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The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. III v2.

The IMSPE is a LDTRGF in the Cartesian coordinates of vector displacements between any two design points

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Abstract

In this Part III of a five-Roman-numeralled-part series [1-5], we demonstrate that the $IMSPE$ objective function of a twin-point design is almost always a low-degree–truncated, rational, generalized function of the coordinates of the separation of the twins.

Key Words: Nu approximant, Chisholm approximant, landscape, post, computer experiments, Gaussian process, covariance matrix, twin points, clustered designs.

1. Outline

2. Introduction

We reported previously [1] that the $IMSPE$ of a design containing a pair of twin points is almost always (a.a.) a pole-free, low-degree–truncated, rational, generalized function, in the coordinates of the twin-point separation, and that this $IMSPE$ includes a.a. an essential discontinuity. After preliminaries in the present paper's Sections 2 through 6, Section 7 provides a proof that the $IMSPE$ is a low-degree–truncated, rational, generalized-function in the coordinates of either half-vector displacement between the loci of two design points, whether proximal or not. Sec. 8 provides examples of the related essential discontinuities.

3. Matrix identities

For NxN matrix $\boldsymbol{A}$, $(N+1)x(N+1)$ invertible symmetric matrix $\boldsymbol{L}$, and $(N+1)x(N+1)$ symmetric matrix $\boldsymbol{R}$, we have the following four identities.

$tr(\boldsymbol{L}^{-1}\boldsymbol{R}) = \sum_{i=0}^{N}\sum_{j=0}^{N}(L^{-1})_{i,j}\, R_{j,i} = \sum_{i,j=0}^{N}(L^{-1})_{i,j}\, R_{i,j}$. (MI3.1)

$(L^{-1})_{i,j} = \frac{\left[(-1)^{i+j}|\boldsymbol{L}_{-i,-j}|\right]^{\mathrm{T}}}{|\boldsymbol{L}|} = \frac{(-1)^{i+j}|\boldsymbol{L}_{-j,-i}|}{|\boldsymbol{L}|} = \frac{(-1)^{i+j}|\boldsymbol{L}_{-i,-j}|}{|\boldsymbol{L}|}$, where $\boldsymbol{L}_{-i,-j}$ is matrix $\boldsymbol{L}$ with Row i and Column j removed. [Eqs. 2-5 and 2-13 of Ref. 6]. (MI3.2)

Leibniz formula: $|\boldsymbol{A}| = \sum_{\sigma\in S_N}\left[sgn(\sigma)\prod_{i=1}^{N} a_{i,\sigma_i}\right]$, where the sum is over all permutations of the symmetric group S_N; $sgn(\sigma)$ denotes the signature of σ; and, in any of the $N!$ summands, the factor $\prod_{i=1}^{N} a_{i,\sigma_i}$ denotes the product of the entries at positions (i,σ_i), where i ranges from 1 to N [Page 24 of Ref. 6]. (MI3.3)

Laplace formula (a.k.a. cofactor expansion): For any given row index i, $|\boldsymbol{A}| = \sum_{j=1}^{N} A_{i,j}(-1)^{i+j}\left|\boldsymbol{A}_{-i,-j}\right|$, or for any given column index j, $|\boldsymbol{A}| = \sum_{i=1}^{N} A_{i,j}(-1)^{i+j}\left|\boldsymbol{A}_{-i,-j}\right|$ [Page 27 of Ref. 6]. (MI3.4)

4. Assumptions and notation

We use the assumptions and notation of [1,7], as listed and extended in this section.

Vectors and matrices are typeset in a bold font, whereas scalars are not.

$N \geq 2$ point, D-factor designs for computer experiments are the subject of interest.

Design: $\{\boldsymbol{x_1}, \boldsymbol{x_2}, \cdots, \boldsymbol{x_N}\} = \left\{\left(x_{1,1}, x_{1,2}, \cdots, x_{1,D}\right),\ \left(x_{2,1}, x_{2,2}, \cdots, x_{2,D}\right), \cdots, \left(x_{N,1}, x_{N,2}, \cdots, x_{N,D}\right)\right\}$.

Coincident design domain and prediction domain: $[-1,1]^D$, i.e., $-1 \leq x_{i,j} \leq 1$.

The loci of the two design points, with midpoint $\boldsymbol{x_m}$, whose half-separation coordinates, Δ, are used for the expansions: $\boldsymbol{x_m} \pm \Delta$.

Model function, with a constant trend: $Y(\boldsymbol{x}) = \beta_0 + Z(\boldsymbol{x})$.

Normalized objective function (from Eq. 2.9 of [7]): $IMSPE = 1 - tr(\boldsymbol{L}^{-1}\boldsymbol{R})$. (4.1)

NxN correlation matrix of design: $\boldsymbol{V} = \begin{pmatrix} \vdots & \vdots & \vdots \\ \cdots & e^{-\sum_{k=1}^{D} \theta_k (x_{i,k} - x_{j,k})^2} & \cdots \\ \vdots & \vdots & \vdots \end{pmatrix},\ 1 \le i, j \le N,$

where $\boldsymbol{\theta} \equiv [\theta_1, \theta_2, \cdots, \theta_D]^{\mathsf{T}}$ are positive covariance parameters.

$(N+1)x(N+1)$ symmetric matrix $\boldsymbol{L}$, with row and column indices 0 through N, follows:

$$L \equiv \begin{pmatrix} 0 & | & 1 & \cdots & 1 \\ -- & | & -- & -- & -- \\ 1 & | & & & \\ \vdots & | & & \boldsymbol{V} & \\ 1 & | & & & \end{pmatrix}.$$

$(N+1)x(N+1)$ symmetric matrix $\boldsymbol{R}$, with row and column indices to account for integration over the prediction domain:

$$\boldsymbol{R} \equiv \frac{1}{2^D} \int_{-1}^{1} \int_{-1}^{1} \cdots \int_{-1}^{1} \begin{pmatrix} 1 & | & v_1 & v_2 & \cdots & v_N \\ -- & | & --- & --- & --- & --- \\ v_1 & | & v_1^2 & v_1 v_2 & \cdots & v_1 v_N \\ v_2 & | & v_1 v_2 & v_2^2 & \cdots & v_2 v_N \\ \vdots & | & \vdots & \vdots & \ddots & \vdots \\ v_N & | & v_1 v_N & v_2 v_N & \cdots & v_N^2 \end{pmatrix} dx_1 dx_2 \cdots dx_D,$$

where $\boldsymbol{v}_i \equiv e^{-\sum_{k=1}^{D} \theta_k (x_{i,k} - x_k)^2}$.

N.B. $x_{i,k}$ is a design-point coordinate, while x_k is an independent variable.

The integrals, immediately above, were detailed in [8], as follows:

$$\boldsymbol{R} = \begin{pmatrix} 1 & | & \cdots & S_1(\boldsymbol{x_j}, \boldsymbol{\theta}) & \cdots \\ - & | & -- & ---------------- & -- \\ \vdots & | & \cdots & \vdots & \cdots \\ \cdot & | & \vdots & S_2\left(\frac{\boldsymbol{x_i} + \boldsymbol{x_j}}{2}, \boldsymbol{\theta}\right) e^{\frac{-\sum_{k=1}^{D} \theta_k (x_{i,k} - x_{j,k})^2}{2}} & \vdots \\ \vdots & | & \cdots & \vdots & \cdots \end{pmatrix}, \text{ where}$$

$$S_\ell(\boldsymbol{x_i}, \boldsymbol{\theta}) = \prod_{k=1}^{D} \sqrt{\frac{\pi}{16 \ell \theta_k}} \left\{ erf\left[\sqrt{\ell \theta_k}(1 + x_{i,k})\right] + erf\left[\sqrt{\ell \theta_k}(1 - x_{i,k})\right] \right\},\ \ell = 1,2.$$

Taylor-series expansions of e^x and $erf(x)$ have infinite radii of convergence. Such expansions are carried out, in this paper, in powers of $\sqrt{\theta_k}\Delta_k$ or $\sqrt{\theta_k}\delta_k,\ k = 1,2,\cdots,D$.

Indices of the pair of points, in $\boldsymbol{V}$ or $\boldsymbol{R}$, whose half-separation coordinates are used for the Taylor-series expansions: $N-1$ and N.

For a matrix $\boldsymbol{A}$ with elements Taylor-series expandable in powers of $\sqrt{\theta_k}\Delta_k,\ k = 1,2,\cdots,D$; $\boldsymbol{A}^{(\boldsymbol{p})}$ is defined as $\boldsymbol{A}$, but including only p-degree terms $\left(\sqrt{\theta_k}\Delta_k\right)^p,\ k = 1,2,\cdots,D$.

"$O(\Delta^2)$" is shorthand for the terms $O(\theta_1 \Delta_1^2), O(\theta_2 \Delta_2^2), \cdots, O(\theta_D \Delta_D^2)$.

"$O(\delta^2)$" is shorthand for the terms $O(\theta_1 \delta_1^2), O(\theta_2 \delta_2^2), \cdots, O(\theta_D \delta_D^2)$.

"Low-degree–truncated function" is defined in Proposition 1 of Section 6.

"The landscape," local region," "post," and "Nu approximant" are defined in Section 8.

5. Expanding in the dimensionless coordinates $\sqrt{\boldsymbol{\theta_k}}\Delta_{\boldsymbol{k}}$, $\boldsymbol{k = 1, 2, \cdots, D}$

The focus in this paper is on expansions in the coordinates of the half-vector displacement, Δ, between the loci of two arbitrarily chosen design points, $\boldsymbol{x_m} \pm \Delta$.

Matrix $\boldsymbol{V}$

$\boldsymbol{V}$ can be divided into blocks $\boldsymbol{V} \equiv \begin{pmatrix} \boldsymbol{V_D} & | & \boldsymbol{V_E} \\ -- & | & -- \\ \cdot & | & \boldsymbol{V_F} \end{pmatrix}$. The $(N-2)x2$ URH block is

$$\boldsymbol{V_E} = \begin{pmatrix} \vdots & \vdots \\ e^{-\sum_{k=1}^{D}\theta_k\left(x_{i,k}-x_{m,k}-\Delta_k\right)^2} & e^{-\sum_{k=1}^{D}\theta_k\left(x_{i,k}-x_{m,k}+\Delta_k\right)^2} \\ \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots \\ a_i\begin{bmatrix} 1 \\ +A_i \\ +O\left(\Delta^2\right) \end{bmatrix} & a_i\begin{bmatrix} 1 \\ -A_i \\ +O\left(\Delta^2\right) \end{bmatrix} \\ \vdots & \vdots \end{pmatrix},$$

where $a_i \equiv e^{-\sum_{k=1}^{D}\theta_k\left(x_{i,k}-x_{m,k}\right)^2}$ $i = 1, 2, \cdots, N-2$; and $A_i \equiv 2\sum_{k=1}^{D}\sqrt{\theta_k}\left(x_{i,k}-x_{m,k}\right)\sqrt{\theta_k}\Delta_k$. N.B.: We intentionally have $\sqrt{\theta_k}$ appears twice.

The $2x2$ LRH block is $\boldsymbol{V_F} = \begin{pmatrix} 1 & \begin{bmatrix} 1 \\ +O\left(\Delta^2\right) \end{bmatrix} \\ \begin{bmatrix} 1 \\ +O\left(\Delta^2\right) \end{bmatrix} & 1 \end{pmatrix}$.

Then writing symmetric $\boldsymbol{V}$, using index i but not index j,

$$\boldsymbol{V} \equiv \begin{pmatrix} 1 & \cdots & V_{1,i} & \cdots & V_{1,N-2} & | & a_1\begin{bmatrix} 1 \\ +A_1 \\ +O(\Delta^2) \end{bmatrix} & a_1\begin{bmatrix} 1 \\ -A_1 \\ +O(\Delta^2) \end{bmatrix} \\ \vdots & \ddots & \vdots & \vdots & \vdots & | & \vdots & \vdots \\ V_{1,i} & \cdots & 1 & \cdots & V_{i,N-2} & | & a_i\begin{bmatrix} 1 \\ +A_i \\ +O(\Delta^2) \end{bmatrix} & a_i\begin{bmatrix} 1 \\ -A_i \\ +O(\Delta^2) \end{bmatrix} \\ \vdots & \vdots & \vdots & \ddots & \vdots & | & \vdots & \vdots \\ V_{1,N-2} & \cdots & V_{i,N-2} & \cdots & 1 & | & a_{N-2}\begin{bmatrix} 1 \\ +A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & a_{N-2}\begin{bmatrix} 1 \\ -A_{N-2} \\ +O(\Delta^2) \end{bmatrix} \\ ------ & - & ------ & - & ------- & | & ------- & ------- \\ a_1\begin{bmatrix} 1 \\ +A_1 \\ +O(\Delta^2) \end{bmatrix} & \cdots & a_i\begin{bmatrix} 1 \\ +A_i \\ +O(\Delta^2) \end{bmatrix} & \cdots & a_{N-2}\begin{bmatrix} 1 \\ +A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & | & 1 & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} \\ a_1\begin{bmatrix} 1 \\ -A_1 \\ +O(\Delta^2) \end{bmatrix} & \cdots & a_i\begin{bmatrix} 1 \\ -A_i \\ +O(\Delta^2) \end{bmatrix} & \cdots & a_{N-2}\begin{bmatrix} 1 \\ -A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & | & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} & 1 \end{pmatrix}. \tag{5.1}$$

Matrix $\boldsymbol{L}$

It follows that matrix $\boldsymbol{L}$ can be expressed in similar, but more abbreviated, form as,

$$\boldsymbol{L} \equiv \left(\begin{array}{c|cccc|cc} 0 & 1 & & \cdots & 1 & 1 & 1 \\ - & --- & & ------- & --- & ------- & ------- \\ 1 & 1 & & \cdots & V_{1,N-2} & \vdots & \vdots \\ \vdots & \vdots & & \ddots & \vdots & a_i\begin{bmatrix} 1 \\ +A_i \\ +O(\Delta^2) \end{bmatrix} & a_i\begin{bmatrix} 1 \\ -A_i \\ +O(\Delta^2) \end{bmatrix} \\ 1 & V_{1,N-2} & & \cdots & 1 & \vdots & \vdots \\ - & --- & & ------- & --- & ------- & -------- \\ 1 & \cdots & & a_i\begin{bmatrix} 1 \\ +A_i \\ +O(\Delta^2) \end{bmatrix} & \cdots & 1 & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} \\ 1 & \cdots & & a_i\begin{bmatrix} 1 \\ -A_i \\ +O(\Delta^2) \end{bmatrix} & \cdots & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} & 1 \end{array}\right).$$

Matrix $\boldsymbol{R}$

Matrix $\boldsymbol{R}$ can be divided into blocks as $\boldsymbol{R} \equiv \left(\begin{array}{c|c|c} \boldsymbol{R_A} & \boldsymbol{R_B} & \boldsymbol{R_C} \\ -- & -- & -- \\ & \boldsymbol{R_D} & \boldsymbol{R_E} \\ -- & -- & -- \\ & & \boldsymbol{R_F} \end{array}\right)$, where

$$\boldsymbol{R_F} = \begin{pmatrix} S_2(\boldsymbol{x_m} + \Delta, \boldsymbol{\theta}) + O(\Delta^2) & S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) + O(\Delta^2) \\ S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) + O(\Delta^2) & S_2(\boldsymbol{x_m} - \Delta, \boldsymbol{\theta}) + O(\Delta^2) \end{pmatrix}$$

$$= \begin{pmatrix} S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) + \Delta \cdot \boldsymbol{\nabla_x} S_2(\boldsymbol{x}, \boldsymbol{\theta})|_{\boldsymbol{x}=\boldsymbol{x_m}} & S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) \\ S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) & S_2(\boldsymbol{x_m}, \boldsymbol{\theta}) - \Delta \cdot \boldsymbol{\nabla_x} S_2(\boldsymbol{x}, \boldsymbol{\theta})|_{\boldsymbol{x}=\boldsymbol{x_m}} \end{pmatrix} + \left(O(\Delta^2)\right), \quad (5.2)$$

and where $\Delta \equiv (\Delta_1, \Delta_2, \cdots, \Delta_D)$; "$\cdot$" denotes inner product; $\boldsymbol{\nabla_x}$ is the gradient operator defined as $\boldsymbol{\nabla_x} f \equiv \sum_{k=1}^{D} \frac{\delta f}{\delta x_k} \boldsymbol{i_k}$, where $\boldsymbol{i_k}$, $k = 1,2,\cdots,D$ is the standard unit vector in the direction of the $x_{m,k}$ coordinate.

6. Proposition 1: $|\boldsymbol{V}|$ and $|\boldsymbol{L}|$ are low-degree–truncated functions

Proposition 1: Given a D-factor, N-point design that includes a pair of not-necessarily-proximal points with midpoint $\boldsymbol{x_m}$*, viz.,* $\boldsymbol{x_{N-1}} = \boldsymbol{x_m} + \Delta$ *and* $\boldsymbol{x_N} = \boldsymbol{x_m} - \Delta$*; and given the design's corresponding Gaussian-correlation matrix,* $\boldsymbol{V}$*, with elements* $V_{i,j} \equiv e^{-\sum_{k=1}^{D} \theta_k (x_{i,k} - x_{j,k})^2}$*,* $i,j = 1,2,\cdots,N$*; the expansion of* $|\boldsymbol{V}|$ *in the dimensionless Cartesian components,* $\sqrt{\theta_k}\Delta_k$*, contains no* *constant or linear terms. In other words, $|\boldsymbol{V}|$ is a low-degree–truncated function of minimum degree two.*

Proof: We use "Type-0" and "Type-1" arguments, defined by examples:

<u>Type-0 argument</u>
By the Leibniz formula of Matrix Identity MI3.1, a constant term in $|\boldsymbol{V}|$ can only arise from a product of N constants in the power-series of $\boldsymbol{V}$, and thus $|\boldsymbol{V}|^{(0)} = \left|\boldsymbol{V}^{(\mathbf{0})}\right|$. Then, because $\boldsymbol{V}^{(\mathbf{0})}$, based on Eq. 5.1.1, above, has two identical columns, $\left|\boldsymbol{V}^{(\mathbf{0})}\right| = 0$. Thus, $|\boldsymbol{V}|$ contains no constant term.

<u>Type-1 argument</u>
Now consider whether $|\boldsymbol{V}|$ can contain first-degree term in the $\sqrt{\theta_k}\Delta_k$. If $N = 2$, $\boldsymbol{V}$ consists solely of the LRH $2x2$ block of Eq. 5.1, above, where there are no such terms, and the proof is complete. If $N > 2$, refer to Eq. 6.1, immediately below, and consider the linear term a_1A_1 in Row $N-1$ and Col. 1 of the full matrix $\boldsymbol{V}^{(\mathbf{1})}$. This term can appear in isolation in $|\boldsymbol{V}|$ only via the signed product of itself and $N-1$ constants, each of the latter of which may be 1; a_ℓ, $\ell = 1, \cdots, N-2$; or $V_{i,j}$, $i = 2, \cdots, N-2$ & $j = 1, \cdots, N-2$. In Eq. 6.1, we highlight in green the specific a_1A_1 term and proceed by crossing out its element's row and column to leave $\boldsymbol{V}$ with both Row $N-1$ and Col. 1 removed, which we define as $\boldsymbol{V}^{(\mathbf{1})}_{-(\boldsymbol{N}-\mathbf{1}),-\mathbf{1}}$. The desired linear term in A_1 will appear as sgn[element at Row $(N-1)$ and Col. 1] $\cdot \left|\boldsymbol{V}^{(\mathbf{1})}_{-(\boldsymbol{N}-\mathbf{1}),-\mathbf{1}}\right|$, where sgn is the relevant signature of the term in the Laplace formula (cf. MI4) for $|\boldsymbol{V}|$.

$$\boldsymbol{V}_{-(\boldsymbol{N}-\mathbf{1}),-\mathbf{1}} = \left\{\begin{array}{cccc|cc}
1 & V_{1,2} & \cdots & V_{1,N-2} & \begin{bmatrix} a_1 \\ +a_1A_1 \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} a_1 \\ -a_1A_1 \\ +O(\Delta^2) \end{bmatrix} \\
V_{1,2} & 1 & \cdots & V_{2,N-2} & \begin{bmatrix} a_2 \\ +a_2A_2 \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} a_2 \\ -a_2A_2 \\ +O(\Delta^2) \end{bmatrix} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
V_{1,N-2} & V_{2,N-2} & \cdots & 1 & \begin{bmatrix} a_{N-2} \\ +a_{N-2}A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} a_{N-2} \\ -a_{N-2}A_{N-2} \\ +O(\Delta^2) \end{bmatrix} \\
\hdashline
\begin{bmatrix} a_1 \\ +\boldsymbol{a_1A_1} \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} a_2 \\ +a_2A_2 \\ +O(\Delta^2) \end{bmatrix} & \cdots & \begin{bmatrix} a_{N-2} \\ +a_{N-2}A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & 1 & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} \\
\begin{bmatrix} a_1 \\ -a_1A_1 \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} a_2 \\ -a_2A_2 \\ +O(\Delta^2) \end{bmatrix} & \cdots & \begin{bmatrix} a_{N-2} \\ -a_{N-2}A_{N-2} \\ +O(\Delta^2) \end{bmatrix} & \begin{bmatrix} 1 \\ +O(\Delta^2) \end{bmatrix} & 1
\end{array}\right\}. \tag{6.1}$$

To simplify the determination of $\left|\boldsymbol{V}^{(\mathbf{1})}_{-(\boldsymbol{N}-\mathbf{1}),-\mathbf{1}}\right|$, we drop the other A_1's and all A_i $i \neq 1$, as these would contribute second-degree-or-higher terms to $\left|\boldsymbol{V}^{(\mathbf{1})}_{-(\boldsymbol{N}-\mathbf{1}),-\mathbf{1}}\right|$, and such terms are not of current interest. Thus,

$$\left|{}_{N}\boldsymbol{V}^{(\mathbf{1})}_{-(\boldsymbol{N-1}),-\mathbf{1}}\right| = \left|\begin{array}{ccc|cc} V_{1,2} & \cdots & V_{1,N-2} & a_1 & a_1 \\ 1 & \cdots & V_{2,N-2} & a_2 & a_2 \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ V_{2,N-2} & \cdots & 1 & a_{N-2} & a_{N-2} \\ \hline a_2 & \cdots & a_{N-2} & 1 & 1 \end{array}\right|,$$

and this is zero, because the ultimate expression has two identical rows or columns. Also, its contribution to linear terms of $|\boldsymbol{V}|$ is zero. The same argument is true, *mutatis mutandis*, for any other A_i in Eq. 6.1. Thus, $|\boldsymbol{V}|$ contains no linear term in $\sqrt{\theta_k}\Delta_k,\ k = 1,2,\cdots,D.$ □

A relevant corollary follows.

Corollary: The expansion of $|\boldsymbol{L}|$ in the dimensionless Cartesian components, $\sqrt{\theta_k}\Delta_k$, contains no constant or linear terms. Proof: Follows from the same reasoning as that of Proposition 1.

7. *Proposition 2: $IMSPE$ is a low-degree–truncated (generalized) rational function with minimum-degree two*

Proposition 2: Given the design and correlation matrix in the statement of Proposition 1; then the normalized, integrated, mean-squared error of the design, $IMSPE = 1 - tr(\boldsymbol{L}^{-\mathbf{1}}\boldsymbol{R})$; when expanded in the Cartesian components $\sqrt{\theta_k}\Delta_k$ of either half-vector (or vector) between any two distinct design points; and when expressed as a rational, possibly generalized, function; contains neither constant nor linear terms in its numerator or denominator.

Proof: From Eq. 4.1, Matrix Identities MI3.1 and MI3.2, and the symmetries of $\boldsymbol{R}$ and $\boldsymbol{L}^{-\mathbf{1}}$,

$$IMSPE = 1 - tr(\boldsymbol{L}^{-\mathbf{1}}\boldsymbol{R}) = 1 - \sum_{i,j=0}^{N}(\boldsymbol{L}^{-\mathbf{1}})_{i,j}\, R_{i,j} = \frac{|\boldsymbol{L}| - \sum_{i,j=0}^{N}(-1)^{i+j}|\boldsymbol{L}_{-i,-j}|R_{i,j}}{|\boldsymbol{L}|}.$$

Because the Taylor-series expansions of e^x and $erf(x)$ are convergent, $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|$ and $R_{i,j}$ can be expanded in power-series of $\sqrt{\theta_k}\Delta_k$ into terms of order-zero, order-one, etc., as follows: $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right| = \left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(0)} + \left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(1)} + \left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(2)} + \cdots$ and $R_{i,j} = R^{(0)}_{i,j} + R^{(1)}_{i,j} + R^{(2)}_{i,j}$. Then,

$$IMSPE = \frac{|\boldsymbol{L}| - \sum_{i,j=0}^{N}(-1)^{i+j}\left\{\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(0)}\left[R^{(0)}_{i,j} + R^{(1)}_{i,j}\right] + \left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(1)}R^{(0)}_{i,j}\right\} + O(\Delta^2)}{|\boldsymbol{L}|}. \quad (7.1)$$

We explore $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(0)}$ and $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(1)}$, in turn.

$\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}\right|^{(0)}$:

Reducing the elements of Eq. 5.1 to just its constant terms, gives,

$$\boldsymbol{L}^{(\mathbf{0})} \equiv \left(\begin{array}{c|ccc|cc} 0 & 1 & \cdots & 1 & 1 & 1 \\ -- & --- & -- & --- & -- & -- \\ 1 & 1 & \cdots & V_{1,N-2} & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & a_i & a_i \\ 1 & V_{1,N-2} & \cdots & 1 & \vdots & \vdots \\ -- & --- & -- & --- & -- & -- \\ 1 & \cdots & a_i & \cdots & 1 & 1 \\ 1 & \cdots & a_i & \cdots & 1 & 1 \end{array}\right)$$, with blocks

$\boldsymbol{L}^{(\mathbf{0})} \equiv \left(\begin{array}{c|c} \boldsymbol{L}_{\boldsymbol{A}}^{(\mathbf{0})} & \boldsymbol{L}_{\boldsymbol{C}}^{(\mathbf{0})} \\ -- & -- \\ \cdot & \boldsymbol{L}_{\boldsymbol{F}}^{(\mathbf{0})} \end{array}\right)$. We can draw conclusions about the values of various $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right|$, $0 \leq i,j \leq N$.

When N=2, $\boldsymbol{L}^{(\mathbf{0})} \equiv \left(\begin{array}{c|cc} 0 & 1 & 1 \\ -- & -- & -- \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{array}\right)$. By inspection, when indices i and j are not both in Block $\boldsymbol{L}_{\boldsymbol{F}}^{(\mathbf{0})}$, there are two identical rows or columns, and $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right| = 0$; whereas for indices i and j both in Block $\boldsymbol{L}_{\boldsymbol{F}}^{(\mathbf{0})}$, $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right|$ is immune to intra-block changes in i and j, and $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right|$ is a constant that we dub ${}_N L$. It is clear that ${}_2 L = -1$, but for the purpose of the proof at hand, this specific value is not needed.

When N>2, the argument is the same.

We conclude the following, for arbitrary $N \geq 2$:

When indices i and j are not both in Block $\boldsymbol{L}_{\boldsymbol{F}}^{(\mathbf{0})}$: $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right| = 0$. (7.2)

Otherwise: $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{0})}\right| = {}_N L$. (7.3)

$\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{1})}\right|$:

Via a Type-1 argument, $\left|\boldsymbol{L}_{-\boldsymbol{i},-\boldsymbol{j}}^{(\mathbf{1})}\right| = 0$. (7.4)

Using Eqs. 7.2 through 7.4, Eq. 7.1 becomes $IMSPE = \frac{|\boldsymbol{L}| - {}_N L \sum_{i,j=N-1}^{N} (-1)^{i+j} \left[R_{i,j}^{(0)} + R_{i,j}^{(1)}\right] + O(\Delta^2)}{|\boldsymbol{L}|}$, so it remains to show $\sum_{i,j=N-1}^{N} (-1)^{i+j} \left[R_{i,j}^{(0)} + R_{i,j}^{(1)}\right] = 0$. Examination of Eq. 5.2 leads to the conclusion that this sum is indeed zero. □

8. Simple $D = N = 2$ examples with $(\theta_1, \theta_2) = (1.0, 1.0)$

From Proposition 2, the $IMSPE$ of a D-factor, $N \geq 2$ design, when expanded in the Cartesian components $\sqrt{\theta_k}\Delta_k$ of either half-vector (or vector) between any two distinct design points is a low-degree-truncated rational function (properly “generalized function” - see two paragraphs, below) in those components, with minimum degrees two in both numerator and denominator.

We dub these degrees m_ℓ and n_ℓ, respectively, where the "ℓ" subscripts denote "lower." We also truncate the numerator and denominator with maximum degrees that we dub m_h and n_h, respectively, where the "h" subscripts denote "higher." We introduce the resulting "$\left[\frac{m_\ell,m_h}{n_\ell,n_h}\right]$ Nu approximant" of the $IMSPE$, in rough analogy to a Padé approximant, as follows:

$$\left[\frac{m_\ell,m_h}{n_\ell,n_h}\right]_{IMSPE}(\delta_1,\delta_2) \equiv \frac{(terms\ of\ total\ \ power\ \ m_\ell)+(terms\ of\ tot.\ pow.\ m_\ell+1)+\cdots+(terms\ of\ tot.\ pow.\ m_h)}{(terms\ of\ total\ \ power\ \ n_\ell)+(terms\ of\ tot.\ pow.\ n_\ell+1)+\cdots+(terms\ of\ tot.\ pow.\ n_h)}.$$

We now provide three, simple, $D = N = 2$, examples. For each example, 3D plots of the $IMSPE$ are provided in the following four ways:

(a) the exact $IMSPE$ of Eq. 4.1 plotted over the full prediction domain, $-1 \le (x_{m,1} + \Delta_1) \le 1$ and $-1 \le (x_{m,2} + \Delta_2) \le 1$, which we dub "the landscape;"

(b) the same as (a), but with Δ_k replaced with δ_k, and plots made over $-0.1 \le \delta_1 \le 0.1$ and $-0.1 \le \delta_2 \le 0.1$, which we dub "the local region;"

(c) $\left[\frac{2,2}{2,2}\right]_{IMSPE}(\delta_1,\delta_2)$; and

(d) $\left[\frac{2,4}{2,4}\right]_{IMSPE}(\delta_1,\delta_2)$.

The examples, except for the highly symmetric first one, show that the local regions are dominated by non-analytic, pole-free essential discontinuities at limit-zero-distance point separation (in this limit we can write alternatively "twin-point separation"), where the $IMSPE$ takes on multiple values dependent upon the direction of approach of the twins. In the second and third examples these multiple values lie on a vertical line, which we dub a "post." Because of this almost-always (a.a) multivaluedness, $IMSPE$ is properly considered as a.a. a "generalized function" [9]. Outside its local region, each $IMSPE$ connects smoothly with its corresponding landscape.

Maple [10] was used for making 3D plots and for symbolic algebra. Small gaps in the 3D plots are artifacts of the plotting and should be disregarded.

Greater detail and generalization, including connections with related Padé, Chisholm, and Canterbury approximants, shall be provided in Part IV of this series of papers.

8.1 $(x_{m,1}, x_{m,2}) = (0.0, 0.0)$

The center of the two points is the origin.

Landscape: A 3D $IMSPE$ landscape plot is shown as the left-hand plot of Fig. 8.1, below. The dominant feature is an origin-centered, dome-shaped, analytic, local maximum.

Local region: The $IMSPE$ is shown as the center-left plot of Fig. 8.1. $\left[\frac{2,2}{2,2}\right]_{IMSPE}(\delta_1,\delta_2) \cong \frac{5.96\delta_1^2+5.96\delta_2^2}{8(\delta_1^2+\delta_2^2)}$, which factors to the constant shown in the center-right plot; whereas $\left[\frac{2,4}{2,4}\right]_{IMSPE}(\delta_1,\delta_2) \cong \frac{(5.96\delta_1^2+5.96\delta_2^2)-(24.21\delta_1^4+48.79\delta_1^2\delta_2^2+24.22\delta_2^4)}{8(\delta_1^2+\delta_2^2-2\delta_1^4-4\delta_1^2\delta_2^2-2\delta_2^4)}$, which does not factor. The latter approximant is shown on the right-hand plot of Fig. 8.1. We expect successive, higher-order Nu approximants converge to the true local-region (center-left plot) $IMSPE$.

8.2 $(\boldsymbol{x_{m,1}}, \boldsymbol{x_{m,2}}) = (\mathbf{0.6}, \mathbf{0.0})$

The center of the two points lies on the abscissa but not on the ordinate. The dominant feature is an origin-centered, dome-shaped, non-analytic, pole-free, local maximum with a post. Mentions of plots are to those in Fig. 8.2, below. A portion of this example first appeared in [11].

Landscape: A 3D $IMSPE$ landscape plot is shown as the left-hand plot.

Local region: The $IMSPE$ is shown on the center-left, and its post, shown in the center plot, has height numerically computed to be ≅ 1.19% of the local-region maximum. $\left[\frac{2,2}{2,2}\right]_{IMSPE}(\delta_1, \delta_2) \cong \frac{7.7403\delta_1^2+7.6485\delta_2^2}{8\left(\delta_1^2+\delta_2^2\right)}$, is shown in the center-right plot, and its post height is $\lim_{\substack{\delta_1\to 0\\ \delta_2=0}} IMSPE_{2,2}(\delta_1, \delta_2) - \lim_{\substack{\delta_1=0\\ \delta_2\to 0}} IMSPE_{2,2}(\delta_1, \delta_2) \cong 1.19\%$ of the local-region maximum, notably matching the post height computed without expansion. $\left[\frac{2,4}{2,4}\right]_{IMSPE}(\delta_1, \delta_2) \cong \frac{\left(7.7403\delta_1^2+7.6485\delta_2^2\right)-\left(29.41\delta_1^4+57.61\delta_1^2\delta_2^2+28.19\delta_2^4\right)}{8\left(\delta_1^2+\delta_2^2-2\delta_1^4-4\delta_1^2\delta_2^2-2\delta_2^4\right)}$ is shown on the right-hand plot. Again, we expect that successive, higher-order Nu approximants converge to the true local-region (center-left plot) $IMSPE$.

8.3 $(\boldsymbol{x_{m,1}}, \boldsymbol{x_{m,2}}) = (\mathbf{0.6}, \mathbf{0.2})$

In this example, we have the following:

The center of the two points lies on neither the abscissa nor the ordinate.

Plots similar to those of Fig. 8.2 are given in Fig. 8.3, below.

Local region: $$\left[\frac{2,4}{2,4}\right]_{IMSPE}(\delta_1, \delta_2) \cong \frac{\left[\begin{array}{c}\left(7.9010\delta_1^2-0.0799\delta_1\delta_2+7.8346\delta_2^2\right)\\ -\left(29.7764\delta_1^4+0.8765\delta_1^3\delta_2+58.4490\delta_1^2\delta_2^2+0.9399\delta_1\delta_2^3+28.7110\delta_2^4\right)\end{array}\right]}{8\left(\delta_1^2+\delta_2^2-2\delta_1^4-4\delta_1^2\delta_2^2-2\delta_2^4\right)},$$

where the numerical values are truncated after four digits to the right of the decimal point.

The post height is ≅ 1.31% of the local full-scale $IMSPE$.

9. Summary

We have demonstrated that $|\boldsymbol{V}|$ and $|\boldsymbol{L}|$ are low-degree–truncated functions and that the $IMSPE$ objective function is almost always a low-degree–truncated, rational, generalized function.

10. Research reproducibility

We support the recommendations of ICERM's Workshop on Reproducibility in Computational and Experimental Mathematics Workshop [12]. All data and figure-generation files used in this research are available to responsible parties, upon request to selden_crary (at) yahoo (dot) com.

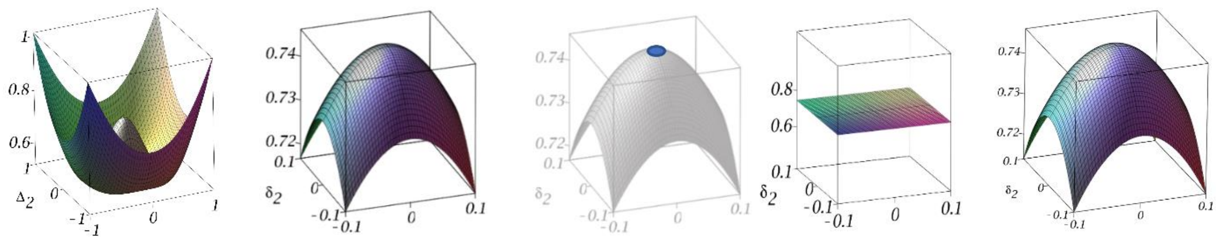

Fig. 8.1. $(x_{m,1}; x_{m,2}) = (0.0,0.0)$. The $IMSPE$ in the landscape (leftmost) and local region (left of center) show a dome-shaped, post-free local maximum. (center) The absent, or zero-height, post is represented as a circular blue disk. (right of center) The $\left[\frac{2,2}{2,2}\right]$ Nu approximant captures only the value of the maximum, while the $\left[\frac{2,4}{2,4}\right]$ Nu approximant (right) demonstrates incipient convergence to the local-region $IMSPE$.

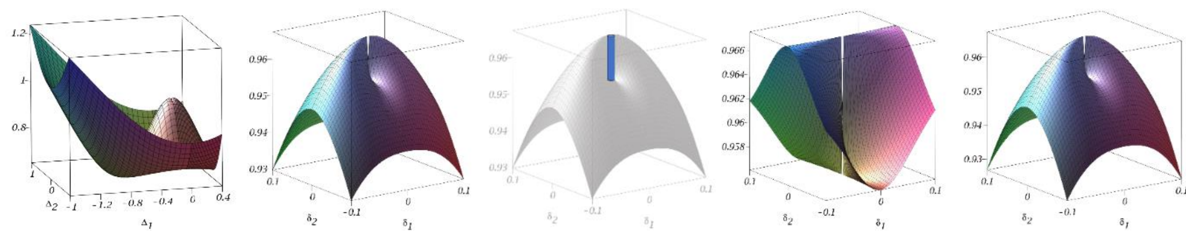

Fig. 8.2. $(x_{m,1}; x_{m,2}) = (0.6; 0.0)$. The $IMSPE$ in the landscape (leftmost) and local region (left of center) show a local maximum with an essential discontinuity including a post (center) represented as a blue cylinder with height $\approx$ 1.19% of the local-region $IMSPE$ maximum. (right of center) The $\left[\frac{2,2}{2,2}\right]$ Nu approximant captures the discontinuity and post height, while the $\left[\frac{2,4}{2,4}\right]$ Nu approximant (rightmost) demonstrates the incipient convergence.

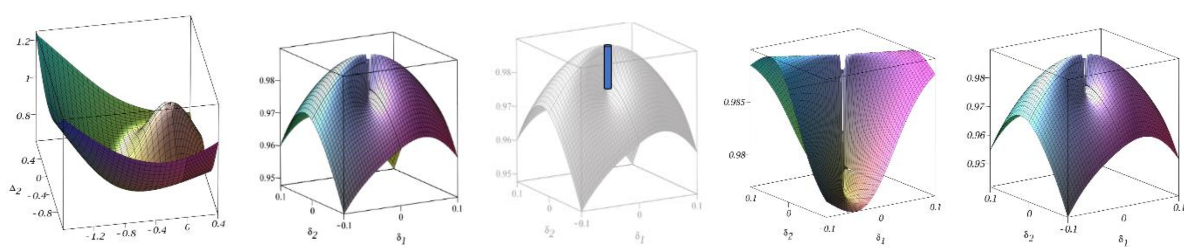

Fig. 8.3. $(x_{m,1}; x_{m,2}) = (0.6; 0.2)$. The $IMSPE$ in the landscape (leftmost) and local region (left of center) show an essential discontinuity with a post (center) represented as a blue cylinder with height $\approx$ 1.31% of the local-region $IMSPE$ maximum. (right-of-center) The $\left[\frac{2,2}{2,2}\right]$ Nu approximant captures the discontinuity and post height, while the $\left[\frac{2,4}{2,4}\right]$ Nu approximant (rightmost) demonstrates the incipient convergence.

11. Revision history

V2 corrections: Some coefficients in Sec. 8, some typos, and the rightmost 3D plot in Fig. 8.1.

References

1. Selden Crary, "The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. I. IMSPE in Design of Computer Experiments: Integrals and Very-Low-N, Single-Factor, Free-Ranging Designs," arXiv:1604.05278 [stat.ME] 18 Apr 2016.
2. Selden Crary, Tatiana Nizhegorodova, and Michael Saunders, "The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. Ia. "MINOS for IMSPE Evaluation and Optimal-IMSPE-Design Search," arXiv: 1704.06250 [stat.ME] 20 Apr 2017.
3. Selden Crary, Richard Diehl Martinez, Michael Saunders, "The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. Ib. "Integrals of Matérn-correlation functions for all odd–half-integer class parameters," arXiv: 1707.00705 [stat.ME] 3 Jul 2017.
4. Nikoloz Chkonia and Selden Crary, "The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. Ic. IMSPE-optimal designs with circular-disk prediction domains," arXiv:1709.09599 [stat.ME] 27 Sep 2017.
5. Selden Crary, Richard Diehl Martinez, Michael Saunders, Amin Mobasher, and Nikoloz Chkonia, The Nu Class of Low-Degree-Truncated, Rational, Generalized Functions. II. IMSPE in design of computer experiments: low-N, multifactor, free-ranging, optimal designs. Authorea. July 10, 2019. DOI: https://doi.org/10.22541/au.156277706.69664177.
6. Anthony J. Pettofezzo, Matrices and Transformations, Dover, New York, 1966.
7. Jerome Sacks, Susannah B. Schiller, and William J. Welch, "Designs for Computer Experiments," *Technometrics* **31** (1), pp. 41-47 (1989).
8. Selden Crary and Jan Stormann, "Four-Point, 2D, Free-Ranging, IMSPE-Optimal, Twin-Point Designs," arXiv:1510.01685 [stat.ME] 6 Oct 2015.
9. I. M. Gel'fand and G.E. Shilov, Generalized Functions, Vol. 1, Academic Press, New York, 1964.
10. Maple 2018 [Computer Software], Maplesoft Software, Waterloo, ON Canada.
11. Selden B. Crary and Rachel Johnson, "Validation of the Twin-Point-Design Concept in the Design of Computer Experiments," Section on Statistical Computing – JSM 2011, pp. 5495-5505.*
12. V. Stodden, D.H. Bailey, J. Borwein, R. J. LeVeque, and W. Stein, eds., "Setting the Default to Reproducible: Reproducibility in Computational and Experimental Mathematics," webpage of the Reproducibility in Computational and Experimental Mathematics Workshop, held Dec. 9-14, 2012 at the Institute for Computational and Experimental Research in Mathematics, Providence, RI, and available at https://www.carma.newcastle.edu.au/jon/icerm12.pdf.

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