf{x}_1), y(\mathbf{x}_2), \dots, y(\mathbf{x}_n)$$

(untried point)

$$y(\mathbf{x}) \quad \text{가}$$

$$\text{predictor) } \hat{y}(\mathbf{x})$$

(linear

(4)

$$\hat{y}(\mathbf{x}) = c(\mathbf{x})^T \mathbf{Y} \quad (6)$$

$$\hat{y}(\mathbf{x}) \quad \text{BLUP 가}$$

$$\hat{y}(\mathbf{x})$$

(unbiasedness condition)

가 가

$$\hat{y}(\mathbf{x}) - y(\mathbf{x}) = c(\mathbf{x})^T \mathbf{Y} - y(\mathbf{x})$$

(7)

$$= c(\mathbf{x})^T (\mathbf{F}\beta + \mathbf{Z}) - (f(\mathbf{x})^T \beta + z)$$

$$\beta$$

$$\mathbf{F}^T c(\mathbf{x}) = f(\mathbf{x}) \quad (8)$$

(2)

(8)

$$\text{E}[(y(\mathbf{x}) - y(\mathbf{x}))^2] = \text{E}[(c^T \mathbf{Z} - z)^2]$$

(9)

$$= \sigma^2 [1 - 2c^T \mathbf{r} + c^T \mathbf{R}c]$$

$$\mathbf{r}(\mathbf{x})$$

$$\mathbf{x}^i$$

$$\mathbf{x}$$

$$\mathbf{r}(\mathbf{x}) = \{R(\mathbf{x}, \mathbf{x}_1, \boldsymbol{\theta}), R(\mathbf{x}, \mathbf{x}_2, \boldsymbol{\theta}), \dots, R(\mathbf{x}, \mathbf{x}_n, \boldsymbol{\theta})\}^T \quad (10)$$

(Lagrange multiplier)

$$(8) \quad (9)$$

$$A = \sigma^2 [1 - 2\mathbf{c}^T \mathbf{r} + \mathbf{c}^T \mathbf{R} \mathbf{c}] + \lambda^T (\mathbf{F}^T \mathbf{c} - f) \quad (11)$$

$$\frac{\partial A}{\partial \mathbf{c}}: \sigma^2 [-2\mathbf{r} + 2\mathbf{R} \mathbf{c}] + \mathbf{F} \lambda = 0 \quad (12)$$

$$\frac{\partial A}{\partial \lambda}: \mathbf{F}^T \mathbf{c} - f = 0$$

$$\begin{bmatrix} \mathbf{0}_{p \times p} & \mathbf{F}^T_{p \times n} \\ \mathbf{F}_{n \times p} & \mathbf{R}_{n \times n} \end{bmatrix} \begin{Bmatrix} \lambda' \\ \mathbf{c} \end{Bmatrix}_{(p+n) \times 1} = \begin{Bmatrix} f \\ \mathbf{r} \end{Bmatrix}_{(p+n) \times 1} \quad (13)$$

$$\lambda = 2\sigma^2 \lambda' \quad (13)$$

$$\lambda' = (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{r} - f) \quad (14)$$

$$\mathbf{c} = \mathbf{R}^{-1} [\mathbf{r} - \mathbf{F} (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{r} - f)]$$

$$(14) \quad (6)$$

$$\hat{\mathbf{y}}(\mathbf{x}) = \{\mathbf{r} - \mathbf{F} (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{r} - f)\}^T \mathbf{R}^{-1} \mathbf{Y} \quad (15)$$

$$\hat{\mathbf{y}}(\mathbf{x}) = f^T \hat{\boldsymbol{\beta}} + \mathbf{r}^T \mathbf{R}^{-1} (\mathbf{Y} - \mathbf{F} \hat{\boldsymbol{\beta}}) \quad (16)$$

$$\hat{\boldsymbol{\beta}} = (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{R}^{-1} \mathbf{Y}$$

(generalized least squared estimate)

2.3 (Maximum Likelihood Method)

$$(3) \quad (10)$$

$\boldsymbol{\theta}$

$\boldsymbol{\theta}$

function)  
distribution)  
density function)

(likelihood  
multivariate normal  
probability

$$\ln L = -\frac{(\mathbf{Y} - \mathbf{F} \hat{\boldsymbol{\beta}})^T \mathbf{R}^{-1} (\mathbf{Y} - \mathbf{F} \hat{\boldsymbol{\beta}})}{2\sigma^2} \quad (17)$$

$$-\frac{n}{2} \ln 2\pi - \frac{n}{2} \ln \sigma^2 - \frac{1}{2} \ln |\mathbf{R}| \quad (17) \quad \sigma^2 \quad \sigma^2$$

$\hat{\sigma}^2$

$$\hat{\sigma}^2 = \frac{(\mathbf{Y} - \mathbf{F} \hat{\boldsymbol{\beta}})^T \mathbf{R}^{-1} (\mathbf{Y} - \mathbf{F} \hat{\boldsymbol{\beta}})}{n} \quad (18)$$

$$(18) \quad (17)$$

$$\ln L = -\frac{n \ln \hat{\sigma}^2 + \ln |\mathbf{R}|}{2} \quad (19)$$

$$(19) \quad \theta \quad 0 \leq \theta \leq \infty \quad (16)$$

$n$

3.

가

(random sampling)

(Latin

hypercube) (Mckay, 1979). Johnson

(maximin distance design)

Johnson et al., 1990), Morris

가

(Maximin Latin Hypercube)

(Morris et al., 1995). Wynn Sacks

(determinant) (entropy)

(Wynn, 1987; Sacks et al., 1989).

3.1

Sacks Wynn  $n$

$$Ent = \int p(\mathbf{x})(-\ln p(\mathbf{x})) d\mathbf{x} \quad (20)$$

$n$   
 $p(\mathbf{x})$

$$Ent(\mathbf{x}) = \frac{1}{2} \ln((2\pi e)^n |\mathbf{V}|) \quad (21)$$

$\mathbf{V}$   $n$   
 $\sigma^2(\mathbf{x})$   $\mathbf{R}$   
Sacks

가

$$\text{Maximize } |\mathbf{R}| \quad (22)$$

$\mathbf{R}$  가

$\theta$   
 $\theta$

$\mathbf{x}_i (i=1, \dots, n)$   $n$   
가 가 Sacks Johnson  
(positive definite)  $\mathbf{R}$  가  
(singular matrix) 가  
가 Sacks  
(condition number)

$$Ent(\mathbf{x}) = -\text{cond}(\mathbf{R}) = -\frac{\lambda_n}{\lambda_1} \quad (\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n) \quad (23)$$

$(\mathbf{R} - \lambda)\mathbf{I} = 0$

Sacks  $\mathbf{R}$   
가  $\lambda_n$   $|\mathbf{R}|$   $\lambda_1$

Sacks  
가  
Fig.1 Fig.2 Sacks

2

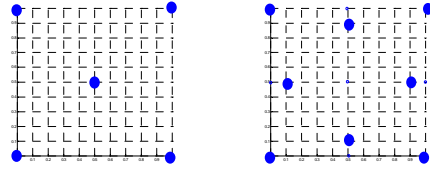


Fig.1 Sampling result using proposed entropy for 2 design variables

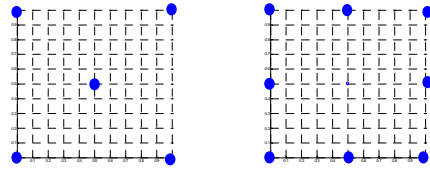


Fig.2 Sampling result using Sacks entropy for 2 design variables

Sacks 가 entropy Sacks

4.

Sacks Johnson  
가 36, 54, 76  
( $E_{avg}$ ), RMS ( $E_{rms}$ ) ( $E_{max}$ )

$$E_{avg} = \frac{1}{N} \sum_i^N |y_i - \hat{y}_i| \quad (25)$$

$$E_{rms} = \sqrt{\frac{1}{N} \sum_i^N (y_i - \hat{y}_i)^2} \quad (26)$$

$$E_{max} = \text{MAX}_i [|y_i - \hat{y}_i|] \quad (27)$$

$N$  가  
 $N = 2500$

$$f = e^{\cos(x_1 - x_2)} \cdot \sin\left(\frac{\cos(x_1 - x_2)^2 + x_1 + x_2}{1 + (x_1 - x_2)^2}\right) \quad (28)$$

$x_1, x_2 \in [0, 4]$

$$f = 2 + 0.01(x_2 - x_1^2)^2 + (1 - x_1)^2 + 2(2 - x_2)^2 + 7 \sin(0.5x_1) \sin(0.7x_1x_2) \quad (29)$$

$x_1, x_2 \in [0, 5]$

$$f = (x_2 - x_1^2)^2 + (1 - x_1)^2 \quad (30)$$

$x_1, x_2 \in [-5, 5]$

$$f = x_1 \sin(4x_1) + 1.1x_2 \sin(2x_2) \quad (31)$$

$x_1, x_2 \in [0, 4]$

$$f = 3(1 - x_1)^2 \times \exp(-x_1^2 - (x_2 + 1)^2) - 10\left(\frac{x_1}{5} - x_1^3 - x_2^5\right) \times \exp(-x_1^2 - x_2^2) - \frac{1}{3} \exp(-(x_1 + 1)^2 - x_2^2) \quad (32)$$

$x_1, x_2 \in [-3, 3]$

$$f = (1 + (x_1 + x_2 + 1)^2 \times (19 - 14x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2)) \times (30 + (2x_1 - 3x_2)^2 \times (18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2)) \quad (33)$$

$x_1, x_2 \in [-2, 2]$

Fig.3~Fig.8 (28)~ (33) 3

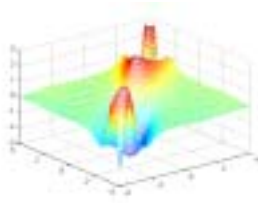


Fig.3 Crane function (Eq.28)

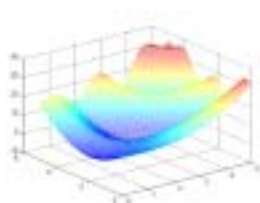


Fig.4 Weichen function (Eq.29)

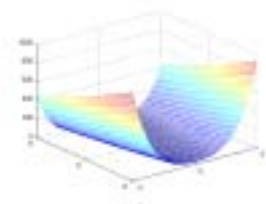


Fig.5 Rosenbrock function (Eq.30)

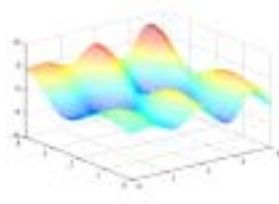


Fig.6 Haupt function (Eq.31)

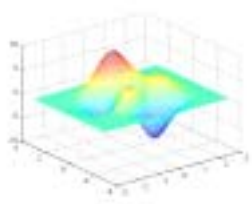


Fig. 7 Peak function (Eq.32)

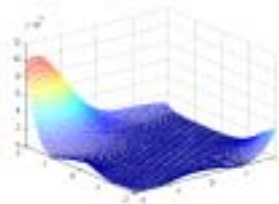


Fig. 8 Goldstein function (Eq.33)

Fig.9~Fig.14

RMS

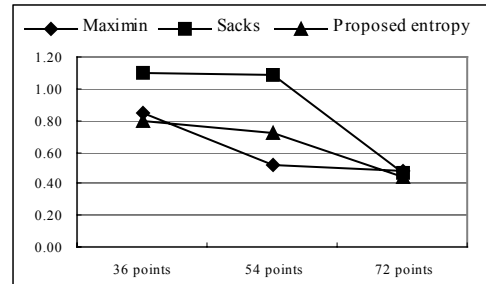


Fig.9 RMS for crane function

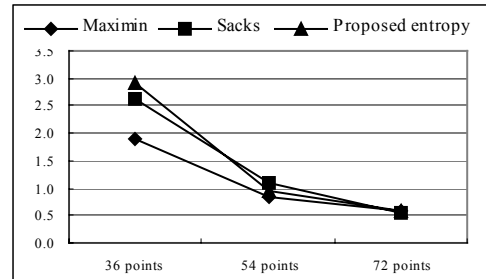


Fig.10 RMS for Weichen function

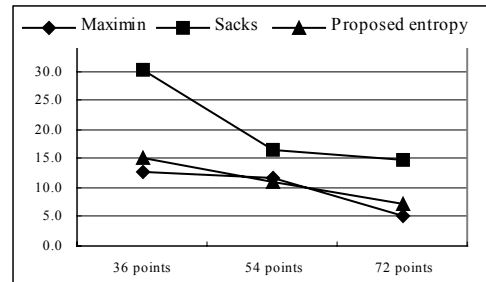


Fig.11 RMS for Rosenbrock function

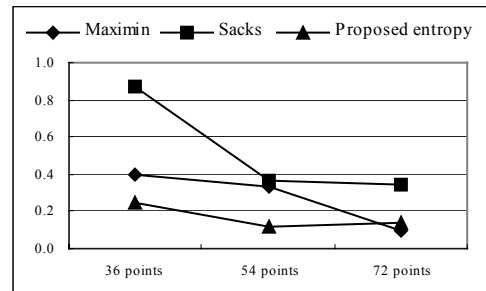


Fig.12 RMS for Haupt function

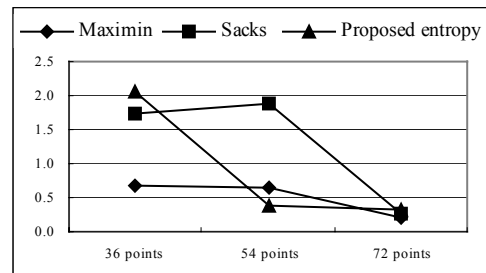


Fig.13 RMS for Peak function

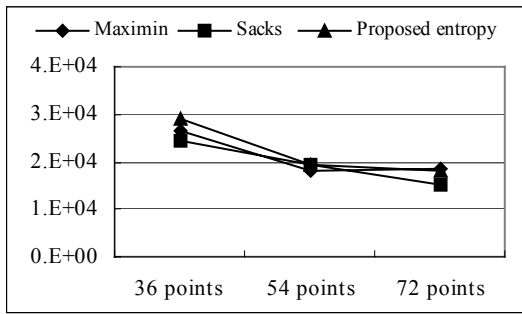


Fig.14 RMS for Peak function

(5) Sacks, J., Welch, W. J., Mitchell, T. J. and Wynn, H. P., 1989, "Design and Analysis of Computer Experiments," *Statistical Science*, Vol. 4, No. 4, pp. 409~435.

(6) Simpson, T. W., Mauery, T. M., Korte, J. J. and Mistree, F., 1998, "Comparison of Response Surface and Kriging Models for Multidisciplinary Design Optimization," *7<sup>th</sup> AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis & Optimization*, St. Louis, MO, AIAA, September 2-4, Vol. 1, pp. 381~391

(7) , 2002, "

5.

가

Sacks

가

2

가

가

(1) Chen, W., Jin, R. and Simpson, T. W., 2000, "Comparative Studies of Metamodeling Techniques Under Multiple Modeling Criteria," *8<sup>th</sup> AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization*, AIAA-2000-4801.

(2) Johnson, M. E., Moore, L. M. and Ylvisaker, D., 1990, "Minimax and Maximin Distance Designs," *Journal of Statistical Planning and Inference*, Vol. 26, No.2, pp.131~148.

(3) Krige, D. G., 1951, "A Statistical Approach to Some Basic Mine Valuation Problems on the Witwatersrand," *Journal of the Chemical, Metallurgical and Mining Society of South Africa*, Vol. 52, pp. 119~139.

(4) Morris, M. D. and Mitchell, T. J., 1995, "Exploratory Designs for Computational Experiments," *Journal of Statistical Planning and Inference*, Vol. 43, No. 3, pp. 381~402.