Extremal Properties of Principal Curves in the Plane

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Abstract

Principal curves were introduced to formalize the notion of “a curve passing through the middle of a dataset”. Vaguely speaking, a curve is said to pass through the middle of a dataset if every point on the curve is the average of the observations projecting onto it. This idea can be made precise by defining principal curves for probability densities. In this paper we study principal curves in the plane. Like linear principal components, principal curves are critical points of the expected squared distance from the data. However, the largest and smallest principal components are extrema of the distance, whereas all principal curves are saddlepoints. This explains why cross-validation does not appear to be a viable method for choosing the complexity of principal curve estimates.
1 Introduction

Principal curves were introduced in Hastie (1984) and Hastie and Stuetzle (1989) to formalize the notion of “a curve passing through the middle of a dataset”. Vaguely speaking, a curve $\Gamma$ is said to pass through the middle of a dataset if every point $x$ on the curve is the average of the observations projecting onto it.

To make this idea precise, Hastie and Stuetzle (1989) define principal curves for probability densities. Let $X$ denote a two-dimensional random vector distributed according to a probability density $p$, and let $\Gamma \subset \mathbb{R}^2$ be a smoothly embedded closed interval (arc) or circle (loop). For each point $x \in \mathbb{R}^2$, let $d(x, \Gamma)$ denote the distance from $x$ to $\Gamma$. Because $\Gamma$ is compact, for each $x \in \mathbb{R}^2$ the distance $d(x, \Gamma)$ is realized by at least one point of $\Gamma$. Of course, there may be several such points; a point $x$ with several closest points on the curve is called an ambiguity point. The projection map

$$\pi_\Gamma : \mathbb{R}^2 \to \Gamma,$$

is the map which assigns to each $x \in \mathbb{R}^2$ a point $\pi_\Gamma(x) \in \Gamma$ realizing the distance from $x$ to $\Gamma$, i.e.

$$d(x, \Gamma) = \| x - \pi_\Gamma(x) \|.$$

The vague notion that every point on the curve should be the average of the observations projecting onto it can now be formalized:

Definition 1 (Hastie and Stuetzle (1989)) A curve $\Gamma$ is called self-consistent or a principal curve of a density $p$ if $E(X \mid \pi_\Gamma(X) = x) = x$ for almost every $x \in \Gamma$.

The notion of projection also leads to a natural definition of the distance between a random vector $X$ or its associated density, and a curve $\Gamma$:

$$d^2(X, \Gamma) = E(\| X - \pi_\Gamma(X) \|^2).$$

The main result proved in Hastie and Stuetzle (1989) is that principal curves are critical points of the distance in the variational sense:

Theorem 1 Let $\Gamma$ be a principal curve, and let $\Gamma_t$ be a smooth family of curves with $\Gamma_0 = \Gamma$, then

$$\left. \frac{d}{dt} d^2(X, \Gamma_t) \right|_{t=0} = 0$$

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Linear principal components share this property if $\Gamma_t$ is restricted to be a smooth family of straight lines. The largest principal component minimizes the distance to $X$, the smallest principal component maximizes the distance (among all lines passing through $E(X)$), and the others are saddle points.

In this paper we show that all principal curves are saddle points of the distance; there are no local minima. This is in notable contrast to the regression problem, where the conditional expectation $\mathbb{E}(Y \mid x)$ minimizes the expected squared distance $\mathbb{E}(Y - f(X))^2$ among all functions $f$. In the regression case, we can choose model complexity by minimizing an estimate of $\mathbb{E}(Y - f(X))^2$, for example the cross-validated residual sum of squares. As principal curves are not minima of the distance, there is no justification for choosing the complexity that minimizes an estimate of the distance, and indeed cross-validation has been observed to fail in practice.

While principal curves are not local minima in general, they are local minima of the distance for “low frequency variations”. However, the definition of “low-frequency” depends on the principal curve itself, and not only on the underlying density. Thus it is not clear how this fact can be used in an operational way.

As our main result is essentially negative, we do not attempt to prove it in greatest generality. To avoid various technical problems, we only consider regular, closed curves for which the support of the density forms a tubular neighborhood. For such curves, the projection map $\pi$ is well defined and smooth.

In a companion paper (Duchamp and Stuetzle (1995)) we show that regular principal curves are solutions of a differential equation. By solving this differential equation, we find principal curves for uniform densities on rectangles and annuli. There are oscillating solutions besides the obvious straight and circular ones, indicating that principal curves in general will not be unique. If a density has several principal curves, they have to cross, a property somewhat analogous to the orthogonality of principal components. Finally, we study principal curves for spherical and elliptical distributions.

**Notation and conventions:** The following notation is used throughout the paper: $L_\Gamma$ denotes the length of $\Gamma$; $\Lambda$ denotes the circle of circumference $L_\Gamma$; $X = x(s)$ denotes an arc length parameterization of $\Gamma$. The unit tangent and normal vector fields to $\Gamma$ are written $T(s)$ and $N(s)$, respectively, and oriented so that the pair $(T(s), N(s))$ is consistent with the standard
orientation of $\mathbb{R}^2$. The support $\Omega$ of the density $p$ is assumed to be a compact, connected region with smooth boundary. The density is assumed to be strictly positive on the interior of $\Omega$ and smooth on all of $\Omega$. The map

$$\lambda : \begin{cases} \Omega & \to \Lambda \\ \mathbf{x} & \mapsto s = \lambda(\mathbf{x}) \end{cases}$$

defined by the formula $\pi_\Gamma(\mathbf{x}) = \mathbf{x}(\lambda(\mathbf{x}))$ is called the projection index (see Hastie and Stuetzle (1989)).

## 2 Regularity, Normal Coordinates and Transverse Moments

Suppose that $\Gamma$ is a curve for which the support $\Omega$ of the density is a tubular neighborhood that does not contain any ambiguity points (see Figure 1). In this case, $\Omega$ can be parameterized in terms of normal coordinates.

![Regular loop](image)

**Figure 1:** A regular loop.

**Definition 2.** The normal coordinate map of $\Gamma$ is the map $\nu_\Gamma : \Lambda \times \mathbb{R} \to \mathbb{R}^2$ defined by the formula

$$\nu_\Gamma(s, v) = \mathbf{x}(s) + v\mathbf{N}(s)$$

and the normal coordinate transformation is the map $\mu_\Gamma : \Omega \to \Lambda \times \mathbb{R}$ defined by the formula

$$\mu_\Gamma(\mathbf{x}) = (\lambda(\mathbf{x}), (\mathbf{x} - \mathbf{x}(\lambda(\mathbf{x})), \mathbf{N}(\lambda(\mathbf{x})))).$$
The components $(s, v)$ of $\mu_\Gamma(x)$ are called the normal coordinates of $x$.

By virtue of our assumption that $\Omega$ does not contain ambiguity points of $\Gamma$, the normal map is a left inverse of the normal coordinate transformation $\mu_\Gamma$:

$$\nu_\Gamma \circ \mu_\Gamma = \text{id}_\Omega.$$ 

We can now state a formal definition of regularity:

**Definition 3.** A smooth curve $\Gamma \subseteq \Omega$ is called regular if the following conditions are satisfied:

1. $\Omega$ contains no ambiguity points of $\Gamma$.
2. The map $\mu_\Gamma : \Omega \to \Lambda \times \mathbb{R}$ is a diffeomorphism onto its image.
3. The image $\mu_\Gamma(\Omega)$ is of the form

$$\mu_\Gamma(\Omega) = \{(s, v) \in \Lambda \times \mathbb{R} \mid v_-(s) \leq v \leq v_+(s)\},$$

where $v_-$ and $v_+$ are smooth and $v_-(s) < 0 < v_+(s)$ on the interior of $\Lambda$.

Regularity implies that for any $s \in \Lambda$ the set $V(s) = \{v \mid (s, v) \in \mu_\Gamma(\Omega)\}$ of points in $\Omega$ projecting onto $x(s)$ is an interval.

Define

$$\mu_\kappa(s) = \int_{V(s)} v^k p(x(s) + vN(s))dv.$$ 

Then $\mu_\perp(s) = \mu_1(s)/\mu_0(s)$ is the mean of the transverse density on $V(s)$ induced by $p$, and $\sigma^2_\perp(s) = \mu_2(s)/\mu_0(s) - \mu^2_\perp$ is its variance.

For later reference, we now calculate the Jacobian determinant of the normal map. Recall the Frenet formulas

$$\frac{dT(s)}{ds} = \kappa(s)N(s) \quad \text{and} \quad \frac{dN(s)}{ds} = -\kappa(s)T(s),$$

where $\kappa(s)$ is the curvature of $\Gamma$. Then $\frac{\partial \nu_\Gamma(s, v)}{\partial s} = x'(s) + vN'(s) = (1 - v\kappa(s))T(s)$ and $\frac{\partial \nu_\Gamma(s, v)}{\partial v} = N(s)$. The Jacobian determinant $\frac{\partial(x, y)}{\partial(s, v)}$ of the normal coordinate map is now easily computed:

$$\frac{\partial(x, y)}{\partial(s, v)} = \left| \frac{\partial \nu_\Gamma(s, v)}{\partial s} \times \frac{\partial \nu_\Gamma(s, v)}{\partial v} \right| = 1 - v\kappa(s).$$

(1)
3 The First Variation

The goal of this section is to compute the first (variational) derivative of the distance functional

\[ I[\Gamma] = d^2(\mathbf{X}, \Gamma) = \int_{\mathbf{x} \in \Omega} \| \mathbf{x} - \pi_\Gamma(\mathbf{x}) \|^2 p(\mathbf{x}) \, d\mathbf{x} \]

at a regular curve \( \Gamma \). For this purpose consider a smooth variation of \( \Gamma \), i.e. a smooth function

\[ \Phi : \Lambda \times (-\epsilon, +\epsilon) \to \mathbb{R}^2 \]

for which \( \Phi(s, 0) \) is the arc-length parametrization of \( \Gamma \). Let \( \Gamma_t \) be the curve parametrized by \( \Phi(s, t) \). Differentiating \( \Phi \) with respect to \( t \) at \( t = 0 \) gives a vector field \( \mathbf{Y} \) defined along \( \Gamma \). The fact that \( I[\Gamma_t] \) is independent of the parametrization of \( \Gamma_t \) implies that \( \Phi \) can be chosen so that \( \mathbf{Y} \) is normal to \( \Gamma \). Thus, \( \mathbf{Y} \) can be assumed to be of the form \( \mathbf{Y} = f \mathbf{N} \) where \( f \) is a real valued function on \( \Lambda \). We call \( f \) an infinitesimal variation of \( \Gamma \).

Let \( \lambda : \Omega \times (-\epsilon, \epsilon) \to \Lambda \) be the projection index associated with the curve \( \Phi(s, t) \). It is defined by the condition

\[ \Phi(\lambda(\mathbf{x}, t), t) = \pi_{\Gamma_t}(\mathbf{x}), \]

where \( \pi_{\Gamma_t} : \Omega \to \Gamma_t \subset \Omega \) is the projection map. One can show that, for sufficiently small \( t \), \( \Gamma_t \) is regular, and thus \( \lambda(\mathbf{x}, t) \) is a smooth function of \( \mathbf{x} \) and \( t \).

**Theorem 2** Let \( \Gamma \) be a regular curve of \( p \) and let \( \Gamma_t \) be a smooth variation of \( \Gamma \). Then

\[ \left. \frac{d[I[\Gamma_t]]}{dt} \right|_{t=0} = -2 \int_\Lambda f(s) \left\{ \mu_+(s) - \kappa(s) \left( \sigma^2_+(s) + \mu^2_+(s) \right) \right\} \mu_0(s) \, ds, \]

where \( f \) is the infinitesimal variation generated by \( \Gamma_t \).

**Proof.** The proof is a direct calculation. Set \( I(t) = I[\Gamma_t] \). Then

\[ I'(t) = \frac{d}{dt} \int_{\Omega} \| \mathbf{x} - \Phi(\lambda(\mathbf{x}, t), t) \|^2 p(\mathbf{x}) \, d\mathbf{x} \]

\[ = -2 \int_{\Omega} \left( \mathbf{x} - \Phi(\lambda(\mathbf{x}, t), t), \left( \frac{\partial \Phi(\lambda(\mathbf{x}, t), t)}{\partial s} \frac{\partial \lambda(\mathbf{x}, t)}{\partial t} + \frac{\partial \Phi(\lambda(\mathbf{x}, t), t)}{\partial t} \right) \right) p(\mathbf{x}) \, d\mathbf{x} . \]
Note that, for $\mathbf{x} \in \Omega$, the vector $\partial \Phi(\lambda(\mathbf{x}, t), t) / \partial s$ is tangential to $\Gamma_t$ at $\Phi(\lambda(\mathbf{x}, t), t)$. Since $\Phi(\lambda(\mathbf{x}, t), t)$ is the point on $\Gamma_t$ nearest $\mathbf{x}$ and since $\Gamma_t$ is regular, it follows that $\mathbf{x} - \Phi(\lambda(\mathbf{x}, t), t)$ is orthogonal to $\partial \Phi(\lambda(\mathbf{x}, t), t) / \partial s$.

Thus,

$$I'(t) = -2 \int_{\Omega} \left( \mathbf{x} - \Phi(\lambda(\mathbf{x}, t), t), \frac{\partial \Phi(\lambda(\mathbf{x}, t), t)}{\partial t} \right) p(\mathbf{x}) \, d\mathbf{x}. \quad (2)$$

By switching to normal coordinates, we obtain

$$I'(0) = -2 \int_{\Omega} \left( \mathbf{x} - \pi(\mathbf{x}), f(\pi(x)) N(\pi(x)) \right) p(\mathbf{x}) \, d\mathbf{x}$$

$$= -2 \int_{\Omega} \left\{ \int_{\mathbb{L}} v f(s) p(\mathbf{x}(s) + v N(s)) \left(1 - \nu(s) \right) \, dv \right\} ds$$

$$= -2 \int_{\Omega} f(s) \left\{ \mu_1(s) - \kappa(s) \left( \sigma^2(s) + \mu_\perp^2(s) \right) \right\} \mu_0(s) \, ds.$$

For $I'$ to be a critical point of the distance functional, $I'(0)$ has to vanish for all choices of $f$. This is equivalent to the condition that

$$\kappa(s) = \frac{\mu_\perp(s)}{\mu_\perp^2(s) + \sigma^2(s)}. \quad (3)$$

4 The Second Variation

We will now compute the second derivative of $I[\Gamma_t]$.

**Theorem 3.** Let $\Gamma$ be a regular principal curve of $p$ and let $\Gamma_t$ be a smooth variation of $\Gamma$. Then

$$\left. \frac{d^2 I[\Gamma_t]}{dt^2} \right|_{t=0} = 2 \int_{\Omega} \left\{ \left( \frac{\sigma^2}{\mu_\perp^2 + \sigma^2} \right) f^2 - \left( \mu_\perp^2 + \sigma^2 \right) f'^2 \right\} \mu_0 \, ds$$

where $f$ is the infinitesimal variation generated by $\Gamma_t$.

**Proof.** By equation (2),

$$I''(t) = -2 \frac{d}{dt} \int_{\Omega} \left( \mathbf{x} - \Phi(\lambda(\mathbf{x}, t), t), \frac{\partial \Phi(\lambda(\mathbf{x}, t), t)}{\partial t} \right) p(\mathbf{x}) \, d\mathbf{x}.$$
Differentiation inside the integral and an application of the chain rule gives:

\[
I''(t) = 2 \int\int_{\Omega} \left< \frac{\partial \Phi(\lambda(x,t),t)}{\partial s}, \frac{\partial \lambda(x,t)}{\partial t} \right> \frac{\partial \Phi(\lambda(x,t),t)}{\partial t} \ p(x) \ dx (4)
\]

\[
+2 \int\int_{\Omega} \left< \frac{\partial \Phi(\lambda(x,t),t)}{\partial t}, \frac{\partial \Phi(\lambda(x,t),t)}{\partial t} \right> \ p(x) \ dx (5)
\]

\[
-2 \int\int_{\Omega} \left< x - \Phi(\lambda(x,t),t), \frac{\partial^2 \Phi(\lambda(x,t),t)}{\partial s \partial t} \right> \ p(x) \ dx (6)
\]

\[
-2 \int\int_{\Omega} \left< x - \Phi(\lambda(x,t),t), \frac{\partial^2 \Phi(\lambda(x,t),t)}{\partial t^2} \right> \ p(x) \ dx . (7)
\]

We will now evaluate the four terms at \( t = 0 \). By construction, \( \partial \Phi(s,0)/\partial s = T(s) \) and \( \partial \Phi(s,0)/\partial t = f(s)N(s) \). Hence the first term (4) vanishes.

Decomposing the vector field \( \partial^2 \Phi(s,0)/\partial t^2 \) into a tangential component \( h_\parallel(s)T(s) \) and a normal component \( h_\perp(s)N(s) \) allows us to rewrite the fourth term (7) as:

\[
-2 \int\int_{\Omega} \langle x - \pi_T(x), h_\perp(\lambda(x,0)) N(\lambda(x,0)) \rangle \ p(x) \ dx
\]

This is a first variation (see Equation (2)) and vanishes because \( \Gamma \) is assumed to be a principal curve.

We can rewrite the second term (5) by changing to normal coordinates and using the fact that \( \Gamma \) is a principal curve:

\[
2 \int\int_{\Omega} \left< \frac{\partial \Phi(\lambda(x,t),t)}{\partial t}, \frac{\partial \Phi(\lambda(x,t),t)}{\partial t} \right> \ p(x) \ dx
\]

\[
= 2 \int\int_{\Omega} f^2(\lambda(x,0)) \ p(x) \ dx
\]

\[
= 2 \int_{\lambda} f^2(s) \left\{ \int_{\nu(s)} (1 - v\kappa(s)) \ p(x(s) + vN(s)) \ dv \right\} ds
\]

\[
= 2 \int_{\lambda} f^2(s) (\mu_0(s) - \mu_1(s) \kappa(s)) \ ds
\]

\[
= 2 \int_{\lambda} f^2(s) \left( \frac{\sigma_1^2(s)}{\mu_1^2(s) + \sigma_1^2(s)} \right) \mu_0(s) \ ds.
\]
It remains to examine the third term (6). We will first rewrite the mixed partial:
\[
\frac{\partial^2 \Phi(\lambda(x, 0), 0)}{\partial s \partial t} = \frac{\partial}{\partial s} \left( f(\lambda(x, 0)) N(\lambda(x, 0)) \right)
= f'(\lambda(x, 0)) N(\lambda(x, 0)) - f(\lambda(x, 0)) \kappa(\lambda(x, 0)) T(\lambda(x, 0))
\]

Hence,
\[
-2 \int \int_{\Omega} \left\{ x - \pi_\Gamma(x), \frac{\partial^2 \Phi(\lambda(x, 0), 0)}{\partial s \partial t} \frac{\partial \lambda(x, 0)}{\partial t} \right\} p(x) \, dx
= -2 \int \int_{\Omega} \left\{ x - \pi_\Gamma(x), f'(\lambda(x, 0)) N(\lambda(x, 0)) \frac{\partial \lambda(x, 0)}{\partial t} \right\} p(x) \, dx \quad (8)
\]
To conclude the calculation, we need a formula for \( \frac{\partial \lambda(x, 0)}{\partial t} \). Observe that
\[
\left\{ x - \Phi(\lambda(x, t), t), \frac{\partial \Phi(\lambda(x, t), t)}{\partial s} \right\} = 0
\]
identically in \( t \), because \( (x - \Phi(\lambda(x, t), t)) \) is normal to \( \Gamma_t \) and \( \frac{\partial \Phi(\lambda(x, t), t)}{\partial s} \) is tangential to \( \Gamma_t \). Differentiating with respect to \( t \) at \( t = 0 \) and solving for \( \frac{\partial \lambda(x, t)}{\partial t} \) gives
\[
\left. \frac{\partial \lambda(x, t)}{\partial t} \right|_{t=0} = f'(\lambda(x, 0)) \frac{\langle x - \pi_\Gamma(x), N(\lambda(x, 0)) \rangle}{1 - \kappa(\lambda(x, 0)) \langle x - \pi_\Gamma(x), N(\lambda(x, 0)) \rangle} \quad (9)
\]
(The calculation is somewhat lengthy, but proceeds along the same lines as the calculations above.) Substituting Equation (9) into Equation (8) and reverting to normal coordinates, we obtain
\[
-2 \int \int_{\Omega} \left\{ x - \pi_\Gamma(x), f'(\lambda(x, 0)) N(\lambda(x, 0)) \frac{\partial \lambda(x, 0)}{\partial t} \right\} p(x) \, dx
= -2 \int \int_{\Omega} f'^2(\lambda(x, 0)) \frac{\langle x - \pi_\Gamma(x), N(\lambda(x, 0)) \rangle^2}{1 - \kappa(\lambda(x, 0)) \langle x - \pi_\Gamma(x), N(\lambda(x, 0)) \rangle} p(x) \, dx
= -2 \int \int_{\Omega} f'^2(\lambda(x, 0)) \frac{\sigma_1^2(s) + \mu_1^2(s)}{\mu_0(s)} \, ds
\]
Collecting terms gives the final formula for the second variation. \( \Box \)

From Theorem 3 it is easy to see why all regular principal curves are saddle points of \( I \): Choosing a variation with constant \( f \) leads to a positive second derivative, while choosing a variation with large \( f'^2 \) and small \( f \) (in the \( L^2 \) sense), leads to a negative second derivative. In particular, regular principal curves are never local minima.
5 Low Frequency Variations

In this section we show that principal curves are local minima of the distance, if we restrict ourselves to low frequency variations. We first examine the case of the circular principal curve for the uniform distribution on an annulus, and then discuss the general case.

5.1 The Annulus

Consider the uniform distribution on the annulus

$$\Omega_{R_1,R_2} = \{(r, \phi) : R_1 \leq r \leq R_2\},$$

where \((r, \phi)\) are polar coordinates.

For symmetry reasons, an annulus has a circular principle curve. Using Equation (3) it is not hard to show that

$$r_{circ} = \frac{2 (R_1^2 + R_1 R_2 + R_2^2)}{3 (R_1 + R_2)}.$$

Let \(f(s)\) be the infinitesimal variation generated by a smooth variation \(\Gamma_t\) of the principal circle.

Observing that the moments \(\mu_0, \mu_\perp, \sigma_\perp^2\) are constant, and using Theorem 3, we obtain

$$I''(0) = \frac{2\mu_0 \sigma_\perp^2}{\mu_\perp^2 + \sigma_\perp^2} \int_\Gamma f^2(s) \, ds - 2\mu_0 (\mu_\perp^2 + \sigma_\perp^2) \int_\Gamma f'^2(s) \, ds. \quad (10)$$

We express the second variation \(I''(0)\) in terms of the Fourier expansion of \(f(s)\):

$$f(s) = a_0 + \sum_{n=1}^\infty a_n \cos (\omega_n s) + b_n \sin (\omega_n s)$$

where \(\omega_n = 2\pi n / L_\Gamma\) are the Fourier frequencies. Substituting

$$\int_\Gamma f^2(s) \, ds = \frac{L_\Gamma}{2} \left(2a_0^2 + \sum_{n=1}^\infty (a_n^2 + b_n^2)\right)$$

and

$$\int_\Gamma f'^2(s) \, ds = \frac{L_\Gamma}{2} \sum_{n=1}^\infty \omega_n^2 (a_n^2 + b_n^2)$$
into Equation (10) and simplifying gives

\[ I''(0) = \mu_0 L \Gamma \left\{ \frac{2\sigma^2}{\mu^2 + \sigma^2} a_0^2 + \sum_{n=1}^{\infty} \left( \frac{\sigma^2}{\mu^2 + \sigma^2} - \omega^2_n (\mu^2 + \sigma^2) \right) (a_n^2 + b_n^2) \right\}. \]

Thus, \( I''(0) \) will be positive, and the principal circle will be a local minimum of the distance, within the space of variations with frequency

\[ \omega_n < \frac{\sigma^2}{\mu^2 + \sigma^2}. \]

5.2 The General Case

In the previous example the transverse moments were constant along the principal curve \( \Gamma \). This allowed us to obtain a simple expression for the second variation \( I''(0) \) in terms of the Fourier coefficients of \( f \). Similar computations can be carried out if the transverse moments are approximately constant. In this case, \( I''(0) \) can be expressed in terms of a (generalized) Fourier expansion of the infinitesimal variation \( f \) with respect to a basis \( \{ f_n \}_{n=1}^{\infty} \) of functions on \( \Gamma \) that is naturally associated with the transverse moments of \( p \). The details of how this basis is constructed can be found in Duchamp and Stuetzle (1993).

There are three important features of this basis:

1. The functions \( f_n \) are approximately periodic functions whose frequencies increase with increasing \( n \).

2. If \( f = \sum_{n=1}^{\infty} a_n f_n \), then

\[ I''(0) = \sum_{n=1}^{\infty} (1 - \lambda_n) |a_n|^2, \]

where \( \lambda_n \) is a monotone non-decreasing sequence of positive real numbers.

3. \( \lambda_n > 1 \) when the frequency is greater than \( \sigma_\perp(s)/(\mu_\perp^2(s) + \sigma_\perp^2(s)) \) and \( \lambda_n < 1 \) when the frequency is smaller than \( \sigma_\perp(s)/(\mu_\perp^2(s) + \sigma_\perp^2(s)) \).

Thus, \( I''(0) > 0 \) if the Fourier expansion of \( f \) only contains terms of frequency lower than \( \sigma_\perp(s)/(\mu_\perp^2(s) + \sigma_\perp^2(s)) \). Therefore \( \Gamma \) is a local minimum of \( I \) within the class of such variations. A more precise statement and a proof are presented in Duchamp and Stuetzle (1993).
6 Conclusion

Principal curves were invented to formalize the concept of “a curve passing through the middle of a data set”. In this paper we show that, while principal curves are critical points of the distance function, they are never local minima. Thus there is no justification for the use of cross-validation to determine the complexity of principal curve estimates, and indeed cross-validation has been observed to fail in practice.

To our knowledge, nobody has as yet suggested a reasonably motivated, automatic method for choice of model complexity in the context of manifold estimation or nonparametric orthogonal distance regression. This remains an important open problem.

References


