A Statistical Characterization of Regular Simplices

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1 INTRODUCTION.

Picture three points at the vertices of an equilateral triangle in two dimensions, or four points at the vertices of a regular tetrahedron in three dimensions. Thought of as scatterings of data they wouldn’t seem to reveal strong linear associations between the coordinates. There are no clear axes of elongation in the scatterplots, which would suggest that change in some variable is predictable as a function of the others. In general, such associations are usually indicated by the covariance matrix $S_u$ of the set of points $u = \{x_1, \ldots, x_n\}$ in $\mathbb{R}^p$, which is given by

$$S_u = \frac{1}{|u|} \sum_{x \in u} (x - \bar{x}_u)(x - \bar{x}_u)',$$

where

$$\bar{x}_u = \frac{1}{|u|} \sum_{x \in u} x.$$

The off-diagonal entries of $S_u$, the pairwise covariances, tell us something about dependencies. If the coordinate variables are independent these entries are zero. Though the converse is false, a diagonal covariance matrix roughly says that the coordinates are not mutually linearly predictable from each other. Indeed, for our equilateral triangle in $\mathbb{R}^2$, tetrahedron in $\mathbb{R}^3$, and the generalized configurations in higher dimensions having equal inter-point distances, the covariance matrix turns out to be diagonal. In fact, it’s a scalar multiple of the identity. Furthermore, the converse is also true: any configuration of $n = p + 1$ points in $p$ dimensions whose covariance matrix
is a positive multiple of the identity are equidistant from each other. We formalize this result in the following theorem:

**Theorem.** Let \( u = \{x_1, \ldots, x_n\} \) be a set of \( n \) points in \( \mathbb{R}^p \), with \( n = p + 1 \geq 2 \), and let \( \sigma^2 \) be an arbitrary positive number. Then the interpoint distances of \( u \) satisfy 
\[ ||x_i - x_j||^2 = 2\sigma^2\delta_{ij} \]
if and only if \( nS_u = \sigma^2 I_p \).

In other words, \( p + 1 \) points in \( p \) dimensions lie at the vertices of a regular simplex if and only if their covariance matrix is a multiple of the identity. A proof of this statistical characterization of regular simplices is given in section 2, after some preliminaries.

## 2 STATISTICAL CHARACTERIZATION OF REGULAR SIMPLICES.

The reader is assumed to be familiar with the basic elements of linear algebra in \( \mathbb{R}^p \) (linear subspaces, span, linear dependence and independence, basis and dimension), as treated, for example, in the text of Seber [1]. For a finite subset \( u \) of \( \mathbb{R}^p \) let \( V_u = \text{span}\{x - \bar{x}_u : x \in u\} \).

**Lemma.** With \( n > 1 \) let \( u \) be any collection of \( n \) points in \( \mathbb{R}^p \) with common squared interpoint distance \( 2\sigma^2 > 0 \). Then \( \dim(V_u) = n - 1 \), and with \( r_{\sigma,n}^2 = \sigma^2(n-1)/n \) and \( s_{\sigma,n}^2 = \sigma^2/(n(n-1)) \), the following are true for each \( x \) in \( u \):
\[ ||x - \bar{x}_u|| = r_{\sigma,n}, \quad ||\bar{x}_u - \bar{x}_{u-\{x\}}|| = s_{\sigma,n}, \quad x - \bar{x}_{u-\{x\}} \perp V_{u-\{x\}}. \]

**Proof.** We argue by induction. The three claims are easily verified if \( n = 2 \). When \( n > 2 \), for every \( x \) in \( u \) the points \( u - \{x\} \) are equidistant from \( x \), and by the induction hypotheses also equidistant from their average \( \bar{x}_{u-\{x\}} \), albeit at a smaller distance. Hence, the points of \( u - \{x\} \) lie on the intersection of two spheres with distinct centers, \( x \) and \( \bar{x}_{u-\{x\}} \), which implies that \( V_{u-\{x\}} \) is perpendicular to the direction vector of the line
\[ L_{u,x}(\alpha) = \bar{x}_{u-\{x\}} + \alpha (x - \bar{x}_{u-\{x\}}) \quad (\alpha \in \mathbb{R}) \]
passing through these centers and that the points of \( u - \{x\} \) are equidistant from each point of \( L_{u,x} \). In particular, all points of \( u - \{x\} \) are equidistant from \( L_{u,x}(1/n) = \bar{x}_u \), hence so are all points of \( u \). Because \( x - \bar{x}_{u-\{x\}} \perp V_{u-\{x\}} \) but \( x - \bar{x}_{u-\{x\}} \in V_u \), \( \dim (V_u) = \dim (V_{u-\{x\}}) + 1 \). By orthogonality \( \| \bar{x}_u - \bar{x}_{u-\{x\}} \|^2 = r_{\sigma,n}^2 - r_{\sigma,n-1}^2 \) and does not depend on \( x \). Using the fact that \( \bar{x}_{u-\{x\}}, \bar{x}_u, \) and \( x \) all lie on \( L_{u,x} \), in tandem with orthogonality gives \( 2\sigma^2 = r_{\sigma,n}^2 - 1 + (s_{\sigma,n} + r_{\sigma,n})^2 \); solving these two equations for \( r_{\sigma,n} \) and \( s_{\sigma,n} \) finishes the induction.

**Proof of the theorem.** Let \( X = (x_1, \ldots, x_n) \), an element of \( \mathbb{R}^{p \times n} \). Since \( S_{T(u)} = S_u \) for any translation \( T \), we can assume without loss of generality that the members of \( u \) have already been centered by subtraction of their mean, so \( \bar{x}_u = 0 \) and in general letting \( B_v := |v|S_v \) we have

\[
B_u = \sum_{x \in u} xx' = XX'.
\]

Assuming that the points are equidistant, we infer from (1) and the lemma that

\[
B_u x = \sum_{y \in u-\{x\}} yy'x + xx'x = (r_{\sigma,n}^2 - \sigma^2) \sum_{y \in u-\{x\}} y + r_{\sigma,n}^2 x
\]

for each \( x \) in \( u \). Hence \( B_u x = \sigma^2 I_p x \) on \( V_u \). Since \( \dim(V_u) = p \) by the lemma, \( B_u = \sigma^2 I_p \).

For the converse, assume that \( B_u = \sigma^2 I_p \). Note that the matrix

\[
A = \sigma^{-2}X'X \in \mathbb{R}^{n \times n}
\]

is symmetric, \( A' = A \), and idempotent, \( A^2 = \sigma^{-4}X'XX'X = \sigma^{-4}X'B_uX = A \). Hence \( A \) is an orthogonal projection, and therefore has rank equal to its trace,

\[
\text{rank}(A) = \text{tr}(A) = \sigma^{-2}\text{tr}(X'X) = \sigma^{-2}\text{tr}(XX') = \sigma^{-2}\text{tr}(B_u) = p,
\]

using the cyclic invariance of the trace. With \( 1_n \in \mathbb{R}^n \) the vector with all components equal to 1, \( A1_n = 0 \) by virtue of \( \bar{x}_u = 0 \). By the rank plus nullity theorem the null space of \( A \) has dimension one, and must therefore equal \( \text{span}(1_n) \), the span of \( 1_n \). Hence \( A = I_n - \frac{1}{n}1_n1_n' \), as this is the unique
orthogonal projection of rank $p$ with null space span($1_n$). As the entries of $A$ are $\sigma^{-2}$ times the inner products of the vectors in $u$, the squared interpoint distances between $x_i \neq x_j$ equals

$$||x_i - x_j||^2 = 2 (x_i'x_i - x_i'x_j) = 2\sigma^2 \left( \left( 1 - \frac{1}{n} \right) + \frac{1}{n} \right) = 2\sigma^2.$$ 

We remark that once the matrix $A$ is determined to have constant off-diagonal entries, the proof may also be completed by induction in the following more geometric way: Assume that $n > 2$, the base case being trivial. Any $p$ points in $\mathbb{R}^p$ lie in a hyperplane of dimension $p-1$, and for $x \in u$ let $\mathcal{H}$ denote the hyperplane which contains $u - \{x\}$, the space $\mathcal{V}_{u-\{x\}}$ translated by $\bar{x}_{u-\{x\}}$. The inner products $x'y$ for all $y \in u - \{x\}$, being the off-diagonal elements of $A$, are equal, and therefore, $x'y = x'\bar{x}_{u-\{x\}}$, so $x \bot y - \bar{x}_{u-\{x\}}$. Hence $x \bot \mathcal{V}_{u-\{x\}}$, and since $\bar{x}_{u-\{x\}} = -x/p$, we conclude $x - \bar{x}_{u-\{x\}} \bot \mathcal{V}_{u-\{x\}} = \mathcal{H} - \bar{x}_{u-\{x\}}$.

Now let $T$ be the translation $Ty = y - \bar{x}_{u-\{x\}}$, and, with $\{e_i\}_{1 \leq i \leq p}$ the standard basis, $O$ the rotation that maps $Tx$ to $\beta e_p$ where $\beta = ||x - \bar{x}_{u-\{x\}}||$. That is, $V(x) = \beta e_p$ for $V = OT$, and

$$B_{V(u-\{x\})} + \beta^2 e_p e'_p = O \left( B_{T(u-\{x\})} + Tx(Tx)' \right) O' \quad (2)$$

$$= O \left( B_{u-\{x\}} + Tx(Tx)' \right) O' = OB_{u}O' = \sigma^2 O I_p O' = \sigma^2 I_p.$$ 

Since $\mathcal{V}_{u-\{x\}} \bot x - \bar{x}_{u-\{x\}}$, $V(\mathcal{H}) \subset \mathbb{R}^{p-1} \times \{0\}$, and we can consider the points $V(u - \{x\})$ as lying in $\mathbb{R}^{p-1}$. By (2), the $(p-1) \times (p-1)$ submatrix $[B_{V(u-\{x\})}]_{1 \leq i,j \leq p-1}$ equals $\sigma^2 I_{p-1}$, so applying the induction hypotheses to $V(u - \{x\})$ we conclude that the interpoint distances of $u - \{x\}$, unchanged by $V$, are all $2\sigma^2$. The induction is completed by noting that this is true for each $x$ in $u$.

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References

[1] G. A. F. Seber and A. J. Lee Linear Regression Analysis, John Wiley, New York, 2003.
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