

Nonparametric Inference for Geometric Objects

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Outline:

- inference for geometric features/objects - overview
- distribution theory for filament estimation
- suprema of gaussian processes on growing manifolds

Inference for geometric objects

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- Estimation of integral curves

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- Estimation of level sets

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- Estimation and inference for persistent homology
(topological data analysis)

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Consider $\hat{V}(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right) V_i$ and estimate $\mathcal{X}(t)$ via

$$\frac{d}{dt}\hat{\mathcal{X}}(t) = \hat{V}(\hat{\mathcal{X}}(t)), \quad \hat{\mathcal{X}}(0) = x_0.$$

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Koltchinskii et al. (2007) show that under appropriate assumptions

$$\sqrt{nh^{d-1}} (\hat{\mathcal{X}}(t) - x(t)) \rightarrow_{\mathcal{D}} G(t), \quad 0 \leq t \leq T,$$

where $T > 0$, $\{G(t), 0 \leq t \leq T\}$ mean zero Gaussian process.

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Heuristics underlying the derivation of the rate:

- Integral curve: $\mathcal{X}(t) = x_0 + \int_0^t V(\mathcal{X}(s)) ds;$
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integration \rightsquigarrow gain of one power of h .

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Note also that

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Further work: Carmichael and Sakhanenko (2015, 2015), Qiao and WP (2015)

Integral curves driven by second eigenvector of Hessian

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Motivation: Filament (ridge line) estimation.

More later.

Estimation of level sets

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Level sets of a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ are given by

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- **plug-in approach via kernel density estimation:** Baillo et al. (2000), Cuevas et al. (2001, 2006, 2007, 2009), Cadre (2006), Scott et al. (2006), Mason and WP (2009), Rigollet and Vert (2009), Bouka et al. (2015)...

Confidence regions for density level sets

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$X_1, \dots, X_n \sim f$. Fix $\lambda > 0$ and $\gamma \in [0, 1]$.

GOAL: Find region \hat{C}_n with $P(f^{-1}(\lambda) \subset \hat{C}_n) \rightarrow \gamma$.

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Two different approaches in literature, based on

- vertical variation
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- vertical variation
- horizontal variation

Both approaches are based on kernel density estimation:

Let $\widehat{f}_n(x) = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{X_i - x}{h}\right)$, and

$$\Gamma_{\widehat{f}}(\lambda) = \{x \in \mathbb{R}^d : \widehat{f}_n(x) \geq \lambda\}.$$

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Construct confidence region of the form

$$\widehat{C}_n = \Gamma_{\widehat{f}}(\lambda - \beta_n) \setminus \Gamma_{\widehat{f}}(\lambda + \beta_n) = \widehat{f}_n^{-1}[\lambda - \beta_n, \lambda + \beta_n].$$

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because

$$\begin{aligned} f^{-1}(\lambda) &\subset \widehat{f}_n^{-1}[\lambda - \beta_n, \lambda + \beta_n] \\ &\Leftrightarrow \\ -\beta_n &\leq \widehat{f}_n(x) - \lambda \leq \beta_n \quad \text{for all } x \in f^{-1}(\lambda) \end{aligned}$$

Vertical variation

One might consider two approximations of distribution of $\sup_{x \in f^{-1}(\lambda)} |\hat{f}_n(x) - f(x)|$:

- bootstrap
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Mammen and WP (2013) use related approach and construct bootstrap approximation of $\sup_{x \in f^{-1}[\lambda - b_n, \lambda + b_n]} |\hat{f}_n(x) - f(x)|$, for appropriately chosen sequence $b_n \rightarrow 0$.

Horizontal variation

Chen et al. (2015a), Qiao and WP (2015)

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 confidence regions by using quantiles of Hausdorff distance

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 confidence regions by using quantiles of Hausdorff distance

$$d_H(f^{-1}(\lambda), \hat{f}_n^{-1}(\lambda)) = \max \left[\sup_{x \in f^{-1}(\lambda)} d(x, \hat{f}_n^{-1}(\lambda)), \sup_{x \in \hat{f}_n^{-1}(\lambda)} d(x, f^{-1}(\lambda)) \right].$$

Inference for modes / modal clustering

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- excess mass approach, Hartigan's dip \rightsquigarrow testing for modes

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- integral curves driven by gradient fields \rightsquigarrow modal clustering

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- integral curves driven by gradient fields \rightsquigarrow modal clustering
- existence of antimodes \rightsquigarrow testing for modes

Hartigan (1975, 1985, 1987, 2000); Müller and Sawitzki (1991); WP (1995); Burman & WP (2009); Chacón (2013), Chen et al. (2015b)

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Distinguish between signal and noise by using *persistence*.

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Bubenik and Kim (2006); Balakrishnan et al. (2011, 2013); Chazal et al. (2014a,b), Fasy et al. (2013); Bauer et al. (2014), Bobrowski et al. (2015), Boissonat et al. (2015), ...

Filament or ridge line estimation

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- What is a filament?

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Definition: A point is said to be a ridge point or a *filament point* if

$$\lambda_2 < 0$$
$$H \nabla f = \lambda_1 \nabla f$$

where $\lambda_1 > \lambda_2$ are the two eigenvalues of the Hessian $H(x)$.

A *filament* consists of filament points and is an integral curve of the gradient.

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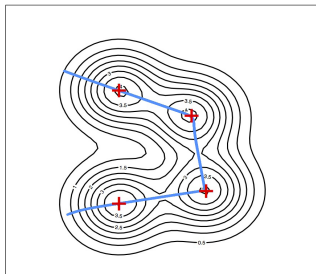
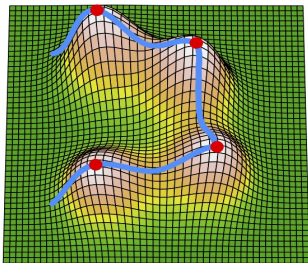
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Let $V(x)$ denote *second* eigenvector of Hessian H .

On the filament, either $\nabla f = 0$ or $\nabla f \parallel V^\perp$, i.e. $\langle \nabla f, V \rangle = 0$.



From Chen et al. (2014).



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Application areas

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- seismology: analysis of fault lines
- analysing road or river networks
- cosmology: cosmic web
- medical imaging: e.g. blood vessels network
-
-
-

Related literature

- Minimum spanning tree, Barrow et al. (1985)
- Candy model, Stoica et al. (2005)
- Principal curves ; Hastie and Stuetzle (1989), Kegl et al. (2000), Sandilya and Kulkarni (2002), and Smola et al. (2001)
- Local principal curve; Einbeck, Tutz and Evers (2005), Einbeck, Evers, and Bailer-Jones (2007)
- Skeleton; Novikov et al. (2006)
- Nonparametric penalized maximum likelihood; Tibshirani (1992)
- Beamlets; Donoho and Huo (2002), Arias-Castro et al. (2006)
- feature detection in point clouds (Engineering/CS): e.g. Weber et al. (2006), Daniels et al. (2007) ...
-
-

Related other concepts

Conceptually related to other statistical concepts:

- mode hunting

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- beamlets, curvelets, ridgelets . . . (Candés 1999; Candés and Donoho, 1999; Donoho and Huo, 2002).

Statistical literature

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Statistical literature:

- Cheng, Hall and Hartigan (2004);
- Arias-Castro, Donoho, and Huo (2006);
- Genovese et al. (2009, 2012, 2014);
- Chen et al. (2013, 2014)
- Qiao and WP (2015)

Genovese et al. (2009): Path density

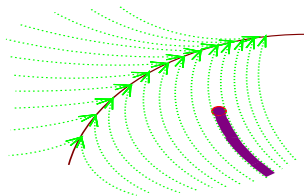
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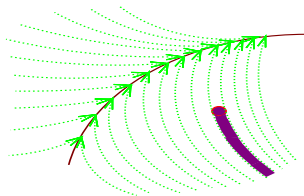
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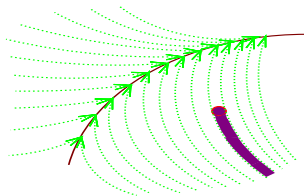


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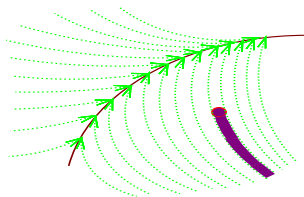
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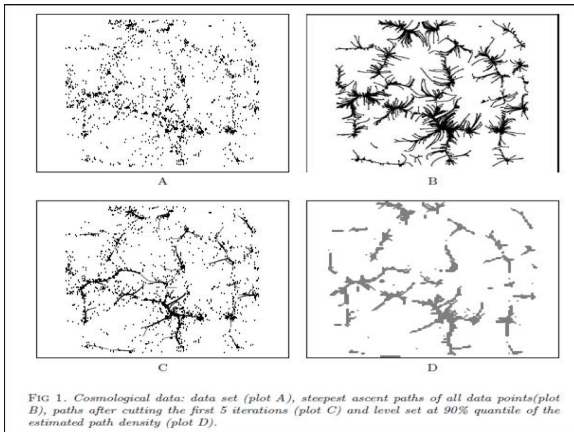
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- Consider level set of estimated path density as 'estimator'.

Path density

Galaxy distribution in a slice



Data source: www.mpa-garching.mpg.de

A different model

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Genovese et al. (2012b) consider the medial axis of the level set to estimate the filament.

Medial axis

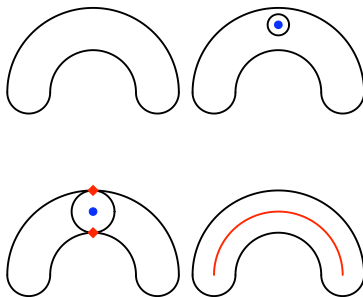


FIG 3. *The Medial Axis. Top left: a set S . Top right: a non-medial ball contained in S ; Bottom left: a medial ball that touches the boundary of S in 2 places. Bottom right: the medial axis consists of the centers of the medial balls.*

From Genovese et al. 2012.

Distribution theory for filament estimation

Qiao and WP (2015)

$$\mathbf{d} = 2$$

Ridge estimation via bump hunting

We now consider filament estimation based on iid observations from a density f assuming the existence of a ridge line. Recall

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Definition: A point is said to be a ridge point or a *filament point* if

$$\lambda_2 < 0$$
$$H \nabla f = \lambda_1 \nabla f$$

where $\lambda_1 > \lambda_2$ are the two eigenvalues of the Hessian $H(x)$.

$V(x)$ denotes *second* eigenvector of Hessian H .

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Same idea is used in Chen et al. (2015c).

Some notation

Hessian

$$H = H(x) = \begin{pmatrix} f_{11}(x) & f_{12}(x) \\ f_{12}(x) & f_{22}(x) \end{pmatrix}$$

Let

$$V = \begin{pmatrix} f_{11} - f_{22} + f_{12} - \sqrt{(f_{22} - f_{11})^2 + 4f_{12}^2} \\ \frac{1}{2} \left(f_{22} - f_{11} + f_{12} - 4\sqrt{(f_{22} - f_{11})^2 + 4f_{12}^2} \right) \end{pmatrix}.$$

then $V(x)$ is eigenvectors for $\lambda_2(x)$.

Some notation

Use kernel density estimator based on $X_1, X_2, \dots, X_n \stackrel{\text{iid}}{\sim} f$

$$\hat{f}(x) = \frac{1}{nh^2} \sum_{i=1}^n K\left(\frac{x - X_i}{h}\right).$$

The kernel estimator of Hessian is

$$\begin{aligned} \hat{H}(x) &= \begin{pmatrix} \hat{f}_{11}(x) & \hat{f}_{12}(x) \\ \hat{f}_{12}(x) & \hat{f}_{22}(x) \end{pmatrix} \\ &= \frac{1}{nh^4} \sum_{i=1}^n \begin{pmatrix} K_{11}\left(\frac{x-X_i}{h}\right) & K_{12}\left(\frac{x-X_i}{h}\right) \\ K_{12}\left(\frac{x-X_i}{h}\right) & K_{22}\left(\frac{x-X_i}{h}\right) \end{pmatrix} \end{aligned}$$

with second eigenvalue $\hat{\lambda}_2$ corresponding second eigenvector $\hat{V}(x)$.

More notation

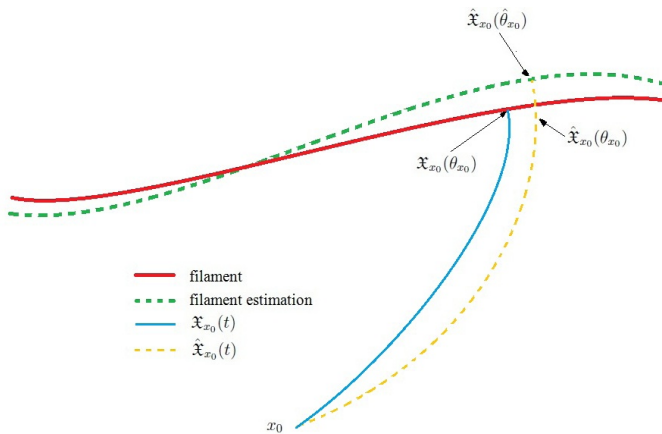
For each $x_0 \in \mathcal{G}$ let

- $\mathcal{X}_{x_0}(t), t \in [0, T]$ integral curve corresponding to vector field $V(x)$ starting at x_0 ;
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Mathematical problems

Integral curve estimation:

Find asymptotic distribution of (appropriately normalized)

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↪ involves finding limit of the distribution of the supremum over (increasing) manifolds of a sequence non-stationary Gaussian process .

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Estimation of integral curves: Assumptions

(K1) The kernel K is a symmetric probability density function with support $\{x : \|x\| < 1\}$. All of its first to fourth order partial derivatives are bounded and $\int_{\mathbb{R}^2} K(x)xx^T dx = \mu_2(K)\mathbf{Id}$ with $\mu_2(K) < \infty$.

(K2) $\mathbf{R}(d^2K) < \infty$, where for any function $g : \mathbb{R}^2 \mapsto \mathbb{R}^3$,
$$\mathbf{R}(g) \equiv \int_{\mathbb{R}^2} g(x)g(x)^T dx.$$

(K3) $\int [K^{(3,0)}(z)]^2 dz \neq \int [K^{(1,2)}(z)]^2 dz.$

(H1) As $n \rightarrow \infty$, $h_n \downarrow 0$, $nh_n^8/(\log n)^3 \rightarrow \infty$, $nh_n^9 \rightarrow \beta$, $\beta \geq 0$.

Estimation of integral curves

Theorem

Under above assumptions and for each $T > 0$, the sequence of stochastic process

$$\sqrt{nh^5}(\hat{\mathcal{X}}_{x_0}(t) - \mathcal{X}_{x_0}(t)), \quad 0 \leq t \leq T$$

converges weakly in $C([0, T], \mathbb{R}^2)$ to a Gaussian process as $n \rightarrow \infty$.

The proof is an adaptation of Koltchinskii et al. (2007).

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$$\bullet \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) = \underbrace{\left[\hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\hat{\theta}) \right]}_{O_P(1/\sqrt{nh^5})} + \underbrace{\left[\mathcal{X}(\hat{\theta}) - \mathcal{X}(\theta) \right]}_{O_P(V(\mathcal{X}(\theta))(\hat{\theta}-\theta))}.$$

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- $\hat{\theta} - \theta = O_P(1/\sqrt{nh^6})$ if $\nabla f(\mathcal{X}(\theta)) \neq 0$, and
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Heuristic

A heuristic argument for why estimation of filaments is easier when $\nabla f(x) = 0$ at the filament:

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Recall: on filament $H(x) \nabla f(x) = \lambda_1(x) \nabla f(x)$.

Thus, when replacing H and f by their estimates, then, if $\nabla f(x) = 0$, this equality holds approximately if we can estimate first derivatives well. The estimation of second derivatives is not too important. Thus the rates are driven by how well we can estimate first derivatives as opposed to second derivatives, and the former is easier (faster rates).

Filament estimation: more assumptions

(F6) For any $x_0 \in \mathcal{H}$ with $x_0 \prec \mathcal{L}$, θ_{x_0} exists and
$$\sup_{x_0 \in \mathcal{H}, x_0 \prec \mathcal{L}} T_{x_0} < \infty.$$

(F7) $\nabla \langle \nabla f(x) V(x) \rangle \neq 0$ for all $x \in \mathcal{L}$

(F8) $\{x \in \mathcal{H} : \lambda_2(x) = 0, \nabla f(x) V(x) = 0\} = \emptyset.$

Filament estimation: Pointwise convergence

Theorem

Assume that above assumptions hold, $nh^9 \rightarrow \beta \geq 0$, $h_n \rightarrow 0$. Then for any fixed starting point x_0 :

$$(a) \quad \sqrt{nh^6} \langle V(\mathcal{X}(\theta)), \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) \rangle \rightarrow_{\mathcal{D}} N(0, \sigma_1^2),$$

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(b) If $\nabla f(\mathcal{X}(\theta)) = 0$, then

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$$(a) \quad \begin{aligned} \sqrt{nh^6} \langle V(\mathcal{X}(\theta)), \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) \rangle &\rightarrow_{\mathcal{D}} N(0, \sigma_1^2), \\ \sqrt{nh^5} \langle V(\mathcal{X}(\theta))^\perp, \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) \rangle &\rightarrow_{\mathcal{D}} N(0, \sigma_2^2). \end{aligned}$$

(b) If $\nabla f(\mathcal{X}(\theta)) = 0$, then

$$\begin{aligned} \sqrt{nh^5} \langle V(\mathcal{X}(\theta)), \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) \rangle &\rightarrow_{\mathcal{D}} N(\mu_1, \sigma_3^2), \\ \sqrt{nh^5} \langle V(\mathcal{X}(\theta))^\perp, \hat{\mathcal{X}}(\hat{\theta}) - \mathcal{X}(\theta) \rangle &\rightarrow_{\mathcal{D}} N(\mu_2, \sigma_4^2). \end{aligned}$$

Filament estimation: Pointwise convergence continued

Theorem

Assume that above assumptions hold, $nh^9 \rightarrow \beta \geq 0$, $h \rightarrow 0$. Then for any fixed starting point x_0

$$\sqrt{nh^6}[\hat{\mathcal{X}}_{x_0}(\hat{\theta}_{x_0}) - \mathcal{X}_{x_0}(\theta_{x_0})] \rightarrow Z(\mathcal{X}_{x_0}(\theta_{x_0}))V(\mathcal{X}_{x_0}(\theta_{x_0})),$$

where $Z(\mathcal{X}_{x_0}(\theta_{x_0}))$ is a mean zero normal random variable.

Filament estimation: Pointwise convergence continued

Theorem

Suppose that the assumptions of the above Theorem hold, and in addition assume that $\nabla f(\mathcal{X}_{x_0}(\theta_{x_0})) = 0$. Then there exists $\mu(x_0) \in \mathbb{R}^2$ and $\Sigma(x_0) \in \mathbb{R}^{2 \times 2}$ such that

$$\sqrt{nh^5}[\hat{\mathcal{X}}_{x_0}(\hat{\theta}_{x_0}) - \mathcal{X}_{x_0}(\theta_{x_0})] \rightarrow \mathcal{N}(\mu(x_0), \Sigma(x_0)).$$

Uniform convergence

Theorem

Under the above assumptions there exists a constant $c > 0$ and a function $b(x)$, both depending on f and the kernel K , such that for any fixed z , we have

$$\lim_{n \rightarrow \infty} P \left(\sup_{x_0 \in \mathcal{G}} \left\| b(\mathcal{X}_{x_0}(\theta_{x_0})) \sqrt{nh^6} \left(\hat{\mathcal{X}}_{x_0}(\hat{\theta}_{x_0}) - \mathcal{X}_{x_0}(\theta_{x_0}) \right) \right\| < B_h(z) \right) = \exp\{-2 \exp\{-z\}\},$$

where $B_h(z) = \sqrt{2 \log h^{-1}} + \frac{1}{\sqrt{2 \log h^{-1}}} [z + c]$ and \mathcal{G} is some properly chosen region of starting points.

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First use ideas similar to Bickel and Rosenblatt (1973). Main ingredient to the proof is a generalization of a theorem by Mikhaleva and Piterbarg (1996).

Generalization of a theorem by Mikhaleva and Piterbarg

Definition (Local equi- D_t -stationarity)

Let $X_h(t)$, $t \in \mathcal{G} \subset \mathbb{R}^2$ be a class of process indexed by $h \in \mathbb{H}$ with covariance function $r_h(t_1, t_2)$. The sequence $X_h(t)$ is *locally equi- D_t^h -stationary*, if for any $\epsilon > 0$ there exists a positive $\delta(\epsilon)$ independent of h such that for any $s \in \mathcal{G}$ one can find a non-degenerated matrix D_s^h such that

$$1 - (1 + \epsilon) \|D_s^h(t_1 - t_2)\|^2 \leq r_h(t_1, t_2) \leq 1 - (1 - \epsilon) \|D_s^h(t_1 - t_2)\|^2$$

provided $\|t_1 - s\| < \delta(\epsilon)$ and $\|t_2 - s\| < \delta(\epsilon)$ where $\|\cdot\|$ is Frobenius norm.

Generalization of a theorem by Mikhaleva and Piterbarg

Theorem

Let $\mathcal{M}_1 \subset \mathcal{H}$ be a smooth compact 1-dimensional manifold with bounded curvature, $\{X_h(t), t \in \mathbb{R}^2, 0 < h \leq 1\}$ a class of centered, locally D_t^h -stationary Gaussian fields. Under below assumptions, there exists $M > 0$ such that with $x_h(z) = (2 \log \frac{1}{h})^{\frac{1}{2}} (1 + \frac{M+z}{2 \log \frac{1}{h}})$ we have

$$\lim_{h \rightarrow 0} P\left\{ \sup_{t \in \mathcal{M}_h} |X_h(t)| \leq x_h(z) \right\} = \exp\{-2 \exp\{-z\}\}$$

where $\mathcal{M}_h = \frac{\mathcal{M}_1}{h}$.

Generalization of a theorem by Mikhaleva and Piterbarg

ASSUMPTIONS:

$\mathcal{M}_1 \subset \mathcal{H}$ smooth compact 1-dimensional manifold with bounded curvature.

Generalization of a theorem by Mikhaleva and Piterbarg

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- D_t^h positive definite and $(t, h) \rightarrow D_t^h$, continuous;

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- D_t^h positive definite and $(t, h) \rightarrow D_t^h$, continuous;
- $\inf_{0 < h \leq 1, hs \in \mathcal{H}} \lambda_2(\{D_s^h\}' D_s^h) \geq C$;

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- $\inf_{0 < h \leq 1, hs \in \mathcal{H}} \lambda_2(\{D_s^h\}' D_s^h) \geq C$;
- $\lim_{h \rightarrow 0, ht = t^*} D_t^h = D_{t^*}^0$ uniformly in $t^* \in \mathcal{H}$;

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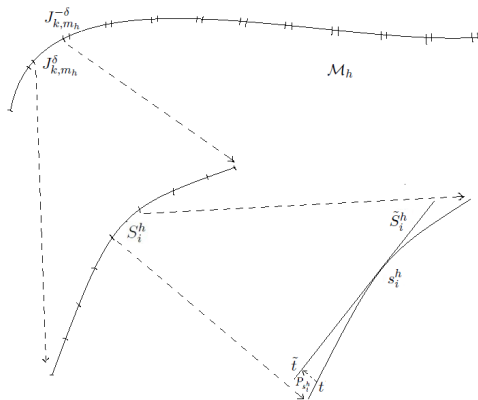
With
$$Q(\delta) := \sup_{0 < h \leq 1} \{|r_h(x+y, y)|, \|x\| > \delta\},$$

where $r_h(x, y)$ the covariance function of $\mathcal{X}_h(t)$, we have

$$0 \leq Q(\delta) < 1$$

$$\exists \tilde{\delta} > 0 : Q(\delta) = 0 \quad \text{for all } \delta \geq \tilde{\delta}.$$

Heuristics of the proof.



A more general result

Definition (Local equi- (α, D_t) -stationarity)

Let $X_h(t)$, $t \in \mathcal{G} \subset \mathbb{R}^d$ be a class of process indexed by $h \in \mathbb{H}$ with covariance function $r_h(t_1, t_2)$. The sequence $X_h(t)$ is *locally equi- (α, D_t^h) -stationary*, if for any $\epsilon > 0$ there exists a positive $\delta(\epsilon)$ independent of h such that for any $s \in \mathcal{G}$ one can find a non-degenerated matrix D_s^h such that

$$1 - (1 + \epsilon) \|D_s^h(t_1 - t_2)\|^\alpha \leq r_h(t_1, t_2) \leq 1 - (1 - \epsilon) \|D_s^h(t_1 - t_2)\|^\alpha$$

provided $\|t_1 - s\| < \delta(\epsilon)$ and $\|t_2 - s\| < \delta(\epsilon)$ where $\|\cdot\|$ is Frobenius norm.

Generalization of a theorem by Mikhaleva and Piterbarg

ASSUMPTIONS:

$\mathcal{M}_1 \subset \mathcal{H}$ smooth compact r -dimensional manifold with **positive condition number**.

Generalization of a theorem by Mikhaleva and Piterbarg

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$\mathcal{M}_1 \subset \mathcal{H}$ smooth compact r -dimensional manifold with **positive condition number**. $\{X_h(t), t \in \mathbb{R}^d, 0 < h \leq 1\}$ sequence of centered, locally (α, D_t^h) -stationary Gaussian fields with

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- D_t^h positive definite and $(t, h) \rightarrow D_t^h$, continuous in $h \in (0, 1]$, $t \in \mathbb{R}^2$;
- $\inf_{0 < h \leq 1, h s \in \mathcal{H}} \lambda_2(\{D_s^h\}' D_s^h) \geq C$,
- $\lim_{h \rightarrow 0, ht = t^*} D_t^h = D_{t^*}^0$ uniformly in $t^* \in \mathcal{H}$;
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- $t^* \rightarrow D_{t^*}^0$, $t^* \in \mathcal{H}$ is continuous.

With $Q(\delta)$ as above

$$Q(\delta) < 1 \quad \text{for all } \delta > 0,$$

$$Q(\delta) |(\log \delta)^{2r/\alpha}| \leq (\log \delta)^{-\beta} \quad \text{for some } \beta > 0.$$

Generalization of a theorem by Mikhaleva and Piterbarg

Theorem

There exists $M > 0$ such that with

$$x_h(z) = (2r \log \frac{1}{h})^{\frac{1}{2}} \left(1 + \frac{M+z+(\frac{r}{\alpha}-\frac{1}{2}) \log \log \frac{1}{h}}{2r \log \frac{1}{h}} \right)$$

we have

$$\lim_{h \rightarrow 0} P \left\{ \sup_{t \in \mathcal{M}_h} |X_h(t)| \leq x_h(z) \right\} = \exp \{ -2 \exp \{ -z \} \}$$

where $\mathcal{M}_h = \frac{\mathcal{M}_1}{h}$.

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