Electronic Supplementary Material (ESI) for Nanoscale

Supporting Information

Spatial Modeling for Refining and Predicting Surface Potential Mapping with Enhanced Resolution

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S1: Mathematical Details

Kriging Method

Let $S = \{s_i, i = 1, \ldots, n\}$ with $s_i = (u_i, v_i)$ denoting the design sites with observed potential and topography. Give the topography information (including derivative information) on $s_0 = (u_0, v_0) \notin S$, the corresponding potential value can be predicted by

$$\hat{z}(s_0) = \sum_{i=1}^{n} c_i(s_0) z(s_i), \tag{1}$$

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where the $c_i(s_0)$s are calculated by minimizing

$$\mathrm{E}\Big[\sum_{i=1}^{n} c_i(s_0)z(s_i) - z(s_0)\Big]^2 \ \text{ s.t. } \ \mathrm{E}\Big[\sum_{i=1}^{n} c_i(s_0)z(s_i)\Big] = \mathrm{E}[z(s_0)]. \tag{2}$$

By solving (3), we have

$$\hat{z}(s_0) = \hat{\mu} + g(s_0)^\top \hat{\beta} + v_{s_0}^\top V_D^{-1}\{Z_D - \hat{\mu} - G_D\hat{\beta}\}, \tag{3}$$

where

$$Z_D = \{z(s_1),\ldots,z(s_n)\}^\top \ \text{ and } \ G_D = \big(g(s_1)^\top,\ldots,g(s_n)^\top\big)^\top,$$

$$v_{s_0} = \big\{\mathrm{cov}\{\varepsilon(s_0),\varepsilon(s_1)\},\ldots,\mathrm{cov}\{\varepsilon(s_0),\varepsilon(s_n)\}\big\}^\top,$$

$$(V_D)_{ij} = \mathrm{cov}\{\varepsilon(s_i),\varepsilon(s_j)\}, \ \text{ for } \ i,j = 1,\ldots,n$$

and $\hat{\mu}$ and $\hat{\beta}$ are generalized least squares estimates for μ and β. The covariance parameters θ_u, θ_v and σ^2 are estimated by maximizing the liklihood function.

Derivative Approximation

The derivative $\partial x/\partial u$ is estimated though the five points method[1]

$$\frac{\partial x(u_i,v_j)}{\partial u} = \frac{-x(u_{i+2},v_j) + 8x(u_{i+1},v_j) - 8x(u_{i+1},v_j) + x(u_{i-2},v_j)}{12(u_i - u_{i-1})}.$$

Similarly, we can estimate $\partial x/\partial v$. Since the derivative estimation of the edge can not be achieved, we cut out points measured on u_1, u_2, u_{255} and u_{256} or v_1, v_2, v_{255}, and v_{256}. Then the model region shrinks to 252×252 grids.

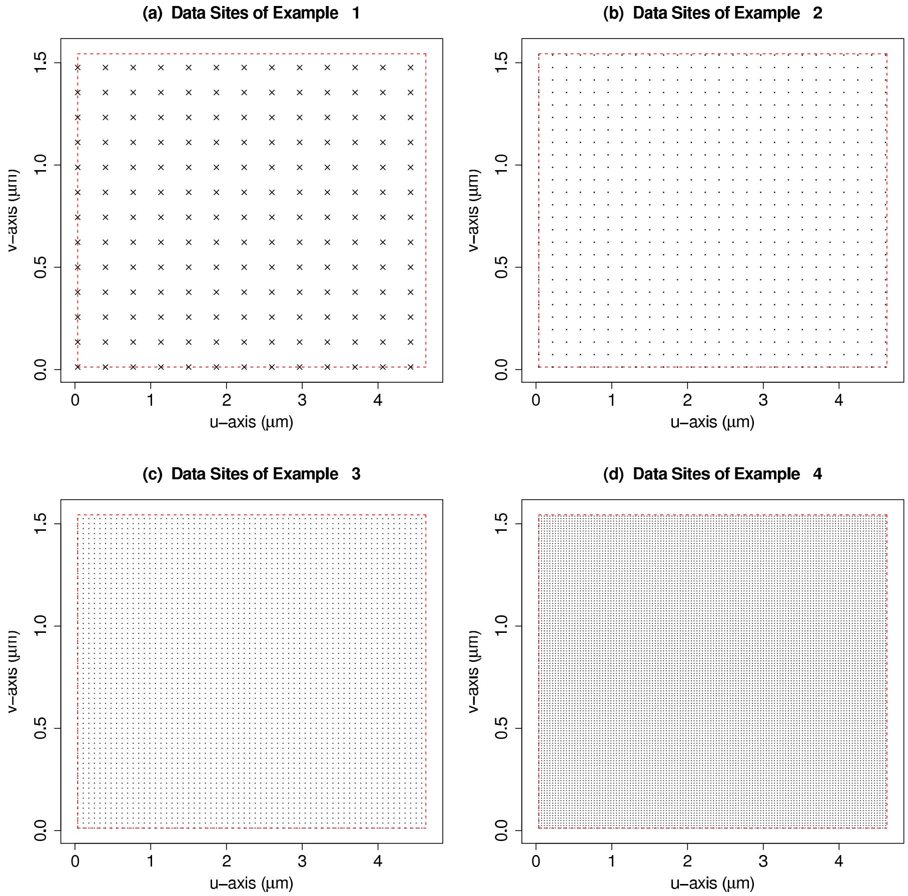

Figure S1: Distribution of the data sites for Examples 1-4 in Table 1.

References

1. Abramowitz, M.; Stegun, I. A. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*; Dover, 1970.