Efficient design of computer experiments

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Designs for linear models with correlated observations

A distinct feature of optimal designs is that points near the boundary have a larger weight than points at the middle of the design interval.

Consider the model

$$y_j = y_j(t_j) = \theta_1 f_1(t) + \ldots + \theta_k f_k(t) + \varepsilon_j$$

where $t_j \in [-T,T]$, $j=1,...,N$ and $\mathbf{E}\varepsilon_j\varepsilon_i = \sigma^2\rho(t_j - t_i)$.
For the estimate

$$\hat\theta_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T Y$$

the exact design problem has the form

$$\operatorname{Var}\left(\hat\theta_{\text{OLS}}\right) = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T R\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1} \to \min_{t_1,\ldots,t_N}.$$

Let the design points $\{t_1,\ldots,t_N\}$ be generated by the quantiles of a distribution function,

$$t_{iN} = a\left((i-1)/(N-1)\right),\ i = 1,\ldots,N,$$

where the function $a:[0,1]\to[-T,T]$ is the inverse of a distribution function.
Let ξ be a design measure corresponding to $a(\cdot)$.
Under asymptotic settings, the design problem has the form

$$D(\xi) = W^{-1}(\xi)R(\xi)W^{-1}(\xi) \to \min_\xi$$

where $W(\xi) = \int f(u)f^T(u)\xi(du)$ and $R(\xi) = \iint \rho(u-v)f(u)f^T(v)\xi(du)\xi(dv)$.
As example, consider the location model

$$y_j = y_j(t_j) = \theta + \varepsilon_j$$

where $t_j \in [-1,1]$, $\mathbf{E}\varepsilon_j = 0$ and $\mathbf{E}\varepsilon_j\varepsilon_i = \sigma^2\rho(t_j - t_i)$.

Exponential corr. function

For $\rho(t) = e^{-\lambda|t|}$ the optimal design has the form

$$\frac{1}{1+\lambda}\left(\frac{1}{2}\delta_1(du) + \frac{1}{2}\delta_{-1}(du)\right) + \frac{\lambda}{1+\lambda}\frac{1}{2}\mathbf{1}_{[-1,1]}(du)$$

Triangular corr. function

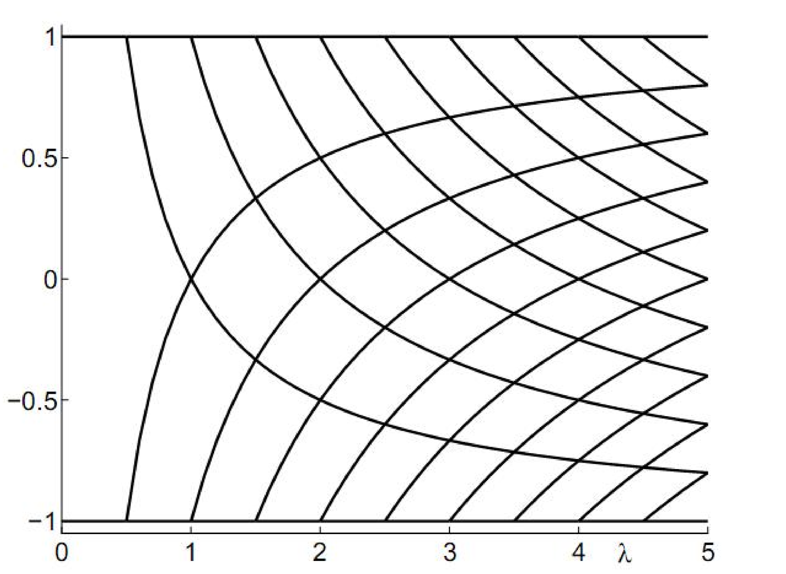
For $\rho(t) = \max\{0, 1-\lambda|t|\}$ the optimal design ξ^* is a discrete symmetric measure supported at $2n$ points

$$\pm t_1, \pm t_2, \ldots, \pm t_n$$

with weights $w_1,\ldots,w_n$ at $t_1,\ldots,t_n$, where $n = \lceil 2\lambda \rceil$,

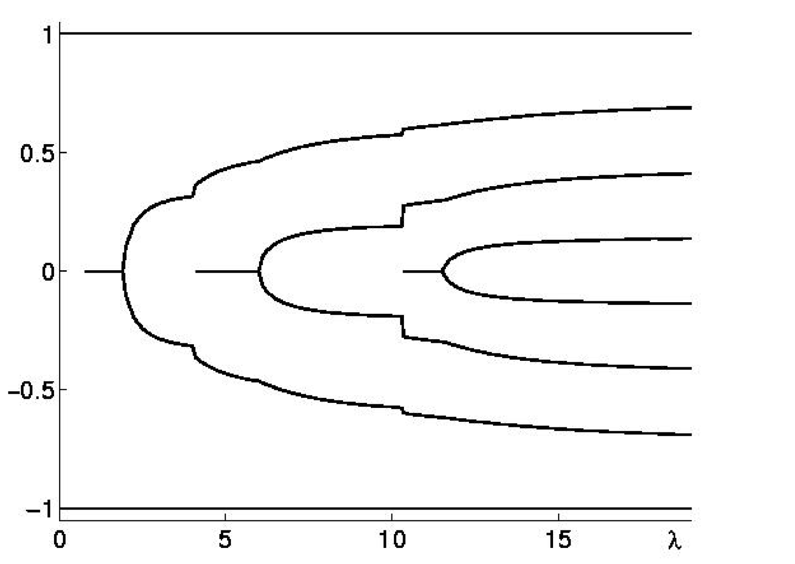
$$(w_1,\ldots,w_n) = \frac{1}{n(n+1)}(\lceil n/2 \rceil, \ldots, 3, n-2, 2, n-1, 1, n),$$

$t_1,\ldots,t_n$ are the ordered quantities $|u_1|,\ldots,|u_n|$, where $u_j = -1 + j/\lambda$, $j = 1,\ldots,n-1$, $u_n = 1$. Support points of the optimal design are depicted.



Gaussian corr. function

For $\rho(t) = e^{-\lambda t^2}$ the optimal design is a discrete measure; support points of the optimal design are depicted.

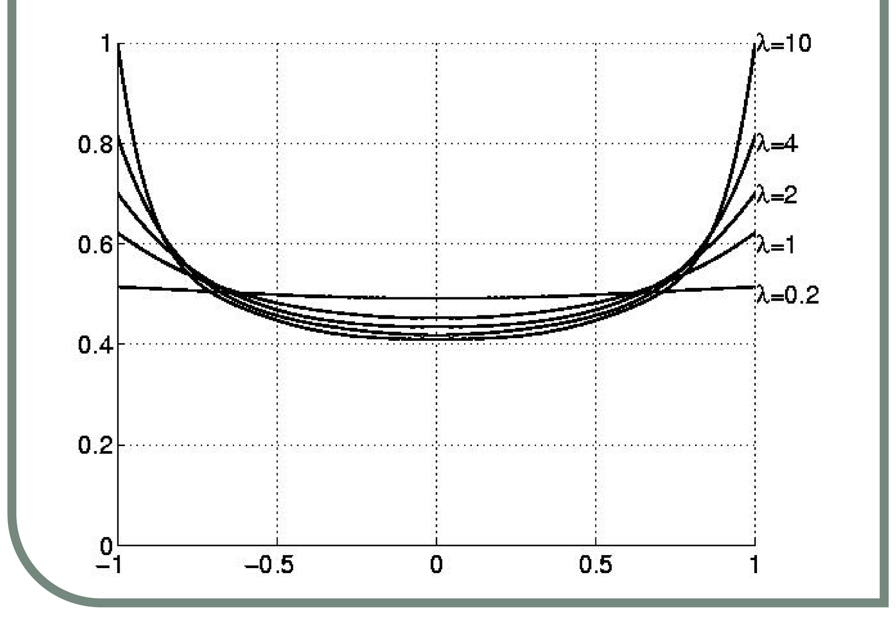


Cauchy corr. function 1

For $\rho(t) = 1/\sqrt{1+\lambda|t|}$ the optimal design has the form

$$\omega^*\left(\frac{1}{2}\delta_1(du) + \frac{1}{2}\delta_{-1}(du)\right) + (1-\omega^*)\xi_0(du).$$

The density of $\xi_0(du)$ is depicted.

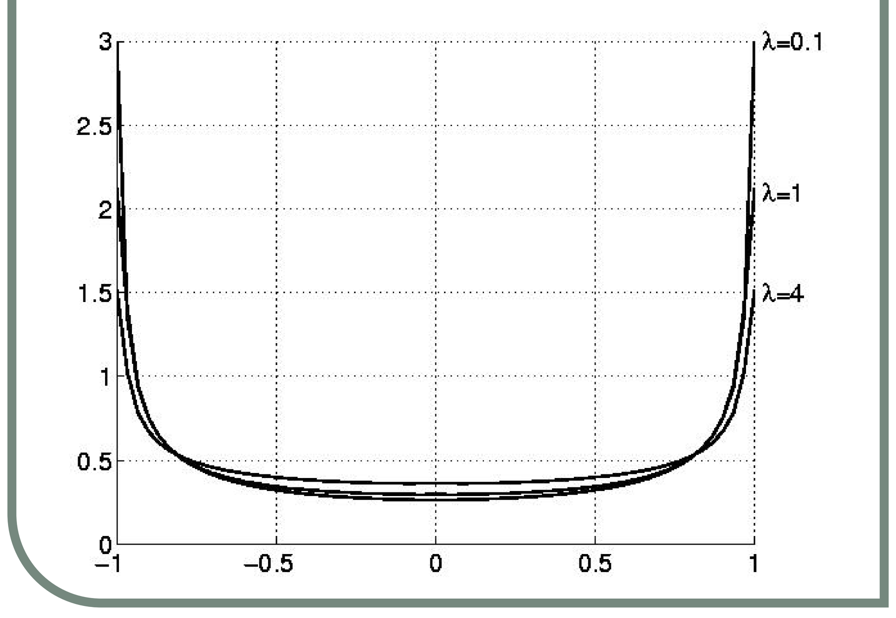


Cauchy corr. function 2

For $\rho(t) = 1/(1+\lambda|t|^{0.5})$ the optimal design has the form

$$\omega^*\left(\frac{1}{2}\delta_1(du) + \frac{1}{2}\delta_{-1}(du)\right) + (1-\omega^*)\xi_0(du).$$

The density of $\xi_0(du)$ is depicted.



Singular corr. kernel 1

For $\rho_\infty(t) = \frac{1}{|t|^\alpha}$, $\alpha \in (0,1)$, the density of the optimal design is a Beta density

$$p^*(t) = \frac{2^{-\alpha}}{B(\frac{1+\alpha}{2},\frac{1+\alpha}{2})}(1-t^2)^{\frac{\alpha-1}{2}}.$$

Singular corr. kernel 2

For $\rho_\infty(t) = -\ln(t^2)$ the density of the optimal design is the arcsine density

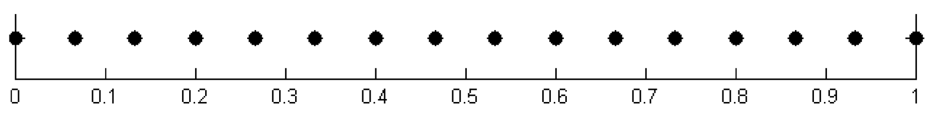
$$p^*(t) = \frac{1}{\pi\sqrt{1-t^2}}.$$

Design of computer experiments

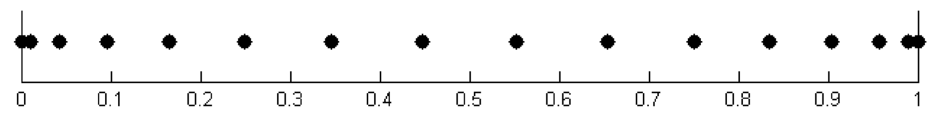
Designs, in which points are located more densely near the boundary, provide a smaller mean squared error than uniform space-filling designs.

The arcsine transformation

Uniform density $p(t) = 1$



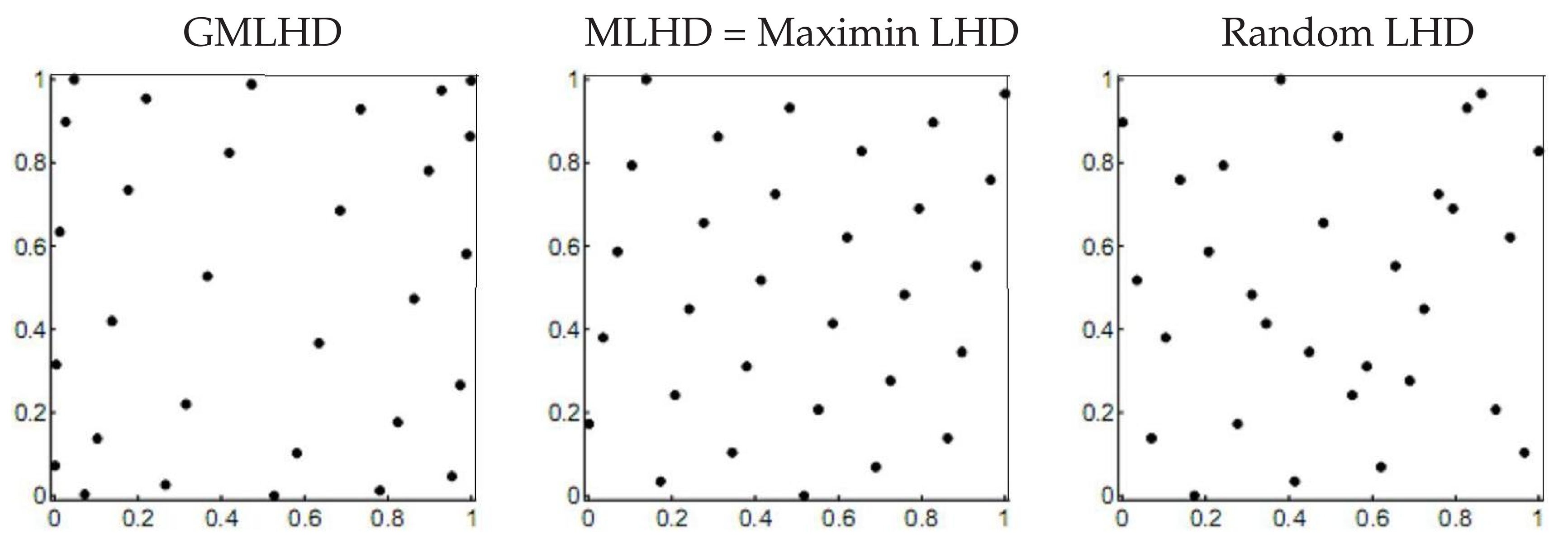
Arcsine density $p(t) = 1\Big/\left(\pi\sqrt{t(1-t)}\right)$



For $x \in [0,1]^d$, apply the transformation to the one-dimensional projections of designs,

$$\tilde x_i = (1-\cos(\pi x_i))/2.$$

30-point LHDs in 2D



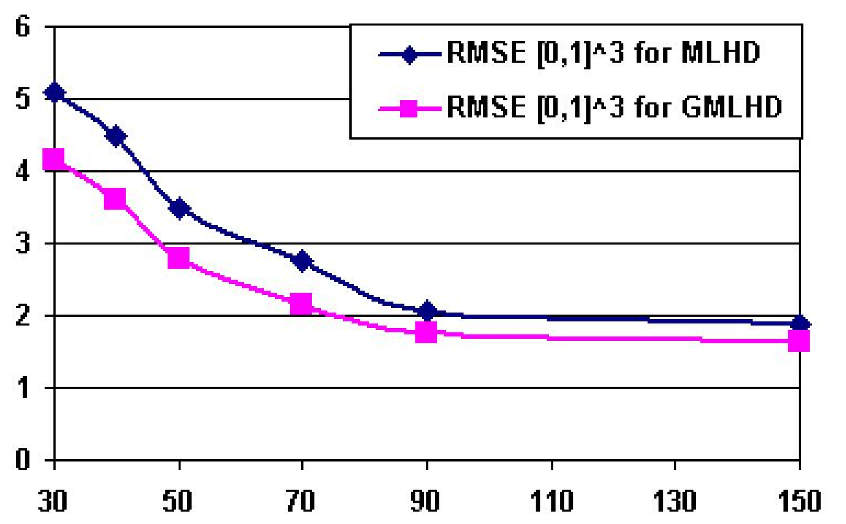
GMLHD = Generalized Maximin LHD which is obtained by modifying MLHD using the arcsine transformation

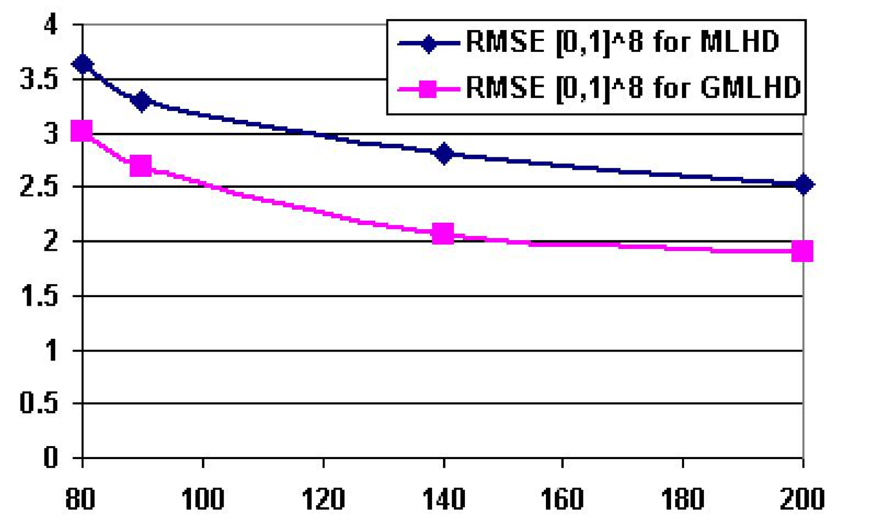
The performance of designs

Compare designs using the MSE criterion and the meta-model given by the posterior mean of a Gaussian process with the Gaussian correlation function, parameters are estimated according to the Bayesian analysis.

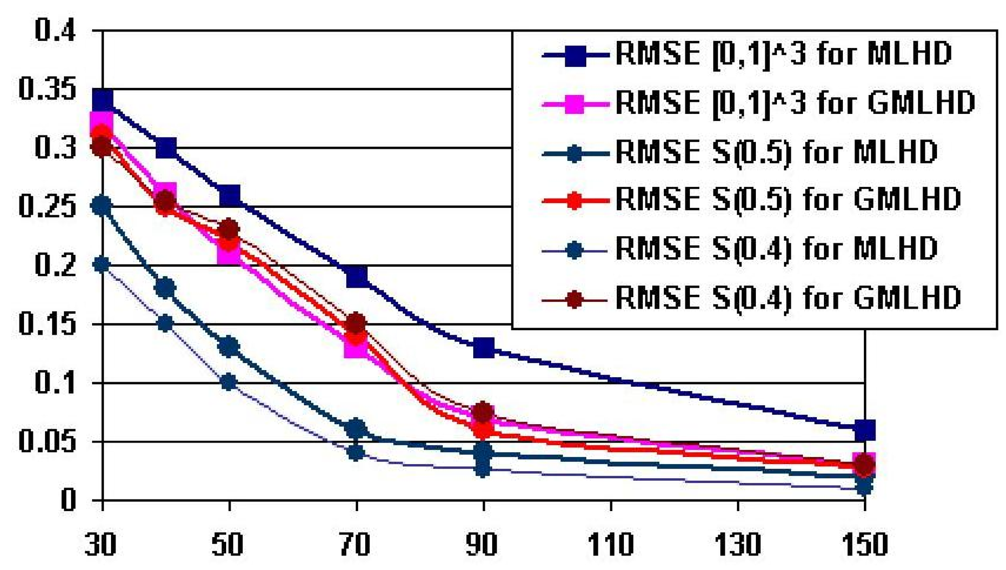
$$\text{MSE}_\Omega(L) = \int_\Omega (\eta(x) - \hat\eta(x))^2\,\mathrm{d}x$$

The square root of the mean squared error, obtained by the generalized maximin Latin hypercube designs, is substantially smaller (about 15%-30%) than the square root of the mean squared error, obtained by the maximin Latin hypercube designs.



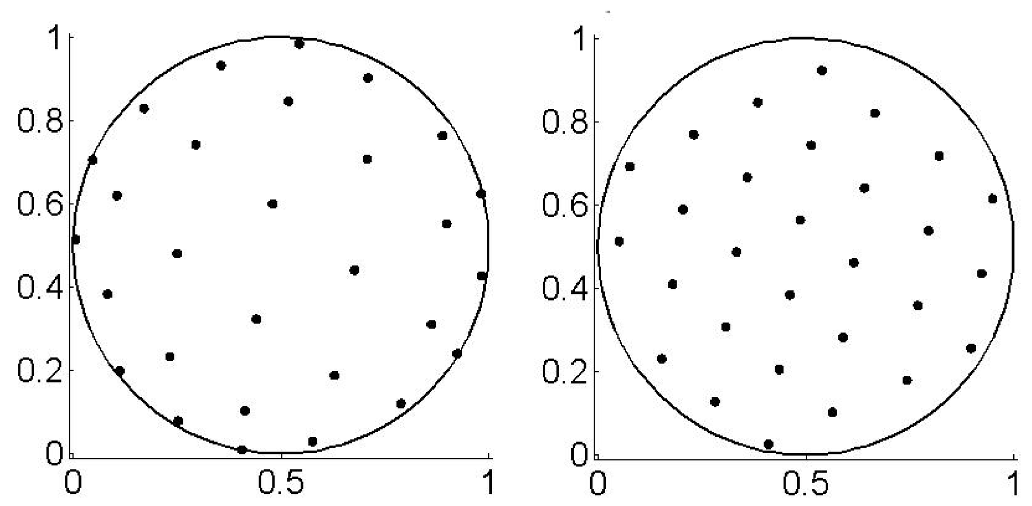


For the MLHD, the mean squared error at the middle of the design space is considerably smaller than the mean squared error over the full design space. For the GMLHD, the mean squared error is almost constant among different subdomains of the design space.



Algorithm for computing efficient designs

- Compute n points which are uniformly distributed on a given domain.
- Shift each point to the boundary, perhaps, using the arcsine transformation.



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