Factorization of the Determinant of the Gaussian-Covariance Matrix of Evenly Spaced Points Using an Inter-dimensional Multiset Duality

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Abstract

We prove our earlier conjecture that the determinant of a Gaussian-covariance matrix $\boldsymbol{V}$ with elements $V_{i.j} = \sigma_z^2 e^{-\theta(i-j)^2\delta^2}$ $(\sigma_z, \theta \in \mathbb{R};\ \sigma_z, \theta > 0;\ i, j \in \mathbb{N}_{\geq 1};\ 1 \leq i, j \leq n)$, of evenly spaced points with nearest-neighbor distance $\delta > 0$, is $\sigma_z^2 C(n)\delta^{n(n-1)}$ + higher-degree terms in δ. We show that $C(n) = SF(n-1) \cdot (2\theta)^{n(n-1)/2}$, where SF is the superfactorial operator. The proof uses Neville elimination to determine all elements of the upper triangular matrix $\boldsymbol{U}$ of $\boldsymbol{V}$ and provides a factorization of $det(\boldsymbol{V})$. The proof makes use of an inter-dimensional multiset duality, which involves simplices that emerge during the factorization. We conjecture that $\boldsymbol{V}$ (for this evenly spaced case) is strictly totally positive.

Note with v2: After v1 appeared, Prof. Michael L. Stein of the Univ. of Chicago pointed us to a Y2000 paper by Wei-Liem Loh and Tao-Kai Lam [7] that had proved, using a different method, Part b of the Lemma presented here.

1 Motivation

We presented a conjecture, two years ago, that the determinant of the Gaussian-covariance matrix $\boldsymbol{V}$ with elements $V_{i.j} = \sigma_z^2 e^{-\theta(i-j)^2\delta^2}$ $(\sigma_z^2, \theta \in \mathbb{R};\ \sigma_z^2, \theta > 0;\ i, j \in \mathbb{N}_{\geq 1};\ 1 \leq i, j \leq n)$, of evenly spaced points with nearest-neighbor distance $\delta > 0$, is $C(n)\delta^{n(n-1)/2}$ + higher-degree terms in δ [1]. This paper provides a proof of this conjecture.

2 Outline

After a few simple definitions and two elementary algebraic identities, we prove six multiset identities, the ultimate of which relates the union of a pair of multisets, defined on the lattice points of an n-simplex, to the union of a corresponding pair of multisets defined on an $(n+1)$-simplex. This identity, which can be considered variously as a lifting transformation or a duality, is key to the proof of our earlier conjecture, which we state as a lemma. The proof proceeds via Neville elimination and provides a complete determination of the upper triangular matrix $\boldsymbol{U}$ of $\boldsymbol{V}$, as well as a complete factorization of $det(\boldsymbol{V})$. We end by conjecturing that the 1D Gaussian-covariance matrix of evenly spaced points, under the conditions used in this paper, is strictly totally positive [2].

3 Definitions and Algebraic Identities

Definitions:

$\mathbb{N}_{\geq 0}$ denotes the set of whole numbers $\{0,1,2,\cdots\}$.

$\mathbb{N}_{\geq 1}$ denotes the set of natural numbers $\{1,2,3,\cdots\}$.

$\mathbb{R}$ denotes the set of real numbers.

$\eta \equiv e^{-\theta\delta^2}$ $(\delta^2, \theta \in \mathbb{R};\ \delta^2, \theta > 0)$.

$h_q \equiv 1 - \eta^{2q}$ $(q \in \mathbb{N}_{\geq 1})$.

$SF(n) \equiv \prod_{k=1}^{n} k!$ $(n \in \mathbb{N}_{\geq 1})$ is the superfactorial operator [3].

Neville-elimination: Neville elimination is pivot-free Gaussian elimination of the nxn upper triangular matrix $\boldsymbol{U}$ in LU-decomposition and uses the following formula for the relevant Stage $s+1$, Row i, and Column j elements, in terms of elements at the immediately prior stage*:*

$U(s+1,i,j) = U(s,i,j) - \frac{U(s,i,s)U(s,s,j)}{U(s,s,s)}$ $(s,i,j \in \mathbb{N}_{\geq 1}, s \leq i, j \leq n)$ [4].

Algebraic identities:

AI1: $(i-n)^2 + (j-n)^2 = 2(i-n)(j-n) + (i-j)^2$ $(i,j,n \in \mathbb{N}_{\geq 1})$.

AI2: $h_{j-1} \sum_{k=0}^{i-2} \eta^{2k(j-1)} = 1 - \eta^{2(i-1)(j-1)}$ $(i,j \in \mathbb{N}_{\geq 1},\ i \geq 2,\ j \geq 1)$.

Proof: $h_{j-1} \sum_{k=0}^{i-2} \eta^{2k(j-1)} = \left[1 - \eta^{2(j-1)}\right]\left[1 + \eta^{2(j-1)} + \cdots + \eta^{2(i-2)(j-1)}\right]$

$= 1 - \eta^{2(i-1)(j-1)}$.

4 Notation for Simplicial Multisets

Consider an array of points from a 2x1 rectangular lattice aligned commensurately with the axes and vertices of a Manhattan-aligned 2-simplex of size 6x3, as show in Fig. 1, below. The multiset of L_1-norm distances from the simplex's lower-left vertex to each of the overlying lattice points is

$\{0,2,3,4,5,6,6,7,8,9\}$, or, written somewhat differently, $\left\{\begin{matrix} & & 0 & & \\ & 2 & & 3 & \\ 4 & & 5 & & 6 \\ 6 & 7 & & 8 & 9 \end{matrix}\right\}$. We are interested in generalizations of such multisets, as they will prove useful in the proof of the lemma.

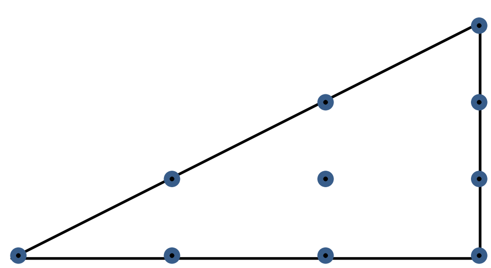

Figure 1: A simple example of a point lattice aligned commensurately with the axes and vertices of a simplex is a rectangular lattice of points aligned with a right-isosceles triangle.

We define the following notation for the multiset of L_1-norm distances, added to a possibly non-zero constant α, from an apex of an n-simplex to the points of a hyper-rectangular lattice aligned commensurately with the axes and vertices of the simplex, with $k, k', \cdots, k^{(n-1)'}$ being the geometric coordinates, where the notation $k^{(n-1)'}$ denotes the letter k appended with $n-1$ prime symbols. We note that all coordinates, save the first, enter on roughly equal footing, with each unit increase in any coordinate resulting in a unit increase in L_1-norm distances to which it is relevant, all other coordinates held fixed. By contrast, each unit increase of the first coordinate, viz. k, results in a β-unit increase in L_1-norm distances.

$$\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta} \equiv \left\{ \begin{matrix} \alpha + \beta k + k' + \cdots + k^{(n-1)'}: \\ k = (\gamma - 1), \cdots, (\delta - 1) \\ k' = \varepsilon[k - (\varepsilon - 1)], \cdots, k - \zeta \\ k'' = 0, \cdots, k' \\ \vdots \\ k^{(n-1)'} = 0, \cdots, k^{(n-2)'} \end{matrix} \right\} \left(\begin{matrix} \alpha, \beta \in \mathbb{N}_{\geq 0};\ n, \gamma, \delta \in \mathbb{N}_{\geq 1}; \\ \gamma \leq \delta;\ \varepsilon, \zeta \in \{0,1\};\ \varepsilon + \zeta = 1; \\ k^{(0)'} \text{ is undefined;} \\ k', \cdots, k^{(n-1)'} \text{ are undefined if not} \\ \text{present in the first} - \text{row list.} \\ \text{Undefined terms are to be neglected.} \end{matrix} \right).$$

Detail for cases with $n = 1, 2$ or 3*:* In the case $n = 1$, all k's with at least one prime symbol, which, reading from left to right as the number of prime symbols increases, are the elements $k', \cdots, k^{(0)'}$, are undefined. Thus, for this case, the first row of the curly bracket is to be read "$\alpha + \beta k$:," and the third and subsequent rows are to be neglected. When $n = 2$, the first row of the bracket is to be read "$\alpha + \beta k + k'$:," and the fourth and subsequent rows are to be neglected. When $n = 3$, the first row of the bracket is to be read "$\alpha + \beta k + k' + k''$:," and the ultimate row is to be neglected.

We note that if $\delta \neq 1$ or $\varepsilon + \zeta \neq 0$, the relevant lattice points for $\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta}$ do not overlie a simplex, but just a contiguous part of one.

The example shown in Fig. 1, above, is, by this definition, $\mathcal{S}_{2,0,2,1,4,0,0}$. Another simple example is $\mathcal{S}_{2,0,4,1,4,0,0} = \left\{ \begin{matrix} 0 \\ 4\ 5 \\ 8\ 9\ 10 \\ 12\ 13\ 14\ 15 \end{matrix} \right\}$, a multiset that will reappear in another example, a few pages below.

$\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta} \uplus \mathcal{S}_{\tilde{n},\tilde{\alpha},\tilde{\beta},\tilde{\gamma},\tilde{\delta},\tilde{\varepsilon},\tilde{\zeta}}$ is the multiset union of $\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta}$ and $\mathcal{S}_{\tilde{n},\tilde{\alpha},\tilde{\beta},\tilde{\gamma},\tilde{\delta},\tilde{\varepsilon},\tilde{\zeta}}$.

$(-1) \otimes \mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta}$ is the multiset $\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta}$, with each element multiplied by -1.

5 Simplex Multiset Identities

We now give six multiset identities (MI1 through MI6) relating $\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta}$ multisets. For identities MI3 through MI6, an example with $(n, \alpha, \beta, \gamma, \delta, \varepsilon, \zeta) = (2,0,4,1,4,0,0)$ is provided.

MI1: $\mathcal{S}_{n,\alpha,\beta,1,\delta,0,0} = \mathcal{S}_{n,\alpha,\beta,1,\delta-1,0,0} \uplus \mathcal{S}_{n,\alpha,\beta,\delta,\delta,0,0}$. (The RHS is the union of the two multisets resulting from slicing off the $k = \delta - 1$ face of the n-simplex on the LHS.)

Proof: By the definition of $\mathcal{S}_{n,\alpha,\beta,\gamma,\delta,0,0}$, the variable k ranges from 0 through $\delta - 1$. This multiset can be decomposed into the union of two mutually exclusive and exhaustive multisets, with different values of the fourth and fifth indices, and with all other indices unchanged. In the former of these constituent multisets, k ranges from 0 through $\delta - 2$, while, in the latter, $k = \delta - 1$. These two constituent multisets are $\mathcal{S}_{n,\alpha,\beta,1,\delta-1,0,0}$ and $\mathcal{S}_{n,\alpha,\beta,\delta,\delta,0,0}$, respectively. Three special cases that will be used later are the following:

MI1a: $\mathcal{S}_{n,0,\beta,1,\delta,0,0} = \mathcal{S}_{n,0,\beta,1,\delta-1,0,0} \uplus \mathcal{S}_{n,0,\beta,\delta,\delta,0,0}$.

MI1b: $\mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-1,0,0} = \mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-2,0,0} \uplus \mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0}$.

MI1c: $\mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta,0,0} = \mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta-1,0,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,\delta,\delta,0,0}$.

MI2: $\mathcal{S}_{n+1,0,\beta-1,1,\delta-1,0,0} = \mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-2,0,0} \uplus \mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0}$. (The RHS is the union of the two multisets resulting from slicing off the $k' = k$ face of the $(n+1)$-simplex on the LHS.)

Proof: By the definition of $\mathcal{S}_{n+1,0,\beta-1,1,\delta-1,0,0}$, the variable k' ranges from 0 through k. This multiset can be decomposed into the union of two exhaustive multisets, with different values of the sixth and seventh indices, and with all other indices unchanged. In the former of these constituent multisets, k' ranges from 0 through $k - 1$, while in the latter $k' = k$. These two constituent multisets are $\mathcal{S}_{n+1,0,\beta-1,1,\delta-1,0,1}$ and $\mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0}$, respectively. However, these two multisets are not mutually exclusive, as they share the 0 element. This element can be removed from the former of the constituent multisets, if that multiset is changed to $\mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-2,0,0}$.

MI3: $\mathcal{S}_{n,0,\beta,1,\delta-1,0,0} = \mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0}$.

In the $(n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta) = (2,0,4,1,4,0,0)$ example, the LHS and RHS of this identity are the

non-crossed-out parts of $\left\{\begin{array}{c} 0 \\ 4\ \ 5 \\ 8\ \ 9\ 10 \\ \cancel{12\ 13\ 14\ 15} \end{array}\right\}$ and $\left\{\begin{array}{r} 0 \\ \cancel{3}\ \ 4\ \ 5 \\ \cancel{6\ \ 7\ \ 8}\ \ 8\ \ 9\ 10 \end{array}\right\}$, respectively.

$$\textit{Proof: } \mathcal{S}_{n,0,\beta,1,\delta-1,0,0} = \left\{\begin{array}{c} \beta k + k' + \cdots + k^{(n-1)\prime}: \\ k\ = 0,\cdots,\delta-2 \\ k' = 0,\cdots,k \\ \vdots \\ k^{(n-1)\prime} = 0,\cdots,k^{(n-2)\prime} \end{array}\right\}.$$

$$\mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0} = \left\{\begin{matrix} (\beta-1)k + k' + \cdots + k^{n\prime}: \\ k\ = 0,\cdots,\delta-2 \\ k' = k,\cdots,k \\ k'' = 0,\cdots,k' \\ \vdots \\ k^{n\prime} = 0,\cdots,k^{(n-1)\prime} \end{matrix}\right\}$$

$$= \left\{\begin{matrix} (\beta-1)k + k + k'' + \cdots + k^{n\prime}: \\ k\ = 0,\cdots,\delta-2 \\ k'' = 0,\cdots,k \\ \vdots \\ k^{n\prime} = 0,\cdots,k^{(n-1)\prime} \end{matrix}\right\}$$

$$= \left\{\begin{matrix} \beta k + k'' + \cdots + k^{n\prime}: \\ k\ = 0,\cdots,\delta-2 \\ k'' = 0,\cdots,k \\ \vdots \\ k^{n\prime} = 0,\cdots,k^{(n-1)\prime} \end{matrix}\right\}.$$

Then, after a change of variables, in the last curly brackets, from $[k'',\cdots,k^{n\prime}]$ to $[k',k'',\cdots,k^{(n-1)\prime}]$,

$$\mathcal{S}_{n+1,\alpha,\beta-1,1,\delta-1,1,0} = \left\{\begin{matrix} \beta k + k' + \cdots + k^{(n-1)\prime}: \\ k\ = 0,\cdots,\delta-2 \\ k' = 0,\cdots,k \\ \vdots \\ k^{(n-1)\prime} = 0,\cdots,k^{(n-2)\prime} \end{matrix}\right\} = \mathcal{S}_{n,0,\beta,1,\delta-1,0,0}\,. \quad \square$$

MI4: $\mathcal{S}_{n,0,\beta,\delta,\delta,0,0} = \mathcal{S}_{n,(\beta-1)(\delta-1),1,\delta,\delta,0,0}$.

In the $(n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta) = (2,0,4,1,4,0,0)$ example, the LHS and RHS of this identity are the non-crossed-out parts of $\left\{\begin{matrix} \cancel{0} \\ \cancel{4\ \ 5} \\ \cancel{8\ \ 9\ 10} \\ 12\ 13\ 14\ 15 \end{matrix}\right\}$ and $\left\{\begin{matrix} \cancel{9} \\ \cancel{10\ 11} \\ \cancel{11\ 12\ 13} \\ 12\ 13\ 14\ 15 \end{matrix}\right\}$, respectively.

Proof: $\mathcal{S}_{n,0,\beta,\delta,\delta,0,0} = \left\{\begin{matrix} \beta k + k' + \cdots + k^{(n-1)\prime}: \\ k\ = (\delta-1),\cdots,(\delta-1) \\ k' = 0,\cdots,k \\ \vdots \\ k^{(n-1)\prime} = 0,\cdots,k^{(n-2)\prime} \end{matrix}\right\}$

$$= \left\{ \begin{matrix} \beta(\delta-1) + k' + \cdots + k^{(n-1)'}: \\ k' = 0, \cdots, (\delta-1) \\ \vdots \\ k^{(n-1)'} = 0, \cdots, k^{(n-2)'} \end{matrix} \right\}.$$

$$\mathcal{S}_{n,(\beta-1)(\delta-1),1,\delta,\delta,0,0} = \left\{ \begin{matrix} (\beta-1)(\delta-1) + k + k' + \cdots + k^{(n-1)'}: \\ k\ = (\delta-1), \cdots, (\delta-1) \\ k' = 0, \cdots, k \\ \vdots \\ k^{(n-1)'} = 0, \cdots, k^{(n-2)'} \end{matrix} \right\}$$

$$= \left\{ \begin{matrix} (\beta-1)(\delta-1) + (\delta-1) + k' + \cdots + k^{(n-1)'}: \\ k' = 0, \cdots, (\delta-1) \\ \vdots \\ k^{(n-1)'} = 0, \cdots, k^{(n-2)'} \end{matrix} \right\}.$$

$$= \left\{ \begin{matrix} \beta(\delta-1) + k' + \cdots + k^{(n-1)'}: \\ k' = 0, \cdots, \delta \\ \vdots \\ k^{(n-1)'} = 0, \cdots, k^{(n-2)'} \end{matrix} \right\} = \mathcal{S}_{n,0,\beta,\delta,\delta,0,0}\,. \quad \square$$

MI5: $\mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0} = \mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta-1,0,0}$.

In the $(n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta) = (2,0,4,1,4,0,0)$ example, the LHS and RHS of this identity are the non-crossed-out parts of $\left\{ \begin{matrix} \cancel{3} \\ \cancel{6\ 7\ 8} \\ 9\ 10\ 11\ 11\ 12\ 13 \end{matrix} \right\}$ and $\left\{ \begin{matrix} 9 \\ 10\ 11 \\ 11\ 12\ 13 \\ \cancel{12\ 13\ 14\ 15} \end{matrix} \right\}$, respectively.

Proof: $$\mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0} = \left\{ \begin{matrix} \beta - 1 + (\beta-1)k + k' + \cdots + k^{n'}: \\ k\ = \delta-2, \cdots, \delta-2 \\ k' = 0, \cdots, k \\ \vdots \\ k^{n'} = 0, \cdots, k^{(n-1)'} \end{matrix} \right\}$$

$$= \left\{ \begin{matrix} \beta - 1 + (\beta-1)(\delta-2) + k' + \cdots + k^{n'}: \\ k' = 0, \cdots, \delta-2 \\ \vdots \\ k^{n'} = 0, \cdots, k^{(n-1)'} \end{matrix} \right\}$$

$$= \left\{ \begin{matrix} (\beta-1)(\delta-1) + k' + \cdots + k^{n'}: \\ k' = 0, \cdots, \delta-2 \\ \vdots \\ k^{n'} = 0, \cdots, k^{(n-1)'} \end{matrix} \right\}$$

$$\mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta-1,0,0} = \left\{ \begin{matrix} (\beta-1)(\delta-1)+1\cdot k+k'+\cdots+k^{(n-1)'}: \\ k \ = 0,\cdots,\delta-2 \\ k' = 0,\cdots,k \\ \vdots \\ k^{(n-1)'} = 0,\cdots,k^{(n-2)'} \end{matrix} \right\}.$$

Then, after changing variables, in the ultimate curly brackets, from $\left[k,k',\cdots,k^{(n-1)'}\right]$ to $[k',k'',\cdots,k^{n'}]$,

$$\mathcal{S}_{n,\beta(\delta+1),1,1,\delta-1,0,0} = \left\{ \begin{matrix} (\beta-1)(\delta-1)+k'+\cdots+k^{n'}: \\ k' = 0,\cdots,\delta-2 \\ \vdots \\ k^{n'} = 0,\cdots,k^{(n-1)'} \end{matrix} \right\} = \mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0}\,. \quad \square$$

MI6: (inter-dimensional simplex duality):

$$\mathcal{S}_{n,0,\beta,1,\delta,0,0} \uplus \mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-1,0,0} = \mathcal{S}_{n+1,0,\beta-1,1,\delta-1,0,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta,0,0}$$

In the $(n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta) = (2,0,4,1,4,0,0)$ example, this equation is

$$\left\{ \begin{matrix} 0 \\ 4\ 5 \\ 8\ 9\ 10 \\ 12\ 13\ 14\ 15 \end{matrix} \right\} \uplus \left\{ \begin{matrix} 3 \\ 6\ 7\ 8 \\ 9\ 10\ 11\ 11\ 12\ 13 \end{matrix} \right\} = \left\{ \begin{matrix} 0 \\ 3\ 4\ 5 \\ 6\ 7\ 8\ 8\ 9\ 10 \end{matrix} \right\} \uplus \left\{ \begin{matrix} 9 \\ 10\ 11 \\ 11\ 12\ 13 \\ 12\ 13\ 14\ 15 \end{matrix} \right\}.$$

Proof: The four simplex multisets in the statement can be expanded, using MI1a, MI1b, MI2, and MI1c, respectively, and the statement can be rewritten as

$$\mathcal{S}_{n,0,\beta,1,\delta-1,0,0} \uplus \mathcal{S}_{n,0,\beta,\delta,\delta,0,0} \uplus \mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-2,0,0} \uplus \mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0}$$
$$= \mathcal{S}_{n+1,\beta-1,\beta-1,1,\delta-2,0,0} \uplus \mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta-1,0,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,\delta,\delta,0,0}\,. \quad (1)$$

In the $(n,\alpha,\beta,\gamma,\delta,\varepsilon,\zeta) = (2,0,4,1,4,0,0)$ example, the first four terms of each side of Eq. 1 are colored respectively red, orange, green, and blue, in the following:

$$\left\{ \begin{matrix} \color{red}{0} \\ \color{red}{4\ 5} \\ \color{red}{8\ 9\ 10} \\ \color{orange}{12\ 13\ 14\ 15} \end{matrix} \right\} \uplus \left\{ \begin{matrix} \color{green}{3} \\ \color{green}{6\ 7\ 8} \\ \color{blue}{9\ 10\ 11\ 11\ 12\ 13} \end{matrix} \right\} = \left\{ \begin{matrix} \color{red}{0} \\ \color{green}{3}\ \color{red}{4\ 5} \\ \color{green}{6\ 7\ 8}\ \color{red}{8\ 9\ 10} \end{matrix} \right\} \uplus \left\{ \begin{matrix} \color{blue}{9} \\ \color{blue}{10\ 11} \\ \color{blue}{11\ 12\ 13} \\ \color{orange}{12\ 13\ 14\ 15} \end{matrix} \right\}. \quad (2)$$

The third multiset of the LHS of Eq. 1 cancels with the first multiset of the RHS, so Eq. 1 can be rewritten as

$$\mathcal{S}_{n,0,\beta,1,\delta-1,0,0} \uplus \mathcal{S}_{n,0,\beta,\delta,\delta,0,0} \uplus \mathcal{S}_{n+1,\beta-1,\beta-1,\delta-1,\delta-1,0,0}$$
$$= \mathcal{S}_{n+1,0,\beta-1,1,\delta-1,1,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,1,\delta-1,0,0} \uplus \mathcal{S}_{n,(\beta-1)(\delta-1),1,\delta,\delta,0,0}\,.$$

In the example, this represents the cancellation of the green terms in Eq. 2.

Then, MI3, MI4, MI5 can be applied, in turn, to show that each multiset on the LHS has exactly one equal multiset on the RHS, and vice versa, as follows: the first multisets on the LHS and RHS (red, in the example) are equal, the second multiset on the LHS is equal to the ultimate multiset on the RHS (yellow, in the example), and the ultimate multiset on the LHS is equal to the second multiset on the RHS (blue, in the example). □

6 Lemma (Factorization of the Determinant of 1D Gaussian-Covariance Matrices)

a. At the end of s stages of Neville elimination, the elements of the upper triangular matrix $\boldsymbol{U}$*, for a Gaussian-covariance matrix* $\boldsymbol{V}$ *with elements* $V_{i,j} = \sigma_z^2 e^{-\theta(i-j)^2\delta^2}$ $(\sigma_z, \theta \in \mathbb{R};\ \sigma_z, \theta > 0;\ i, j \in \mathbb{N}_{\geq 1};\ 1 \leq i, j \leq n)$ *of n evenly spaced points with nearest-neighbor distance* $\delta > 0$*, are the following, where i and j are the integer row and column indices of* $\boldsymbol{U}$*, respectively:*

$\underline{Stage\ s}$	$\underline{Range\ of\ row\ i}$	$\underline{Range\ of\ col.\,j}$	$\underline{Element\ U(s,i,j)/\sigma_z^2}$
1	$1 \leq i \leq p$	$1 \leq j \leq p$	$\eta^{(i-j)^2}$
2	$1 \leq i \leq 1$	$1 \leq j \leq p$	*same as Stage 1*
	$2 \leq i \leq p$	$1 \leq j \leq 1$	0
		$2 \leq j \leq p$	$\eta^{(i-j)^2} h_{j-1} \sum_{k=0}^{i-2} \eta^{2[k(j-2)+k]}$
3	$1 \leq i \leq 2$	$1 \leq j \leq p$	*same as Stage 2*
	$3 \leq i \leq p$	$1 \leq j \leq 2$	0
		$3 \leq j \leq p$	$\eta^{(i-j)^2} h_{j-2} h_{j-1} \sum_{k=0}^{i-3} \sum_{k'=0}^{k} \eta^{2[k(j-3)+k+k']}$
⋮	⋮	⋮	⋮
s	$1 \leq i \leq s-1$	$1 \leq j \leq p$	*same as Stage s-1*
	$s \leq i \leq p$	$1 \leq j \leq s-1$	0
		$s \leq j \leq p$	$\eta^{(i-j)^2} \prod_{x=1}^{s-1} h_{j-x} \sum_{k=0}^{i-s} \sum_{k'=0}^{k} \cdots$
			$\cdots \sum_{k^{(s-2)\prime}}^{k^{(s-3)\prime}} \eta^{2[k(j-s)+k+k'+\cdots+k^{(s-2)\prime}]}.$

b. The determinant of $\boldsymbol{V}/\sigma_z^2$ *can be factored as* $det(\boldsymbol{V}/\sigma_z^2) = \prod_{s=2}^{n} \prod_{x=1}^{s-1} h_x$ *,which is positive.*

c. The lowest-degree term in the expansion of $det(\boldsymbol{V}/\sigma_z^2)$*, in powers of* δ*, is* $det(\boldsymbol{V}/\sigma_z^2) = SF(n-1) \cdot (2\theta)^{n(n-1)/2} \cdot \delta^{n(n-1)}$*, where* SF *is the superfactorial operator.*

Proof of Part a: The elements of $\boldsymbol{V}$ are $V_{i,j} \equiv \sigma_z^2 e^{-\theta(i-j)^2\delta^2} = \sigma_z^2 \eta^{(i-j)^2}$, where $\eta \equiv e^{-\theta\delta^2}$. Neville elimination is carried out in n stages, with the first stage just copying the elements of $\boldsymbol{V}$. Thus, at the end of Stage 1, $U(1,i,j)/\sigma_z^2 = \eta^{(i-j)^2}$, for $1 \leq i, j \leq n$, which is the result sought for this stage. For conciseness, and without loss of generality, we drop the factor σ_z^2 that is common to all elements, in most of the remainder of the proof of this part.

We proceed with a proof by induction. During Stage 2, the first row is unchanged, while the Neville-elimination formula is applied to all other elements. Thus, at the end of Stage 2, excluding the first row, the first column is zero, and the other elements are $U(2,i,j) = U(1,i,j) - \frac{U(1,i,1)}{U(1,1,1)} U(1,1,j) = \eta^{(i-j)^2} - \eta^{(i-1)^2+(j-1)^2}$. Applying AI1, with $n = 1$, gives $U(2,i,j) = \eta^{(i-j)^2}\left[1 - \eta^{2(i-1)(j-1)}\right]$. Next, applying AI2 gives $U(2,i,j) = \eta^{(i-j)^2} h_{j-1} \sum_{k=0}^{i-2} \eta^{2[k(j-2)+k]}$, which is the result sought for this stage.

To complete the proof, we show that if the statement is true for arbitrary Stage $w \geq 2$, then the statement is true for Stage $(w+1) \leq n$. For Stage w, the statement is

$$U(w,i,j) = \eta^{(i-j)^2} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-2)'}=0}^{k^{(w-3)'}} \eta^{2\left[k(j-w)+k+k'+\cdots+k^{(w-2)'}\right]} .$$

During Stage $(w+1)$, the first w rows and $w-1$ columns are unchanged, while the Neville-elimination formula $U(w+1,i,j) = U(w,i,j) - \frac{U(w,i,w)}{U(w,w,w)} U(w,w,j)$ is applied to all other elements, giving, after cancellations,

$$U(w+1,i,j) = \eta^{(i-j)^2} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-2)'}=0}^{k^{(w-3)'}} \eta^{2\left[k(j-w)+k+k'+\cdots+k^{(w-2)'}\right]}$$
$$-\eta^{(i-w)^2+(j-w)^2} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-2)'}=0}^{k^{(w-3)'}} \eta^{2\left[k+k'+\cdots+k^{(w-2)'}\right]}.$$

Collecting common factors, and applying AI1, with n in that identity being w here, the last equation becomes,

$$U(w+1,i,j) = \eta^{(i-j)^2} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-2)'}}^{k^{(w-3)'}} \begin{pmatrix} \eta^{2\left[k(j-w)+k+k'+\cdots+k^{(w-2)'}\right]} \\ -\eta^{2(i-w)(j-w)} \eta^{2\left[k+k'+\cdots+k^{(w-2)'}\right]} \end{pmatrix}$$
$$(w+1 \leq i,j \leq n). \quad (3)$$

Applying MI6, with $(w-1, i-w+1, j-w+1)$ here being (n,δ,β) in the identity, gives

$$\mathcal{S}_{w-1,0,j-w+1,1,i-w+1,0,0} \uplus \mathcal{S}_{w,j-w,j-w,1,i-w,0,0}$$
$$= \mathcal{S}_{w,0,j-w,1,i-w,0,0} \uplus \mathcal{S}_{w-1,(i-w)(j-w),1,1,i-w+1,0,0} ,$$

or, allowing for negative elements in the multisets [5], and after collecting the $(w-1)$-simplices and w-simplices on the LHS and RHS, respectively, we get the lifting transformation,

$$\mathcal{S}_{w-1,0,j-w+1,1,i-w+1,0,0} \uplus (-1) \otimes \mathcal{S}_{w-1,(i-w)(j-w),1,1,i-w+1,0,0}$$
$$= \mathcal{S}_{w,0,j-w,1,i-w,0,0} \uplus (-1) \otimes \mathcal{S}_{w,j-w,j-w,1,i-w,0,0} .$$

The LHS of the last equation is the set of exponents of η^2 in the sum of the two terms in the parenthesis in Eq. 3. Thus, Eq. 3 can be rewritten, using the RHS of the last equation,

$$U(w+1,i,j)$$
$$= \eta^{(i-j)^2} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w-1} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-1)'}}^{k^{(w-2)'}} \begin{pmatrix} \eta^{2\left[k(j-w-1)+k+k'+\cdots+k^{(w-1)'}\right]} \\ -\eta^{2(j-w)} \eta^{2\left[k(j-w-1)+k+k'+\cdots+k^{(w-1)'}\right]} \end{pmatrix}$$
$$= \eta^{(i-j)^2}\left[1-\eta^{2(j-w)}\right] \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w-1} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-1)'}}^{k^{(w-2)'}} \eta^{2\left[k(j-w-1)+k+k'+\cdots+k^{(w-1)'}\right]}$$

$$= \eta^{(i-j)^2} h_{j-w} \prod_{x=1}^{w-1} h_{j-x} \sum_{k=0}^{i-w-1} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-1)'}}^{k^{(w-2)'}} \eta^{2\left[k(j-w-1)+k+k'+\cdots+k^{(w-1)'}\right]}$$

$$= \eta^{(i-j)^2} \prod_{x=1}^{w} h_{j-x} \sum_{k=0}^{i-w-1} \sum_{k'=0}^{k} \cdots \sum_{k^{(w-1)'}}^{k^{(w-2)'}} \eta^{2\left[k(j-w-1)+k+k'+\cdots+k^{(w-1)'}\right]} .$$

$$(w + 1 \leq i, j \leq n)$$

Changing the name of the stage variable from $w + 1$ to s, and including the σ_z^2, which, for conciseness, was dropped earlier, gives

$U(s,i,j)/\sigma_z^2 = \eta^{(i-j)^2} \prod_{x=1}^{s-1} h_{j-x} \sum_{k=0}^{i-s} \sum_{k'=0}^{k} \cdots \sum_{k^{(s-2)'}}^{k^{(s-3)'}} \eta^{2\left[k(j-s)+k+k'+\cdots+k^{(s-2)'}\right]}$, which is the expression in the statement. □

Proof of Part b: The determinant of a real, $n \times n$ matrix with positive elements, as is the case at hand, is the product of the main-diagonal elements of its upper triangular matrix [6], i.e., $det(\boldsymbol{V}/\sigma_z^2) = \prod_{s=1}^{n} U(s,s,s)/\sigma_z^2$, where we have chosen to write the product in terms of the diagonal elements established at the end of each Neville-elimination stage. From the statement of Part a, $U(1,1,1)/\sigma_z^2 = 1$, and $U(s,s,s)/\sigma_z^2 = \prod_{x=1}^{s-1} h_{s-x}$ $(s \geq 2)$, so $det(\boldsymbol{V}/\sigma_z^2) = \prod_{s=2}^{n} \prod_{x=1}^{s-1} h_{s-x}$, which is positive because each h_x is positive. □

Proof of Part c: Substituting the polynomials h_x $(x \in \mathbb{N})$ into the statement of Part b, gives

$det(\boldsymbol{V}/\sigma_z^2) = \prod_{s=2}^{n} \prod_{x=1}^{s-1} \left[1 - \eta^{2(s-x)}\right]$.

By Definition 3, $\eta \equiv e^{-\theta\delta^2}$, so $1 - \eta^{2(s-x)} = 1 - e^{-2(s-x)\theta\delta^2}$, which, for sufficiently small δ, expands to $2(s-x)\theta\delta^2 + O(\theta^2\delta^4)$, giving,

$$\begin{aligned} det(\boldsymbol{V}/\sigma_z^2) &= \prod_{s=2}^{n} \prod_{x=1}^{s-1} [2(s-x)\theta\delta^2 + O(\theta^2\delta^4)] \\ &= \prod_{s=2}^{n} \{(s-1)!\,(2\theta\delta^2)^{s-1} + O[(\theta\delta^2)^s]\} \\ &= SF(n-1) \cdot (2\theta\delta^2)^{n(n-1)/2} + higher - degree\ terms\ in\ \delta, \end{aligned}$$

thus proving the conjecture in [1]. □

7 Interpretation

Part b of the lemma tells us that the determinant is given by a product of h functions, as follows. When there is just one point, i.e. $n = 1$, $Det(\boldsymbol{V}) = 1$. When a second point is added, $Det(\boldsymbol{V})$ increases by a factor h_1 that we can consider as due to the fact that we now have a pair of points. When a third evenly spaced point is added to the previous two, $Det(\boldsymbol{V})$) increases by a factor $h_1 h_2$. This can be interpreted as a factor h_1 due to the newly created, near-neighbor pair, as well as a factor h_2 due to the newly created, second-nearest-neighbor pair. This pairwise, multiplicative, particle-interaction interpretation holds nicely for any number of evenly spaced points.

Part c of the lemma tells us that the expansion of $Det(\boldsymbol{V})$, in powers of δ, commences with a term proportional to $\delta^{n(n-1)}$, i.e. a factor δ^2 for each of the $\binom{n}{2} = n(n-1)/2$ pairs of points. Because $Det(\boldsymbol{V})$ enters the denominator of each element of $\boldsymbol{V}^{-1}$, we can think of each pair of points in the design as contributing a factor δ^2 to the denominator of each element of $\boldsymbol{V}^{-1}$. Of course, the effect of the design also affects the numerator, so the situation is more complex than just naively considering only the denominator. This subject will be taken up in a more-detailed, follow-up report.

8 Conjecture

Based on our experience proving the lemma, as well as simple numerical experiments for $n \leq 8$, we conjecture that $\boldsymbol{V}$ for evenly spaced points is strictly totally positive, i.e., that all sub-matrices (not just the principal minors) of $\boldsymbol{V}$ are positive [2].

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