

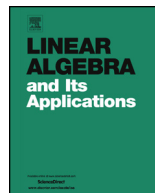


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Geometry of curves in $\mathbb{R}^n$ from the local singular value decomposition [☆]

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ABSTRACT

We establish a connection between the local singular value decomposition and the geometry of n -dimensional curves. In particular, we link the left singular vectors to the Frenet-Serret frame, and the generalized curvatures to the singular values. Specifically, let $\gamma : I \rightarrow \mathbb{R}^n$ be a parametric curve of class C^{n+1} , regular of order n . The Frenet-Serret apparatus of γ at $\gamma(t)$ consists of a frame $e_1(t), \dots, e_n(t)$ and generalized curvature values $\kappa_1(t), \dots, \kappa_{n-1}(t)$. Associated with each point of γ there are also local singular vectors $u_1(t), \dots, u_n(t)$ and local singular values $\sigma_1(t), \dots, \sigma_n(t)$. This local information is obtained by considering a limit, as ϵ goes to zero, of covariance matrices defined along γ within an ϵ -ball centered at $\gamma(t)$. We prove that for each $t \in I$, the Frenet-Serret frame and the local singular vectors agree at $\gamma(t)$ and that the values of the curvature functions at t can be expressed as a fixed multiple of a ratio of local singular values at t . To establish this result we prove a general formula for the recursion relation of a certain class of sequences of

[☆] This paper is dedicated to David Broomhead (1950-2014), a colleague and friend, who conceived many beautiful geometric applications of the singular value decomposition.

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Hankel determinants using the theory of monic orthogonal polynomials and moment sequences.

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1. Introduction

Principal component analysis is typically derived invoking a criterion from statistics, i.e., determine a k -dimensional subspace that captures the most statistical variance in a data set. Data analysts with a more geometric inclination view PCA as containing both statistical and geometric information. For example, it has been shown that local PCA provides information that can be used to determine the topological dimension of a manifold [1,2]. This paper, the first in a series, demonstrates how PCA, and the related singular value decomposition (SVD), rigorously characterizes the geometric information in n -dimensional curves. Here we focus on generalized curvatures and how data sampled from these curves can be used to reconstruct the curves using the SVD. In later work we will show that the philosophy of these ideas carry over to data sampled from hypersurfaces and manifolds [3–5].

We begin this presentation by briefly reviewing the relationship between Principal Component Analysis (PCA) and the Singular Value Decomposition; see also [6]. Recall that PCA is a tool derived in statistics for determining an optimal change of basis, i.e., each coordinate direction captures the maximum variance [7]. This basis inherits its ordering from the amount of variance captured. The first basis vector captures the maximum variance possible for a one-dimensional subspace, the second basis vector captures, in conjunction with the first, the maximum amount of variance possible for a two-dimensional subspace, and so on. The closely related singular value decomposition (SVD) captures the same information as PCA but has the theoretical starting point as the system of equations

$$\begin{aligned} Av &= \sigma u \\ A^T u &= \sigma v \end{aligned}$$

These equations have an associated matrix factorization

$$A = U\Sigma V^T$$

where the U matrix consists of the *left singular vectors*, and the $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$ are the non-zero singular values where A has rank r . These vectors U are also the solutions to

$$AA^T u = \lambda u$$

and hence we recognize them as the principal components. The eigenvalues of PCA and the singular values of the SVD are connected via

$$\lambda = \sigma^2$$

Although the information captured by the SVD and PCA is effectively the same, the numerical linear algebraic algorithms used for computing them are very different. Most importantly, the matrix AA^T is formed in the computation of PCA while this is not the case with SVD. The formation of either the outer product, or inner product, matrices may result in the loss of significant numerical precision. So, in practice it is generally better to compute the principal components in PCA using the SVD [8]. For this reason we choose to refer to the SVD, rather than PCA, although theoretically (but not numerically) we view these as interchangeable.¹

The shape of a curve in n -dimensional Euclidean space can be characterized mathematically in terms of its *generalized curvatures*. These are essentially the features defined at each point on the curve that encode its trajectory. The fundamental theorem of curves connects the shape of a curve to its curvatures. A curve is equivalent to its curvatures in the sense that each can be obtained from the other, at least up to rigid rotations and translations. In three dimensions the curvature κ and torsion τ are the curvatures. Well-known formulae for κ and τ exist which involve the computation of second and third derivatives, respectively. The geometric characterization of curves in $\mathbb{R}^n$ may be done via the formula for the generalized curvatures. A drawback to this approach is that the formula for the j th generalized curvature requires the estimation of the $j + 1$ derivative at each point on the curve. Thus it is of interest in the study of curves to develop additional analytical and computational tools for characterizing these generalized curvatures.

The Frenet-Serret frame is given by the application of the Gram-Schmidt orthogonalization procedure to the derivatives of the curve $\gamma(t) \in \mathbb{R}^n$ denoted by $\gamma^{(1)}(t), \dots, \gamma^{(n)}(t) \in \mathbb{R}^n$. Again, the fundamental theorem of curves holds and the shape of the curve in n dimensions is encoded by the $n - 1$ generalized curvatures denoted $\kappa_i(t)$. There are well-known exact expressions for the associated *generalized* curvature κ_i in terms of the $i + 1$ derivatives of the curve.

In this paper we show that given a curve $\gamma(t) \subset \mathbb{R}^n$ for any $n \in \mathbb{N}$ then the generalized curvatures may be expressed as

$$\kappa_{i-1}(t) = a_{i-1} \frac{\sigma_i(t)}{\sigma_1(t)\sigma_{i-1}(t)}$$

with

¹ Of course, we recognize that for some very large data problems, it is not even possible to load the data matrix A into computer memory while it is possible to compute one of AA^T , or $A^T A$. For these problems the principal components are determined using the algorithms for PCA.

$$a_{i-1} = \frac{i}{i + (-1)^i} \cdot \sqrt{\frac{4i^2 - 1}{3}}$$

for each i between 2 and n where the $\sigma_i(t)$ are the singular values. In addition, the left-singular vectors, i.e., the principal components of the curve, provide the Frenet-Serret frame. Our approach in this paper is theoretical, i.e., our primary purpose is to derive the result stated above. Issues related to approximation accuracy, and the impact of noise in data, are outside the scope of this paper and will be treated elsewhere.

This paper is organized as follows: in Section 2 we summarize the background material on generalized curvatures. In Section 3 we demonstrate the complications of computing curvatures for dimensions three to six using local approximations, an idea we pursue in Section 4 to demonstrate the central results of this paper. In Section 5 we illustrate the application of the results with a basic example and draw conclusions in Section 6. The Appendices contain the details of the proof of the main result including some interesting new lemmas concerning Hankel matrices required to establish the result.

2. Generalized curvatures

Consider an interval $I \subset \mathbb{R}$ and a vector valued function $\gamma : I \rightarrow \mathbb{R}^n$. If γ is k times differentiable, with continuous derivatives, then γ is said to be a parametric curve of class C^k . Let $\gamma^{(k)}$ denote the k th derivative of γ . If for each $t \in I$, the set of vectors $\{\gamma^{(1)}(t), \gamma^{(2)}(t), \dots, \gamma^{(r)}(t)\}$ are linearly independent in $\mathbb{R}^n$, then γ is said to be regular of order r . If $\|\gamma'(t)\| = 1$ for each $t \in I$ then γ is said to be parameterized by arc length.

Let $\gamma : I \rightarrow \mathbb{R}^n$ be a parametric curve of class C^{n+1} , regular of order n , parameterized by arc length. At any point $\gamma(t) \in \gamma(I)$, the Frenet-Serret frame is determined by applying the Gram-Schmidt process to the vectors $\gamma^{(1)}(t), \gamma^{(2)}(t), \dots, \gamma^{(n)}(t)$. Thus the Frenet-Serret frame at $\gamma(t)$ is the ordered sequence of orthonormal vectors $e_1(t), e_2(t), \dots, e_n(t)$, where

$$e_i(t) = \frac{\tilde{e}_i(t)}{\|\tilde{e}_i(t)\|} \quad \text{with} \quad \tilde{e}_i(t) = \gamma^{(i)}(t) - \sum_{k=1}^{i-1} \langle \gamma^{(i)}(t), e_k(t) \rangle e_k(t) \quad \text{for } 1 \leq i \leq n.$$

The generalized curvature functions of γ are defined by

$$\kappa_i(t) = \langle e'_i(t), e_{i+1}(t) \rangle \quad \text{for } 1 \leq i \leq n-1.$$

With this definition, $\kappa_i(t) > 0$ for all i . The frame functions $e_1(t), e_2(t), \dots, e_n(t)$ together with the generalized curvature functions $\kappa_1(t), \dots, \kappa_{n-1}(t)$ is called the Frenet-Serret apparatus of γ . The Frenet-Serret apparatus of a curve characterizes the curve up to translation and rotation.

By the definition of the $e_i(t)$, we have

$$e_i(t) \in \text{span}\{\gamma^{(1)}(t), \dots, \gamma^{(i)}(t)\} \quad \text{for } i = 1, \dots, n-1.$$

Thus,

$$e'_i(t) \in \text{span}\{\gamma^{(1)}(t), \dots, \gamma^{(i+1)}(t)\} = \text{span}\{e_1(t), \dots, e_{i+1}(t)\}.$$

As a consequence,

$$\langle e'_i(t), e_j(t) \rangle = 0 \quad \text{whenever } j \geq i + 2.$$

If we differentiate the expression $\langle e_i(t), e_i(t) \rangle = 1$ then we obtain

$$\langle e'_i(t), e_i(t) \rangle + \langle e_i(t), e'_i(t) \rangle = 0,$$

from which we can conclude that

$$\langle e'_i(t), e_i(t) \rangle = 0 \quad \text{for } 1 \leq i \leq n.$$

In a similar manner, if $i \neq j$ then we differentiate the expression $\langle e_i(t), e_j(t) \rangle = 0$ to obtain

$$\langle e'_i(t), e_j(t) \rangle + \langle e_i(t), e'_j(t) \rangle = 0,$$

from which we can conclude that

$$\langle e'_i(t), e_j(t) \rangle = -\langle e'_j(t), e_i(t) \rangle.$$

Let E denote the orthonormal matrix whose columns are $e_1(t), \dots, e_n(t)$. The above formulas show that $E^T E' = K$ with K a tridiagonal skew symmetric matrix. Since E is orthonormal (thus $EE^T = I$), we can multiply on the left by E to arrive at the expression $E' = EK$. Recalling that $\kappa_i(t) = \langle e'_i(t), e_{i+1}(t) \rangle$ we can express K as:

$$K = \begin{pmatrix} 0 & -\kappa_1(t) & 0 & 0 & 0 \\ \kappa_1(t) & 0 & -\kappa_2(t) & 0 & 0 \\ 0 & \kappa_2(t) & 0 & \ddots & 0 \\ 0 & 0 & \ddots & 0 & -\kappa_{n-1}(t) \\ 0 & 0 & 0 & \kappa_{n-1}(t) & 0 \end{pmatrix}$$

If the generalized curvature functions $\kappa_1(t), \dots, \kappa_{n-1}(t)$ in the matrix K are constant, then the solution to the differential equation, $E' = EK$, can be shown to be (up to translation and rotation) of the form

$$\gamma_e(t) = \begin{bmatrix} a_1 \cos(\alpha_1 t) \\ a_1 \sin(\alpha_1 t) \\ \vdots \\ a_k \cos(\alpha_k t) \\ a_k \sin(\alpha_k t) \end{bmatrix} \quad \text{or} \quad \gamma_o(t) = \begin{bmatrix} a_1 \cos(\alpha_1 t) \\ a_1 \sin(\alpha_1 t) \\ \vdots \\ a_k \cos(\alpha_k t) \\ a_k \sin(\alpha_k t) \\ bt \end{bmatrix} \quad (2.1)$$

with the first equation, $\gamma_e(t)$, covering the case when n is even with $k = n/2$ and the second equation covering the case when n is odd with $k = (n - 1)/2$ [9].

3. Local approximation

Consider a curve $\gamma(t)$ in $\mathbb{R}^n$. Recall that if $\gamma(t)$ is parameterized by arc length then $\gamma(t)$ is a solution to the differential equation $E' = EK$. We would like to understand the associated frame $e_1(t), \dots, e_n(t)$ and curvature functions $\kappa_1(t), \dots, \kappa_{n-1}(t)$ from a different point of view. Specifically, consider points on the curve within an ϵ -ball centered at a point $s_0 = \gamma(t_0)$. The tangent line at s_0 is approximated by taking the span of two points on $\gamma(t)$ in an ϵ -ball centered at s_0 while the *osculating* plane at s_0 is approximated by taking the span of three points on $\gamma(t)$ in an ϵ -ball centered at s_0 . However, points on the curve in a small ϵ -ball are nearly linear. The value of $\kappa_1(t_0)$ can be seen as a measure of the failure of the linearity of such points. In a similar manner, the value of the second curvature function, $\kappa_2(t_0)$ is a measure of the failure of planarity of points in an ϵ -ball on the curve. This point of view will be considered more closely in the next section through the local singular value decomposition. In order to make this connection, it is helpful to replace the curve with an idealized version which agrees, to high order, with the curve at $\gamma(t_0)$.

3.1. Local approximation of curves in $\mathbb{R}^3$ and $\mathbb{R}^4$

Consider a curve $\gamma(t)$ in $\mathbb{R}^3$. The helix of best fit to γ at $\gamma(t_0)$ is the solution to the differential equation $E' = EK_{t_0}$ where K_{t_0} denotes the curvature matrix K evaluated at t_0 . Thus the curvature functions for the helix will be constants $\kappa_1 = \kappa_1(t_0)$ and $\kappa_2 = \kappa_2(t_0)$. In $\mathbb{R}^3$, the general solution, $g(t)$, to the differential equation, $E' = EK_{t_0}$, has the form

$$g(t) = (a \cos(\alpha t), a \sin(\alpha t), bt) + \text{Constant}.$$

The helix of best fit to $\gamma(t)$ at $\gamma(t_0)$ is given by

$$h(t) = g(t) - g(t_0) + \gamma(t_0).$$

If $\|\gamma^{(1)}(t_0)\| = 1$ then we get the condition that

$$a^2\alpha^2 + b^2 = 1.$$

The relationship between the curvature functions of the helix and the parameters a, b, α is:

$$\begin{aligned}\kappa_1^2 &= a^2\alpha^4, \\ \kappa_2^2 &= b^2\alpha^2.\end{aligned}$$

In a similar manner, if we solve the differential equation $E' = EK_{t_0}$ for a curve $\gamma(t)$ in $\mathbb{R}^4$ then we obtain a toroidal curve of best fit at $\gamma(t_0)$ of the form

$$h(t) = g(t) - g(t_0) + \gamma(t_0),$$

where

$$g(t) = (a \cos(\alpha t), a \sin(\alpha t), b \cos(\beta t), b \sin(\beta t)) + Constant.$$

We can relate a, b, α, β to the curvature functions as

$$\begin{aligned}\kappa_1^2 &= a^2\alpha^4 + b^2\beta^4, \\ \kappa_1^2\kappa_2^2 &= a^2\alpha^6 + b^2\beta^6 - \kappa_1^4, \\ \kappa_1^2\kappa_2^2\kappa_3^2 &= a^2\alpha^8 + b^2\beta^8 - \kappa_1^2(\kappa_1^2 + \kappa_2^2)^2,\end{aligned}$$

where again we have assumed that the curve is parameterized by arc length so

$$a^2\alpha^2 + b^2\beta^2 = 1.$$

These equations are derived for $\kappa_1, \kappa_2, \kappa_3$ in [9]. Next we give the corresponding equations for curves in $\mathbb{R}^5$ and $\mathbb{R}^6$. The derivation is straightforward but tedious.

3.2. Curvature relations in $\mathbb{R}^5$ and $\mathbb{R}^6$

If we solve the differential equation $E' = EK_{t_0}$ for a curve $\gamma(t)$ in $\mathbb{R}^5$ then we obtain a curve of best fit at $\gamma(t_0)$ of the form

$$h(t) = g(t) - g(t_0) + \gamma(t_0),$$

where

$$g(t) = (a \cos(\alpha t), a \sin(\alpha t), b \cos(\beta t), b \sin(\beta t), ct) + Constant.$$

We can relate a, b, c, α, β to the curvature functions as

$$\begin{aligned}
1 &= a^2\alpha^2 + b^2\beta^2 + c^2 \\
\kappa_1^2 &= a^2\alpha^4 + b^2\beta^4 \\
\kappa_1^2\kappa_2^2 &= a^2\alpha^6 + b^2\beta^6 - \kappa_1^4 \\
\kappa_1^2\kappa_2^2\kappa_3^2 &= a^2\alpha^8 + b^2\beta^8 - \kappa_1^2(\kappa_1^2 + \kappa_2^2)^2 \\
\kappa_1^2\kappa_2^2\kappa_3^2\kappa_4^2 &= a^2\alpha^{10} + b^2\beta^{10} - \kappa_1^2((\kappa_1^2 + \kappa_2^2 + \kappa_3^2)(\kappa_2^2 + \kappa_3^2) + \kappa_2^2\kappa_3^4).
\end{aligned}$$

In $\mathbb{R}^6$ the curve of best fit has

$$g(t) = (a \cos(\alpha t), a \sin(\alpha t), b \cos(\beta t), b \sin(\beta t), c \cos(\delta t), c \sin(\delta t)) + Constant.$$

Letting $G_k = a^2\alpha^k + b^2\beta^k + c^2\delta^k$, we can relate $a, b, c, \alpha, \beta, \delta$ to the curvature functions as

$$\begin{aligned}
1 &= G_2 \\
\kappa_1^2 &= G_4 \\
\kappa_1^2\kappa_2^2 &= G_6 - \kappa_1^4 \\
\kappa_1^2\kappa_2^2\kappa_3^2 &= G_8 - \kappa_1^2(\kappa_1^2 + \kappa_2^2)^2 \\
\kappa_1^2\kappa_2^2\kappa_3^2\kappa_4^2 &= G_{10} - \kappa_1^2((\kappa_1^2 + \kappa_2^2 + \kappa_3^2)(\kappa_2^2 + \kappa_3^2) + \kappa_2^2\kappa_3^4) \\
\kappa_1^2\kappa_2^2\kappa_3^2\kappa_4^2\kappa_5^2 &= G_{12} - G_{10}(\kappa_1^2 + \kappa_2^2 + \kappa_3^2 + \kappa_4^2) + F_8(\kappa_1^2\kappa_3^2 + \kappa_4^2\kappa_1^2 + \kappa_4^2\kappa_2^2).
\end{aligned}$$

4. The local singular value decomposition

Broomhead et al. showed that the *local* singular value decomposition could be used to compute the topological dimension of a manifold from sampled points lying on the manifold [2]. This provided a powerful tool for many applications that involved modeling data on manifolds. The original setting of [2] concerned the reconstruction of a manifold, via Takens' theorem, from scalar valued time series statistics of a dynamical system on the manifold. The local singular value decomposition is also useful for applying manifold learning algorithms for geometric data analysis, e.g., local models such as charts [10], or global models based on Whitney's embedding theorem [11]. A more detailed discussion may be found in [6,12].

Recall that at each point $\gamma(t) \in \gamma(I)$, the Frenet-Serret frame is determined by applying the Gram-Schmidt orthogonalization process to the set of vectors $\gamma^{(1)}(t), \gamma^{(2)}(t), \dots, \gamma^{(n)}(t)$ (where $\gamma^{(k)}(t)$ denotes the k th derivative of γ evaluated at t). We denote this ordered orthonormal basis $e_1(t), \dots, e_n(t)$ and let E denote the orthonormal matrix whose columns are the $e_i(t)$. The main intuition behind a local singular value analysis (and related PCA) is to exploit the idea that the Frenet-Serret frame may be viewed as finding the subspace of best fit at a point on the curve. We consider the canonical solution of the Frenet-Serret formula where κ_i is assumed to be constant, i.e., the solutions to $E' = EK$ given by Equation (2.1) where K is constant. We use an integral formulation of the principal component analysis, often referred to as the Karhunen-Loève transformation, at a given point on the curve. We then use a Taylor series approximation for $\gamma(t)$ to determine particular eigenvalues of the Karhunen-Loève transformation

in the ϵ -ball. These relationships can be combined with the relationships between the curvature constants and the curve parameters to determine a formula for computing κ_i locally from the eigenvalues of the Karhunen-Loève transformation, or, equivalently, the singular values squared of the local SVD.

4.1. Formulation

Following [1,2], the *mean centered* covariance matrix of $\gamma(t)$ at t is the matrix

$$\overline{C}_\epsilon(t) = \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} (\gamma(s) - \overline{\gamma}_\epsilon(t))(\gamma(s) - \overline{\gamma}_\epsilon(t))^T ds$$

where

$$\overline{\gamma}_\epsilon(t) = \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} \gamma(s) ds.$$

However, we will consider the closely related *on the curve* covariance matrix

$$C_\epsilon(t) = \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} (\gamma(s) - \gamma(t))(\gamma(s) - \gamma(t))^T ds. \quad (4.1)$$

By the eigenvalue decomposition, we have a factorization

$$C_\epsilon(t) = U_\epsilon(t) \Sigma_\epsilon(t) U_\epsilon^T(t)$$

where we assume that the diagonal elements in $\Sigma_\epsilon(t)$ are in monotone decreasing order. The columns of $U_\epsilon(t)$ are the eigenvectors of $C_\epsilon(t)$. Let $U(t) = \lim_{\epsilon \rightarrow 0} U_\epsilon(t)$. The columns of $U(t)$, written $u_1(t), \dots, u_n(t)$, are also the local left singular vectors at $\gamma(t)$. In a similar manner, one can define the local singular vectors $\overline{u}_1(t), \dots, \overline{u}_n(t)$ at $\gamma(t)$ by considering the limiting behavior of the singular vectors in the singular value decomposition of $\overline{C}_\epsilon(t)$ as ϵ tends towards zero.

Theorem 4.1. *Let $\gamma : I \rightarrow \mathbb{R}^n$ be a parametric curve of class C^{n+1} , regular of order n . Let $e_1(t), \dots, e_n(t)$ denote the Frenet-Serret frame at $\gamma(t)$. Let $u_1(t), \dots, u_n(t)$ denote the local left singular vectors at $\gamma(t)$. Then for $i = 1, \dots, n$, $e_i(t) = \pm u_i(t)$.*

Proof. Let $\Gamma(t)$ denote the matrix whose columns are $\gamma^{(1)}(t), \dots, \gamma^{(n)}(t)$. The Frenet-Serret frame, $e_1(t), \dots, e_n(t)$, is obtained by applying the Gram-Schmidt process to the columns of $\Gamma(t)$. Thus $e_i(t)$ is a unit vector orthogonal to the span of $\gamma^{(1)}(t), \dots, \gamma^{(i-1)}(t)$ but lying within the span of $\gamma^{(1)}(t), \dots, \gamma^{(i)}(t)$. Let $\mathbf{v}$ be the $n \times 1$ vector whose k th component is $(s-t)^k/k!$. Then $\Gamma(t)\mathbf{v}$ is the n th order Taylor series expansion for $\gamma(s) - \gamma(t)$

at t . Replacing $\gamma(s) - \gamma(t)$ with its Taylor series expansion leads to the n th order approximation

$$C_\epsilon(t) = \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} (\gamma(s) - \gamma(t))(\gamma(s) - \gamma(t))^T ds \approx \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} (\Gamma(t)\mathbf{v})(\Gamma(t)\mathbf{v})^T ds.$$

We rewrite this as

$$\Gamma(t) \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} \mathbf{v}\mathbf{v}^T ds \Gamma(t)^T = \Gamma(t) \mathcal{E} \Gamma(t)^T.$$

By the definition of $\mathcal{E}$, we compute that

$$\mathcal{E}_{i,j} = \frac{\epsilon^{i+j}}{i!j!(i+j+1)} \quad \text{if } i+j \text{ is even} \quad \text{and} \quad \mathcal{E}_{i,j} = 0 \quad \text{if } i+j \text{ is odd}.$$

We can express $\Gamma(t) \mathcal{E} \Gamma(t)^T$ in terms of the columns of $\Gamma(t)$ and the entries of $\mathcal{E}$ as

$$\frac{\epsilon^2}{3}(c_1 c_1^T) + \frac{\epsilon^4}{5}\left(\frac{1}{6}c_1 c_3^T + \frac{1}{4}c_2 c_2^T + \frac{1}{6}c_3 c_1^T\right) + \cdots + \frac{\epsilon^{2k}}{2k+1} \sum_{i=1}^{2k-1} \frac{1}{i!(2k-i)!} c_i c_{2k-i}^T + \cdots$$

where $c_i = \gamma^{(i)}(t)$. As ϵ tends towards zero, this expression behaves more and more like the rank one matrix $\frac{\epsilon^2}{3}c_1 c_1^T$. Noting that $c_1 = \gamma^{(1)}(t)$, thus is a multiple of $e_1(t)$, we get $u_1(t) = \pm e_1(t)$. Let $P_1 = I - e_1(t)e_1(t)^T$. Pre and post multiplying $\Gamma(t) \mathcal{E} \Gamma(t)^T$ with P_1 deflates away all terms involving c_1 . More precisely,

$$P_1 \Gamma(t) \mathcal{E} \Gamma(t)^T P_1 = \frac{\epsilon^4}{5}\left(\frac{1}{4}P_1 c_2 c_2^T P_1\right) + \cdots + \frac{\epsilon^{2k}}{2k+1} \sum_{i=2}^{2k-2} \frac{1}{i!(2k-i)!} P_1 c_i c_{2k-i}^T P_1 + \cdots$$

As ϵ tends towards zero, this deflated matrix behaves more and more like the rank one matrix $\frac{\epsilon^4}{5}\left(\frac{1}{4}P_1 c_2 c_2^T P_1\right)$. Noting that $P_1 c_2 = P_1 \gamma^{(2)}(t)$, we see that $P_1 c_2$ is orthogonal to $\gamma^{(1)}(t)$ and is in the span of $\gamma^{(1)}(t), \gamma^{(2)}(t)$ thus is a multiple of $e_2(t)$. This leads to $u_2(t) = \pm e_2(t)$. We now pre and post multiply $P_1 \Gamma(t) \mathcal{E} \Gamma(t)^T P_1$ with $P_2 = I - e_2(t)e_2(t)^T$. Note that since $e_1(t)$ is orthogonal to $e_2(t)$, we have $P_2 P_1 = I - e_1(t)e_1(t)^T - e_2(t)e_2(t)^T$. As ϵ tends towards zero, this doubly deflated matrix behaves more and more like the rank one matrix $\frac{\epsilon^6}{7}\left(\frac{1}{36}P_2 P_1 c_3 c_3^T P_1 P_2\right)$. Noting that $P_2 P_1 c_3 = P_2 P_1 \gamma^{(3)}(t)$, we see that $P_2 P_1 c_3$ is orthogonal to the span of $\gamma^{(1)}(t), \gamma^{(2)}(t)$ but in the span of $\gamma^{(1)}(t), \gamma^{(2)}(t), \gamma^{(3)}(t)$ thus is a multiple of $e_3(t)$. This leads to $u_3(t) = \pm e_3(t)$. Continuing to deflate away previously found singular vectors, we obtain the relationship $e_i(t) = \pm u_i(t)$ for all i . Note that for this to work, $\mathcal{E}_{i,i}$ must be non-zero and $P_i P_{i-1} \cdots P_1 \gamma^{(i+1)}(t)$ must be non-zero for each i . These conditions are satisfied since $\mathcal{E}_{i,i} = \frac{\epsilon^{2i}}{(2i+1)i!i!}$ and γ is regular of order n thus $\gamma^{(1)}(t), \dots, \gamma^{(n)}(t)$ are linearly independent. $\square$

The previous theorem considered the relationship between the local singular vectors of a curve and the Frenet-Serret frame of a curve. We now consider the relationship between the local singular values of a curve and values of the curvature functions. More precisely, in the eigenvalue decomposition

$$C_\epsilon(t) = U_\epsilon(t)\Lambda_\epsilon(t)U_\epsilon^T(t)$$

we considered the limiting behavior of $U_\epsilon(t)$, as ϵ tends towards zero, in order to obtain the local principal components, or equivalent, the left singular vectors of the data matrix. We now consider the limiting behavior of $\Lambda_\epsilon(t)$ as ϵ tends towards zero. Note that the entries of $\Lambda_\epsilon(t)$ tend towards zero as ϵ tends towards zero. Let $\lambda_{i,\epsilon}(t)$ denote the i th diagonal entry of $\Lambda_\epsilon(t)$. We show that for some constant c_i , we can write

$$\lambda_{i,\epsilon}(t) = c_i\epsilon^{2i} + O(\epsilon^{2i+2}).$$

The local singular values of $\gamma(t)$ are then defined as $\sigma_i(t) = \sqrt{c_i}\epsilon^i$.

In Section 2, we have explicitly expressed the curvature, for curves with constant curvature functions, in terms of the parameters of the curves. We now express the leading terms of the eigenvalues $\lambda_{i,\epsilon}(t)$ in terms of the parameters of the curves. This allows us to derive a relationship of the form

$$\kappa_i^2(t) = a_i \lim_{\epsilon \rightarrow 0} \frac{\lambda_{i+1,\epsilon}(t)}{\lambda_{1,\epsilon}(t)\lambda_{i,\epsilon}(t)}, \quad (4.2)$$

where a_i is a constant with known value. From this we obtain

$$\kappa_i(t) = \sqrt{a_i} \frac{\sigma_{i+1}(t)}{\sigma_1(t)\sigma_i(t)}.$$

4.2. Two dimensions

Consider a two dimensional curve with constant curvature $\kappa_1 = 1/a$. This will be a circle of radius a . Up to translation and rotation, its parameterized form is $\gamma(s) = (a \cos(\alpha s), a \sin(\alpha s))$. If we assume that the circle is parameterized by arc length then we obtain the constraint $a^2\alpha^2 = 1$. The components of the covariance matrix $C_\epsilon(0)$ are:

$$C_{11} = \frac{1}{2\epsilon} \int_{-\epsilon}^{\epsilon} (a \cos(\alpha s) - a)^2 ds,$$

$$C_{22} = \frac{1}{2\epsilon} \int_{-\epsilon}^{\epsilon} a^2 \sin^2(\alpha s) ds,$$

with

$$C_{12} = C_{21} = \frac{1}{2\epsilon} \int_{-\epsilon}^{\epsilon} (a \cos(\alpha s) - a) \sin(s) ds = 0$$

since the integrand is an odd function.

We follow the usual convention of ordering the eigenvalues by decreasing magnitude so

$$\begin{aligned}\lambda_{1,\epsilon}(0) &= \frac{1}{3}a^2\alpha^2\epsilon^2 + O(\epsilon^4), \\ \lambda_{2,\epsilon}(0) &= \frac{1}{20}a^2\alpha^4\epsilon^4 + O(\epsilon^6), \\ \lim_{\epsilon \rightarrow 0} \frac{\lambda_{2,\epsilon}(0)}{\lambda_{1,\epsilon}^2(0)} &= \frac{9}{20a^2}.\end{aligned}$$

Given that the curvature $\kappa_1 = 1/a$, we obtain the following expression for κ_1 in terms of the local singular values of the circle:

$$\kappa_1 = \sqrt{\frac{20}{9} \frac{\sigma_2}{\sigma_1^2}} = \frac{\sqrt{20}}{3} \frac{\sigma_2}{\sigma_1^2}.$$

4.3. Three and four dimensions

Here we consider curves in $\mathbb{R}^3$ with constant κ_1, κ_2 . Up to translation and rotation, such a curve will have the form

$$\gamma(s) = (a \cos(\alpha s), a \sin(\alpha s), bs).$$

Assuming the curve is parameterized by arc length we have $a^2\alpha^2 + b^2 = 1$. The covariance matrix, $C_\epsilon(t)$, is a 3×3 matrix with eigenvalues

$$\begin{aligned}\lambda_1 &= \frac{1}{3}\epsilon^2 + O(\epsilon^4) \\ \lambda_2 &= \frac{1}{20}a^2\alpha^4\epsilon^4 + O(\epsilon^6) \\ \lambda_3 &= \frac{1}{1575}a^2\alpha^6b^2\epsilon^6 + O(\epsilon^8)\end{aligned}$$

Recalling from Section 2 the equations for κ_1, κ_2 in terms of the parameters a, α, b , we obtain

$$\kappa_1^2 = \frac{20}{9} \lim_{\epsilon \rightarrow 0} \frac{\lambda_{2,\epsilon}(t)}{\lambda_{1,\epsilon}^2(t)}, \quad \kappa_2^2 = \frac{105}{4} \lim_{\epsilon \rightarrow 0} \frac{\lambda_{3,\epsilon}(t)}{\lambda_{1,\epsilon}(t)\lambda_{2,\epsilon}(t)}.$$

This leads to the expression of κ_1, κ_2 in terms of the singular values as:

$$\kappa_1 = \frac{\sqrt{20}}{3} \frac{\sigma_2}{\sigma_1^2} \quad \text{and} \quad \kappa_2 = \frac{\sqrt{105}}{2} \frac{\sigma_3}{\sigma_1 \sigma_2}.$$

Similarly for curves in $\mathbb{R}^4$, using elimination theory we establish the following representations of the κ_i in terms of the local singular values:

$$\kappa_1 = \frac{\sqrt{20}}{3} \frac{\sigma_2}{\sigma_1^2}, \quad \kappa_2 = \frac{\sqrt{105}}{2} \frac{\sigma_3}{\sigma_1 \sigma_2}, \quad \kappa_3 = \frac{\sqrt{336}}{5} \frac{\sigma_4}{\sigma_1 \sigma_3}.$$

4.4. Higher dimensions

Given that many of the entries of $C_\epsilon(0)$ are odd functions, the covariance matrix has a special structure with many zero entries. For instance, the structure of the covariance matrix for $n = 6$ is

$$\begin{bmatrix} C_{11} & 0 & C_{13} & 0 & C_{15} & 0 \\ 0 & C_{22} & 0 & C_{24} & 0 & C_{26} \\ C_{31} & 0 & C_{33} & 0 & C_{35} & 0 \\ 0 & C_{42} & 0 & C_{44} & 0 & C_{46} \\ C_{51} & 0 & C_{53} & 0 & C_{55} & 0 \\ 0 & C_{62} & 0 & C_{64} & 0 & C_{66} \end{bmatrix}$$

We can permute the columns and rows of this matrix an even number of times to obtain the block matrix

$$\begin{bmatrix} C_{11} & C_{13} & C_{15} & 0 & 0 & 0 \\ C_{31} & C_{33} & C_{35} & 0 & 0 & 0 \\ C_{51} & C_{53} & C_{55} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{22} & C_{24} & C_{26} \\ 0 & 0 & 0 & C_{24} & C_{44} & C_{46} \\ 0 & 0 & 0 & C_{26} & C_{46} & C_{66} \end{bmatrix}$$

Thus we observe the more computationally efficient approach to computing the eigenvalues by computing the eigenvalues of the block submatrices.

For curves in $\mathbb{R}^5$ we obtain:

$$\kappa_1 = \frac{\sqrt{20}}{3} \frac{\sigma_2}{\sigma_1^2}, \quad \kappa_2 = \frac{\sqrt{105}}{2} \frac{\sigma_3}{\sigma_1 \sigma_2}, \quad \kappa_3 = \frac{\sqrt{336}}{5} \frac{\sigma_4}{\sigma_1 \sigma_3}, \quad \kappa_4 = \frac{\sqrt{825}}{4} \frac{\sigma_5}{\sigma_1 \sigma_4}. \quad (4.3)$$

And for curves in $\mathbb{R}^6$ the same expressions for $\kappa_1, \kappa_2, \kappa_3, \kappa_4$ hold plus the additional relationship

$$\kappa_5 = \frac{\sqrt{1716}}{7} \frac{\sigma_6}{\sigma_1 \sigma_5}. \quad (4.4)$$

Throughout this section, we have assumed the curve to be parameterized with respect to arc length. The local computations can still be made without this assumption. What would change in the formulas in the previous section is that we would replace the assumption that $\|\gamma^{(1)}(t_0)\| = 1$ with $\|\gamma^{(1)}(t_0)\| = r$. We obtain the same connection between the higher curvature functions and *ratios* of singular values. We summarize these results in the following theorem whose general proof for all dimensions is given in Appendix B:

Theorem 4.2. *Let $\gamma : I \rightarrow \mathbb{R}^n$ be a parametric curve of class C^{n+1} , regular of order n for any $n \in \mathbb{N}$. Let $\kappa_j(t)$ denote the j th curvature function of γ evaluated at t and let $\sigma_j(t)$ denote the j th local singular value of γ at t . For each $t \in I$ and each $j < n$,*

$$\kappa_j(t) = \sqrt{a_j} \frac{\sigma_{j+1}(t)}{\sigma_1(t) \sigma_j(t)} \quad \text{with} \quad a_{j-1} = \left(\frac{j}{j + (-1)^j} \right)^2 \frac{4j^2 - 1}{3}. \quad (4.5)$$

The formula straightforwardly reproduces the results obtained above for the coefficients

$$a_1 = \frac{20}{9}, \quad a_2 = \frac{105}{4}, \quad a_3 = \frac{336}{25}, \quad a_4 = \frac{825}{16}, \quad a_5 = \frac{1716}{49}.$$

The proof of the general case requires the theory of Hankel determinants using orthogonal polynomials, which is reviewed in Appendix A. Perhaps surprisingly, the numerator of this series arises in the number of Kekulé structures in benzenoid hydrocarbons [13] and the degrees of projections of rank loci [14].

5. An example

We consider the twisted cubic curve in $\mathbb{R}^3$ given parametrically as $\gamma(t) = [t, t^2, t^3]$. The Frenet-Serret frame can be shown to be:

$$e_1(t) = \begin{bmatrix} \frac{1}{\sqrt{1+4t^2+9t^4}} \\ \frac{2t}{\sqrt{1+4t^2+9t^4}} \\ \frac{3t^2}{\sqrt{1+4t^2+9t^4}} \end{bmatrix} \quad e_2(t) = \begin{bmatrix} \frac{t(2+9t^2)}{\sqrt{1+4t^2+9t^4}\sqrt{1+9t^2+9t^4}} \\ \frac{1-9t^4}{\sqrt{1+4t^2+9t^4}\sqrt{1+9t^2+9t^4}} \\ \frac{3t+6t^3}{\sqrt{1+4t^2+9t^4}\sqrt{1+9t^2+9t^4}} \end{bmatrix} \quad e_3(t) = \begin{bmatrix} \frac{3t^2}{\sqrt{1+9t^2+9t^4}} \\ \frac{-3t}{\sqrt{1+9t^2+9t^4}} \\ \frac{1}{\sqrt{1+9t^2+9t^4}} \end{bmatrix}$$

while the functions $\kappa_1(t), \kappa_2(t)$ can be shown to be

$$\kappa_1(t) = \frac{2\sqrt{1+9t^2+9t^4}}{(1+4t^2+9t^4)^{3/2}}, \quad \kappa_2(t) = \frac{3}{1+9t^2+9t^4}.$$

Let $\epsilon = .001$ and let $t = 3$. If we consider the singular value decomposition $C_\epsilon(t) = U_\epsilon(t) \Sigma_\epsilon(t) U_\epsilon^T(t)$ for $\gamma(t)$ then we can consider the singular vectors of $C_\epsilon(t)$ as a proxy

for the local singular vectors of $\gamma(t)$ at $t = 3$ and compare to the exact value for $e_i(t)$ at $t = 3$. For instance, comparing the first singular vector to the first frame vector, we get

$$u_{1,\epsilon}(3) = \begin{bmatrix} .036131465 \\ .216788800 \\ .975549656 \end{bmatrix} \quad e_1(3) = \begin{bmatrix} .036131468 \\ .216788812 \\ .975549654 \end{bmatrix}.$$

The other singular vectors, $u_{2,\epsilon}(3), u_{3,\epsilon}(3)$ are similarly close to $e_2(3), e_3(3)$. If we consider

$$\sqrt{a_i} \frac{\sqrt{\lambda_{i+1,\epsilon}(t)}}{\sqrt{\lambda_{1,\epsilon}(t)}\sqrt{\lambda_{i,\epsilon}(t)}} \text{ as a proxy for } \kappa_i = \sqrt{a_i} \frac{\sigma_{i+1}(t)}{\sigma_1(t)\sigma_i(t)}$$

then we obtain the following estimates:

$$\kappa_1(3) \approx .0026865640, \quad \kappa_2(3) \approx .0036991369,$$

whereas using the exact formulas, we can compare these values to

$$\kappa_1(3) = .0026865644..., \quad \kappa_2(3) = .0036991368...$$

For these approximations, we used $\epsilon = 10^{-3}$. With a choice of $\epsilon = 10^{-6}$, for this example, we observed about 13 digits of accuracy. This example illustrates how the theorems of the previous section can be used to obtain very good approximations of both the Frenet-Serret frame and values of the curvature functions by considering small values of ϵ .

6. Conclusions

In this paper, we established the close connection between the Frenet-Serret apparatus and the local singular value decomposition of regular curves in $\mathbb{R}^n$. The local singular value decomposition was defined as the limit of the singular value decomposition of a family of covariance matrices defined on the curve. In particular, we showed in Theorem 4.1 that the Frenet-Serret frame and the local singular vectors of regular curves in $\mathbb{R}^n$ agree (up to a factor of ± 1). In addition we showed in Theorem 4.2 that values of each of the curvature functions can be expressed in terms of ratios of local singular values for regular curves in $\mathbb{R}^n$ for any dimension, with a proportionality coefficient that was obtained exactly through its relation to Hankel determinants via monic orthogonal polynomials. With this, the techniques allow for highly accurate approximations of the Frenet-Serret apparatus in terms of local SVD computations.

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Appendix A. Hankel matrices and orthogonal polynomials

After the previous explicit examples were worked out, we conjectured the formula 4.2 for a_j and numerically verified the result for $\kappa_6, \kappa_7, \kappa_8$ by generating curves with prescribed non-constant curvature and solving the system $E' = EK$ numerically; then, the local singular values were numerically approximated from the numerically generated curves. The general proof is based on the following key result by F.J. Solis [15] for the expansions to leading order of the singular values:

Lemma Appendix A.1. *Let $\gamma(t)$ be a regular curve in $\mathbb{R}^n$, and let P_0 be a point on the curve, then the eigenvalues associated with C_ϵ at P_0 are given by*

$$\lambda_1^\epsilon = p_1 \epsilon^2 + O(\epsilon^4),$$

$$\lambda_j^\epsilon = \frac{(\kappa_1 \cdots \kappa_{j-1})^2}{(j!)^2} p_j \epsilon^{2j} + O(\epsilon^{2j+2}), \quad j = 2, \dots, n$$

and the eigenvectors are given by the Frenet frame at P_0 . The κ_i 's are the higher curvatures of the curve and p_k is the k -th ($k = 1, \dots, n$) pivot of the $n \times n$ matrix A_n defined by

$$A_{ij} = \begin{cases} \frac{1}{i+j+1}, & \text{if } i+j \text{ is even;} \\ 0 & \text{otherwise.} \end{cases}$$

From his proof, a small typo is corrected for the denominator of λ_j^ϵ in the final statement. With this result we can express the curvatures κ_j in terms of the singular values by expressing the pivots as quotients of the determinants B_j of A_j , that is $p_j = B_j/B_{j-1}$, so that:

$$\lim_{\epsilon \rightarrow 0} \frac{\lambda_{j+1}^\epsilon}{\lambda_1^\epsilon \lambda_j^\epsilon} = \kappa_j^2 \frac{B_{j+1} B_{j-1}}{(j+1)^2 B_1 B_j^2}. \quad (\text{A.1})$$

The determinants B_j are of Hankel type for the sequence $\{\mu_n\}_{n=0}^\infty = \{\frac{1}{3}, 0, \frac{1}{5}, 0, \frac{1}{7}, \dots\}$

$$B_1 = \frac{1}{3}, \quad B_2 = \begin{vmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{5} \end{vmatrix}, \quad B_3 = \begin{vmatrix} \frac{1}{3} & 0 & \frac{1}{5} \\ 0 & \frac{1}{5} & 0 \\ \frac{1}{5} & 0 & \frac{1}{7} \end{vmatrix}, \quad B_j = \begin{vmatrix} \mu_0 & \mu_1 & \mu_2 & \cdots & \mu_{j-1} \\ \mu_1 & \mu_2 & \mu_3 & \cdots & \mu_j \\ \mu_2 & \mu_3 & \mu_4 & \cdots & \mu_{j+1} \\ \vdots & \vdots & \vdots & & \vdots \\ \mu_{j-1} & \mu_j & \mu_{j+1} & \cdots & \mu_{2j-2} \end{vmatrix}.$$

Then to get our coefficient in 4.2 amounts to showing that the aforementioned Hankel determinants satisfy the following recurrence relation:

$$\frac{B_j B_{j-2}}{(B_{j-1})^2} = \frac{(j + (-1)^j)^2}{4j^2 - 1}. \quad (\text{A.2})$$

This is indeed the case after we realize that such a recurrence relation appears in the theory of monic orthogonal polynomials generated from $\{x^n\}_{n=0}^\infty$ by Gram-Schmidt orthogonalization with respect to a measure giving our sequence μ_n as the integral moments. Indeed, choose a nondecreasing function $\lambda(x)$ on $\mathbb{R}$ having finite limits at $\pm\infty$ such that it induces a positive measure $d\lambda$ with finite moments to all orders

$$\mu_n(d\lambda) = \int_{\mathbb{R}} x^n d\lambda(x), \quad n = 0, 1, 2, \dots$$

then apply the Gram-Schmidt orthogonalization procedure to $\{x^n\}_{n=0}^\infty$ using the scalar product

$$\langle p(x), q(x) \rangle = \int_{\mathbb{R}} p(x)q(x)d\lambda(x)$$

to obtain a sequence of monic orthogonal polynomials $P_n(x)$ (without normalization). If the given scalar product is positive-definite, such a sequence is infinite and unique, and this is the case if $B_n > 0$ for all $n \in \mathbb{N}$, see Gautschi [16, th. 1.2, 1.6]. Moreover, in this case, the infinite sequence of monic orthogonal polynomials obtained in this manner obeys the recursion relation [16, th. 1.27]:

$$P_{-1}(x) = 0, P_0(x) = 1, \quad P_{n+1}(x) = (x - \alpha_n)P_n(x) - \beta_n P_{n-1}(x) \quad (\text{A.3})$$

where

$$\alpha_n = \frac{\langle P_n, xP_n \rangle}{\langle P_n, P_n \rangle}, \quad \beta_n = \frac{\langle P_n, P_n \rangle}{\langle P_{n-1}, P_{n-1} \rangle} = \frac{\|P_n(x)\|^2}{\|P_{n-1}(x)\|^2}, \quad \text{for } n = 1, 2, \dots$$

The importance of this result is that the recursion coefficients β_n are precisely the recursion coefficients of the Hankel determinants B_n for the sequence μ_n , as it is proved in [16, eq. 2.1.5]

$$\beta_{j-1} = \frac{B_j B_{j-2}}{(B_{j-1})^2}, \quad \text{for } n = 2, 3, \dots \quad (\text{A.4})$$

so finding a measure to reproduce our sequence as its moments and a way to compute the norms of the corresponding polynomials will yield our coefficient formula. There is a fundamental determinantal representation of the monic orthogonal polynomials generated in the previous way [16, th. 2.1]

$$P_n(x) = \frac{1}{B_n} \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & \vdots & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-1} \\ 1 & x & \vdots & x^n \end{vmatrix}, \quad \|P_n(x)\|^2 = \frac{B_{n+1}}{B_n},$$

that yields Heine's integral representation formula [17, p. 288] by essentially pulling the integrals of each moment out of the determinant and expanding

$$P_n(x) = \frac{1}{n!B_n} \int \cdots \int_{\mathbb{R}^n} \prod_{i=1}^n (x - x_i) \prod_{1 \leq l < k \leq n} (x_k - x_l)^2 d\lambda(x_1) \cdots d\lambda(x_n).$$

Since the polynomials are monic, B_n can be solved equating to 1 the leading coefficient of the previous equation

$$B_n = \frac{1}{n!} \int_{\mathbb{R}^n} \prod_{1 \leq l < k \leq n} (x_k - x_l)^2 d\lambda(x_1) \cdots d\lambda(x_n) \quad (\text{A.5})$$

which is a closed formula for all Hankel determinants of any sequence as long as this can be written as moments of a positive measure.

Appendix B. Proof of Theorem 4.2

Using the theory above for Hankel determinants of particular type we arrive at the following key result.

Theorem Appendix B.1. *For any inverse arithmetic sequence $\left\{ \frac{1}{\alpha n + \beta} \right\}_{n=0}^{\infty}$, where $\alpha, \beta \in \mathbb{R}_{>0}$, the corresponding Hankel determinants*

$$F_n(\alpha, \beta) = \begin{vmatrix} \frac{1}{\beta} & \frac{1}{\alpha+\beta} & \frac{1}{2\alpha+\beta} & \cdots & \frac{1}{(n-1)\alpha+\beta} \\ \frac{1}{\alpha+\beta} & \frac{1}{2\alpha+\beta} & \frac{1}{3\alpha+\beta} & \cdots & \frac{1}{n\alpha+\beta} \\ \frac{1}{2\alpha+\beta} & \frac{1}{3\alpha+\beta} & \frac{1}{4\alpha+\beta} & \cdots & \frac{1}{(n+1)\alpha+\beta} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{1}{(n-1)\alpha+\beta} & \frac{1}{n\alpha+\beta} & \frac{1}{(n+1)\alpha+\beta} & \cdots & \frac{1}{(2n-2)\alpha+\beta} \end{vmatrix} \quad (\text{B.1})$$

are given by

$$F_n(\alpha, \beta) = \frac{1}{\alpha^n} \prod_{k=0}^{n-1} \frac{\Gamma(\beta/\alpha + k)(k!)^2}{\Gamma(\beta/\alpha + n + k)} = \frac{1}{\alpha^n} \prod_{k=0}^{n-1} (k!)^2 \prod_{j=0}^{n-1} \frac{\alpha}{\alpha(k+j) + \beta}, \quad (\text{B.2})$$

and satisfy the recursion relation

$$\frac{F_n F_{n-2}}{F_{n-1}^2} = \frac{\alpha^2 (\alpha(n-2) + \beta)^2 (n-1)^2}{(\alpha(2n-2) + \beta) (\alpha(2n-3) + \beta)^2 (\alpha(2n-4) + \beta)}, \quad (\text{B.3})$$

starting with $F_1 = \frac{1}{\beta}$, $F_2 = \frac{\alpha^2}{\beta(2\alpha + \beta)(\alpha + \beta)^2}$.

Proof. Choose the function $\lambda(x) = x^{\beta/\alpha}/\beta$ which is always nondecreasing in the interval $[0, 1]$ for $\beta/\alpha > 0$, then the corresponding positive measure

$$d\lambda(x) = \chi_{[0,1]} \frac{x^{\beta/\alpha-1}}{\alpha} dx,$$

where χ_I is the characteristic function of a measurable set $I \subset \mathbb{R}$, yields moments

$$\mu_n = \int_{\mathbb{R}} x^n d\lambda(x) = \frac{1}{\alpha} \int_0^1 x^{n+\frac{\beta}{\alpha}-1} dx = \frac{1}{\alpha} \left[\frac{x^{n+\frac{\beta}{\alpha}}}{n+\frac{\beta}{\alpha}} \right]_0^1 = \frac{1}{\alpha n + \beta}.$$

Notice that this solves the Stieltjes moment problem uniquely for these sequences because our measure is infinitely supported on $[0, \infty)$, and its moments satisfy Carleman's condition [18, th. 1.10]. From this, the necessary condition $F_n > 0$ is guaranteed to hold for any dimension n [18, th. 1.2], so the induced inner product is positive definite and thus the sequence of monic orthogonal polynomials $P_n(x)$ is infinite and unique. Thus their recurrence relations (A.3) hold for any $n \in \mathbb{N}$, so we can compute the determinants $F_n(\alpha, \beta)$ of any dimension. This is done by computing equation (A.5)

$$F_n(\alpha, \beta) = \frac{1}{n!} \int_0^1 \cdots \int_0^1 \prod_{i=1}^n \frac{x_i^{\frac{\beta}{\alpha}-1}}{\alpha} \prod_{1 \leq l < k \leq n} (x_k - x_l)^2 dx_1 \cdots dx_n$$

by means of Selberg's integral formula [19, 8.1.1], an extension of Euler's Beta function which has applications in different fields within mathematics and physics:

$$\begin{aligned} & \int_{[0,1]^n} \prod_{i=0}^n x_i^{a-1} (1-x_i)^{b-1} \prod_{1 \leq l < k \leq j} |x_k - x_l|^{2g} dx_1 \cdots dx_n \\ &= \prod_{k=0}^{n-1} \frac{\Gamma(a+kg)\Gamma(b+kg)\Gamma(1+(k+1)g)}{\Gamma(a+b+(n+k-1)g)\Gamma(1+g)}, \end{aligned}$$

when $\Re(a) > 0$, $\Re(b) > 0$ and $\Re(g) > -\min\{1/n, \Re(a)/(n-1), \Re(b)/(n-1)\}$. These conditions are satisfied for our case $a = \beta/\alpha > 0$, and $b = g = 1$. Therefore by substitution of these values

$$F_n(\alpha, \beta) = \frac{1}{n! \alpha^n} \prod_{k=0}^{n-1} \frac{\Gamma(\beta/\alpha + k)\Gamma(1+k)\Gamma(2+k)}{\Gamma(\beta/\alpha + n + k)\Gamma(2)} = \frac{1}{\alpha^n} \prod_{k=0}^{n-1} \frac{\Gamma(\beta/\alpha + k)(k!)^2}{\Gamma(\beta/\alpha + n + k)},$$

where the Gamma functions can be simplified by the factorial property $\Gamma(z+1) = z\Gamma(z)$ to get a closed formula:

$$F_n(\alpha, \beta) = \frac{1}{\alpha^n} \prod_{k=0}^{n-1} (k!)^2 \prod_{j=0}^{n-1} \frac{\alpha}{\alpha(k+j) + \beta}.$$

Finally, the recursion equation (A.4) can be worked out by telescoping the products of Gamma functions:

$$\begin{aligned} \frac{F_n F_{n-2}}{F_{n-1}^2} &= \frac{1}{\alpha^n} \prod_{k=0}^{n-1} \frac{\Gamma(\frac{\beta}{\alpha} + k)(k!)^2}{\Gamma(\frac{\beta}{\alpha} + n + k)} \cdot \alpha^{n-1} \prod_{k=0}^{n-2} \frac{\Gamma(\frac{\beta}{\alpha} + n - 1 + k)}{\Gamma(\frac{\beta}{\alpha} + k)(k!)^2} \\ &= \alpha^{n-1} \prod_{k=0}^{n-2} \frac{\Gamma(\frac{\beta}{\alpha} + n - 1 + k)}{\Gamma(\frac{\beta}{\alpha} + k)(k!)^2} \cdot \frac{1}{\alpha^{n-2}} \prod_{k=0}^{n-3} \frac{\Gamma(\frac{\beta}{\alpha} + k)(k!)^2}{\Gamma(\frac{\beta}{\alpha} + n - 2 + k)} = \\ &= \frac{\Gamma(\frac{\beta}{\alpha} + n - 1)(n-1)!^2}{\Gamma(\frac{\beta}{\alpha} + n - 2)(n-2)!^2} \prod_{k=0}^{n-1} \frac{1}{(\frac{\beta}{\alpha} + n - 1 + k)\Gamma(\frac{\beta}{\alpha} + n - 1 + k)} \prod_{k=0}^{n-2} \Gamma\left(\frac{\beta}{\alpha} + n - 1 + k\right) \cdot \\ &\quad \prod_{k=0}^{n-2} \left(\frac{\beta}{\alpha} + n - 2 + k\right) \Gamma\left(\frac{\beta}{\alpha} + n - 2 + k\right) \prod_{k=0}^{n-3} \frac{1}{\Gamma\left(\frac{\beta}{\alpha} + n - 2 + k\right)} = \\ &= \frac{(\frac{\beta}{\alpha} + n - 2)(n-1)^2 \Gamma(\frac{\beta}{\alpha} + 2n - 4)}{\Gamma(\frac{\beta}{\alpha} + 2n - 2)} \prod_{k=0}^{n-1} \frac{1}{(\frac{\beta}{\alpha} + n - 1 + k)} \prod_{k=0}^{n-2} \left(\frac{\beta}{\alpha} + n - 2 + k\right) \\ &= \frac{(\frac{\beta}{\alpha} + n - 2)^2 (n-1)^2}{(\frac{\beta}{\alpha} + 2n - 2)(\frac{\beta}{\alpha} + 2n - 3)^2 (\frac{\beta}{\alpha} + 2n - 4)} \end{aligned}$$

which yields the stated formula upon multiplying numerator and denominator by α^4 . $\square$

Remarkably, this means that our polynomial recursion coefficients satisfy $\beta_n = \frac{1}{4}\beta_n^J$, where β_n^J are those of the classical monic Jacobi polynomials of type $(\frac{\beta}{\alpha} - 1, 0)$. These are generated by the measure $\chi_{[-1,1]}(1-x)^{\frac{\beta}{\alpha}-1}dx$, which induces a completely different moment sequence and set of orthogonal polynomials.

Our actual determinants B_n have alternating 0's in the even positions of the moment sequence, so a block decomposition is needed to get them into the form of the theorem.

Corollary Appendix B.2. For any sequence of type $\left\{\frac{1}{\alpha n + \beta}, 0\right\}_{n=0}^{\infty}$ with $\alpha, \beta \in \mathbb{R}_{>0}$, where zeros alternate every other position, the corresponding Hankel determinants B_n are given by the following block decomposition for even $n = 2m$ or odd $n = 2m - 1$ dimension, $m \in \mathbb{N}$:

$$B_{2m} = F_m(\alpha, \beta)F_m(\alpha, \beta + \alpha), \quad B_{2m-1} = F_m(\alpha, \beta)F_{m-1}(\alpha, \beta + \alpha),$$

and obey the recurrence relations:

$$\frac{B_{2m}B_{2m-2}}{(B_{2m-1})^2} = \frac{(\alpha(m-1) + \beta)^2}{(\alpha(2m-1) + \beta)(\alpha(2m-2) + \beta)}, \quad (\text{B.4})$$

$$\frac{B_{2m-1}B_{2m-3}}{(B_{2m-2})^2} = \frac{\alpha^2(m-1)^2}{(\alpha(2m-2) + \beta)(\alpha(2m-3) + \beta)}, \quad (\text{B.5})$$

starting with $B_1 = \frac{1}{\beta}$, $B_2 = \frac{1}{\beta(\alpha + \beta)}$.

Proof. The Hankel determinants with 0's at every even position of the first row can be decomposed into blocks by the procedure mentioned in Section 4.4 without altering the overall sign. Notice that the second block has as Hankel sequence the original one but shifted in index by +1, so the blocks are $F_m := F_m(\alpha, \beta)$ and $E_m := F_m(\alpha, \beta + \alpha)$. Analogously for $n = 2m - 1$, but in this case the number of 0's is now $m - 1$, so the size of the second block is $(m - 1)^2$ whereas the first is still m^2 . Thus

$$B_{2m} = F_m E_m, \quad B_{2m-1} = F_m E_{m-1}.$$

Whence the recursion coefficients for the induced polynomials are, for even n ,

$$\beta_{n-1} = \beta_{2m-1} = \frac{B_{2m}B_{2(m-1)}}{B_{2m-1}^2} = \frac{E_m}{E_{m-1}} \frac{F_{m-1}}{F_m},$$

and for odd n :

$$\beta_{n-1} = \beta_{2m-2} = \frac{B_{2m-1}B_{2(m-1)-1}}{B_{2(m-1)}^2} = \frac{E_{m-2}}{E_{m-1}} \frac{F_m}{F_{m-1}}.$$

Therefore using (B.2), that the corresponding β/α for the E_m blocks is $\beta/\alpha + 1$ and the factorial property of the Gamma function, the products can be simplified in the same way as in our previous proof:

$$\begin{aligned} \frac{B_{2m}B_{2(m-1)}}{B_{2m-1}^2} &= \frac{1}{\alpha^m} \prod_{k=0}^{m-1} \frac{\Gamma(\beta/\alpha + 1 + k)(k!)^2}{\Gamma(\beta/\alpha + 1 + m + k)} \cdot \alpha^{m-1} \prod_{k=0}^{m-2} \frac{\Gamma(\beta/\alpha + m + k)}{\Gamma(\beta/\alpha + 1 + k)(k!)^2} \\ &= \frac{1}{\alpha^{m-1}} \prod_{k=0}^{m-2} \frac{\Gamma(\beta/\alpha + k)(k!)^2}{\Gamma(\beta/\alpha + m - 1 + k)} \cdot \alpha^m \prod_{k=0}^{m-1} \frac{\Gamma(\beta/\alpha + m + k)}{\Gamma(\beta/\alpha + k)(k!)^2} = \\ &= (\beta/\alpha + m - 1) \prod_{k=0}^{m-1} \frac{1}{(\beta/\alpha + m + k)} \cdot \prod_{k=0}^{m-2} (\beta/\alpha + m + k - 1) = \\ &= \frac{(\beta/\alpha + m - 1)^2}{(\beta/\alpha + 2m - 1)(\beta/\alpha + 2m - 2)}. \end{aligned}$$

Similarly,

$$\begin{aligned}
 \frac{B_{2m-1}B_{2(m-1)-1}}{B_{2(m-1)}^2} &= \frac{1}{\alpha^{m-2}} \prod_{k=0}^{m-3} \frac{\Gamma(\beta/\alpha + 1 + k)(k!)^2}{\Gamma(\beta/\alpha + m - 1 + k)} \cdot \alpha^{m-1} \prod_{k=0}^{m-2} \frac{\Gamma(\beta/\alpha + m + k)}{\Gamma(\beta/\alpha + 1 + k)(k!)^2} \\
 &= \frac{1}{\alpha^m} \prod_{k=0}^{m-1} \frac{\Gamma(\beta/\alpha + k)(k!)^2}{\Gamma(\beta/\alpha + m + k)} \cdot \alpha^{m-1} \prod_{k=0}^{m-2} \frac{\Gamma(\beta/\alpha + m - 1 + k)}{\Gamma(\beta/\alpha + k)(k!)^2} = \\
 &= \frac{(m-1)!^2 \Gamma(\beta/\alpha + m - 1) \Gamma(\beta/\alpha + 2m - 3)}{(m-2)!^2 \Gamma(\beta/\alpha + m - 1) \Gamma(\beta/\alpha + 2m - 1)} = \\
 &= \frac{(m-1)^2}{(\beta/\alpha + 2m - 2)(\beta/\alpha + 2m - 3)}. \quad \square
 \end{aligned}$$

Finally the coefficient formula of Section 4.2 is obtained from this using (A.1).

Corollary Appendix B.3. *The Hankel determinants of size $n \times n$*

$$B_n = \det(A_n), \quad (A_n)_{ij} = \begin{cases} \frac{1}{i+j+1}, & \text{if } i+j \text{ is even;} \\ 0 & \text{otherwise,} \end{cases}$$

satisfy the recurrence relation

$$\frac{B_n B_{n-2}}{(B_{n-1})^2} = \frac{(n + (-1)^n)^2}{4n^2 - 1}. \quad (\text{B.6})$$

Proof. Notice the matrix entry at $(A_n)_{ij}$ is precisely the element of the sequence $\left\{ \frac{1}{2n+3}, 0 \right\}_{n=0}^{\infty}$ where $n = i+j-2$. Thus substituting $\alpha = 2$ and $\beta = 3$ into the equations (B.4), (B.5) above, the result follows straightforwardly when simplifying the theorem formulas after indices are written in terms of the dimension, $m = n/2$ or $m = (n+1)/2$ for the even and odd cases respectively. $\square$

References

- [1] D. Broomhead, R. Jones, G.P. King, Topological dimension and local coordinates from time series data, *J. Phys. A: Math. Gen.* 20 (9) (1987) L563.
- [2] D. Broomhead, R. Indik, A. Newell, D. Rand, Local adaptive Galerkin bases for large-dimensional dynamical systems, *Nonlinearity* 4 (2) (1991) 159.
- [3] J. Álvarez-Vizoso, M. Kirby, C. Peterson, Manifold curvature from covariance analysis, in: (SSP 2018) 2018 IEEE Statistical Signal Processing Workshop, 2018.
- [4] J. Álvarez-Vizoso, M. Kirby, C. Peterson, Integral invariants from covariance analysis of embedded Riemannian manifolds, preprint, arXiv:1804.10425, submitted for publication.
- [5] J. Álvarez-Vizoso, M. Kirby, C. Peterson, Manifold curvature descriptors from hypersurface integral invariants, preprint, arXiv:1804.04808, submitted for publication.
- [6] M. Kirby, *Geometric Data Analysis: An Empirical Approach to Dimensionality Reduction and the Study of Patterns*, John Wiley & Sons, Inc., 2000.
- [7] I. Jolliffe, *Principal Component Analysis*, Springer, New York, 1986.

- [8] L.N. Trefethen, I. David Bau, *Numerical Linear Algebra*, SIAM, Philadelphia, PA, 1997.
- [9] W. Kühnel, *Differential Geometry: Curves-Surfaces-Manifolds*, vol. 16, American Mathematical Soc., 2006.
- [10] D. Hundley, M. Kirby, R. Miranda, Empirical dynamical system reduction II: neural charts, in: K. Coughlin (Ed.), *Semi-Analytic Methods for the Navier–Stokes Equations*, Montreal, 1995, in: CRM Proc. Lecture Notes, vol. 20, Amer. Math. Soc., Providence, RI, 1999, pp. 65–83.
- [11] D. Broomhead, M. Kirby, A new approach for dimensionality reduction: theory and algorithms, *SIAM J. Appl. Math.* 60 (6) (2000) 2114–2142.
- [12] A.V. Little, J. Lee, Y.-M. Jung, M. Maggioni, Estimation of intrinsic dimensionality of samples from noisy low-dimensional manifolds in high dimensions with multiscale SVD, in: *Statistical Signal Processing*, 2009. SSP'09. IEEE/SP 15th Workshop on, IEEE, 2009, pp. 85–88.
- [13] S.J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, vol. 46, Springer Science & Business Media, 2013.
- [14] P. Aluffi, Degrees of projections of rank loci, arXiv preprint, arXiv:1408.1702.
- [15] F.J. Solis, Geometry of local adaptive Galerkin bases, *Appl. Math. Optim.* 41 (2000) 331–342.
- [16] W. Gautschi, *Orthogonal Polynomials, Computation and Approximation*, Oxford University Press, 2004.
- [17] H.E. Heine, *Handbuch der Kugelfunctionen*, vol. I, Berlin, Georg Reimer, 1861.
- [18] J. Shohat, J. Tamarkin, *The Problem of Moments*, American Mathematical Soc., 1943.
- [19] G.E. Andrews, R. Askey, R. Roy, *Special Functions*, Cambridge University Press, 1999.