

Asymptotic Theory for Density Ridges

Yen-Chi Chen

Christopher R. Genovese Larry Wasserman

Department of Statistics
Carnegie Mellon University

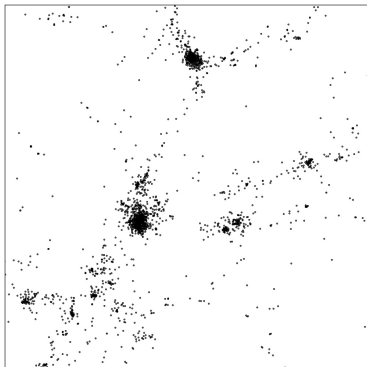
December 13, 2015

Density Ridges: High Density Curves

Density ridges are curves characterizing high density regions.

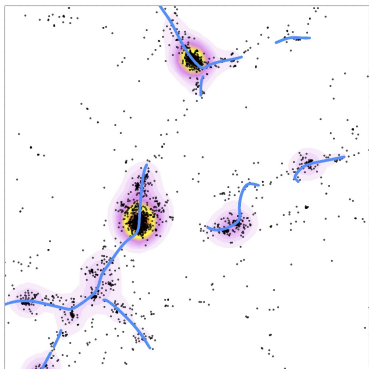
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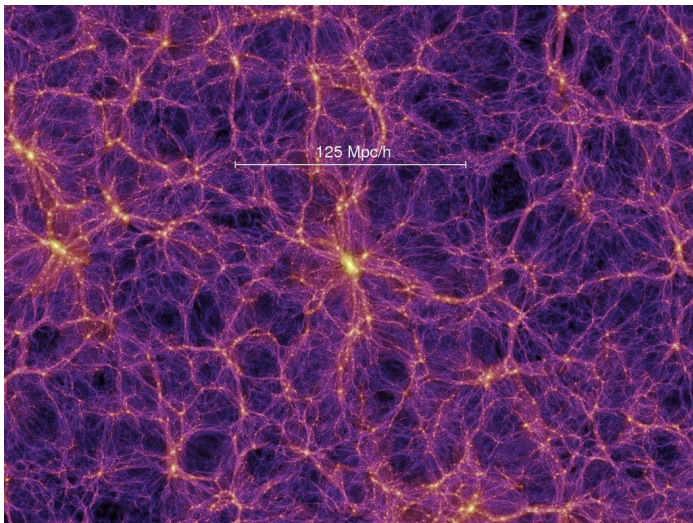


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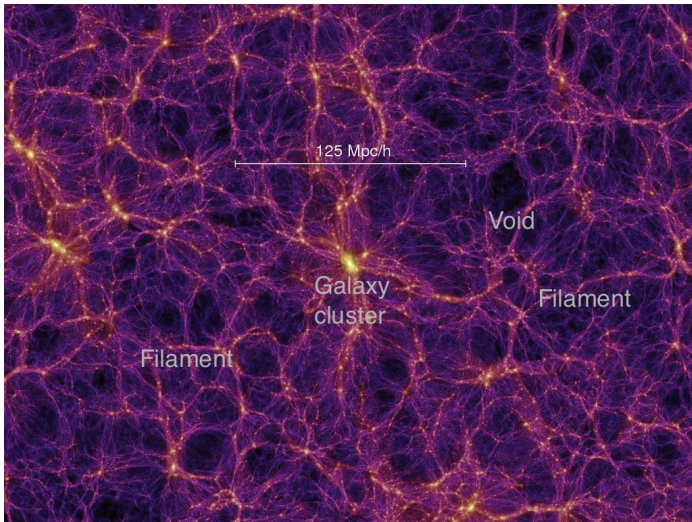


Application of Ridges: Cosmology



Credit: Millennium Simulation

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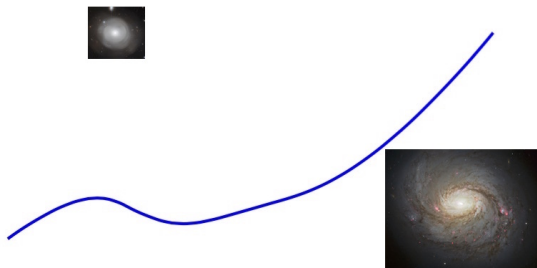
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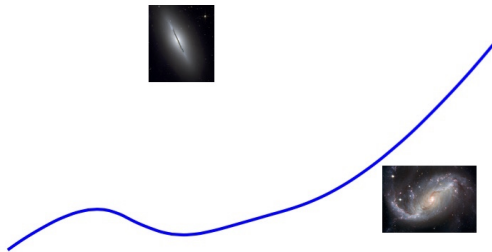


→ **Chen** et al. 'Detecting Effects of Filaments on Galaxy Properties in Sloan Digital Sky Survey III' (2015)

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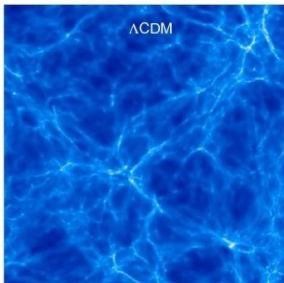
→ **Chen** et al. 'Investigating Galaxy-Filament Alignment in Hydrodynamic Simulations using Density Ridges' (Mon. Not. Roy. Astro. Soc. 2015)

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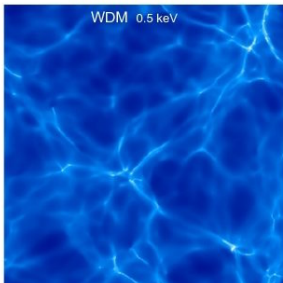
Filaments play key roles in astronomy research.

- A galaxy's brightness, mass, and size are associated with filaments.
- A galaxy's alignment is associated with filaments.
- Filaments can be used to test cosmological models.

cold dark matter



warm dark matter

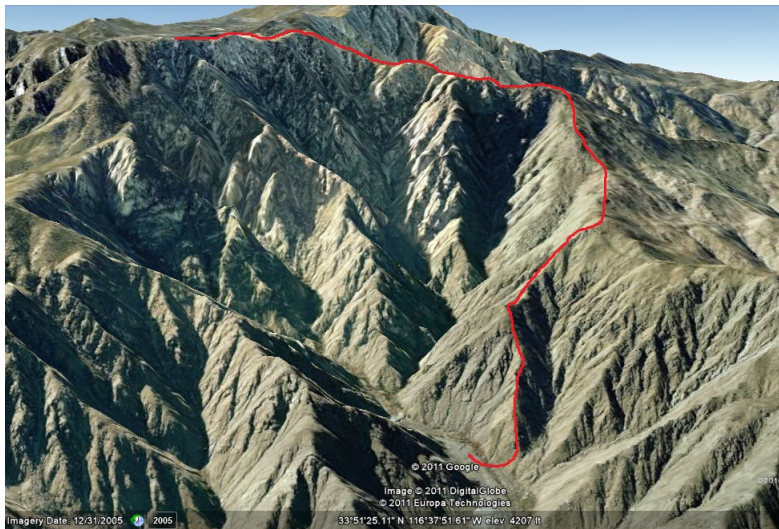


- Credit: Kavli Institute for Cosmology, Cambridge

Density Ridges

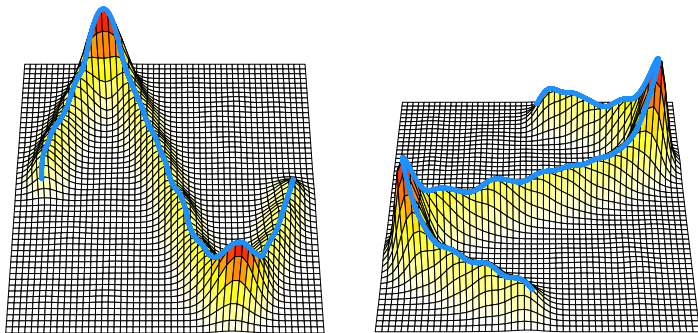
A statistical model for filaments is the *density ridges*.

Example: Ridges in Mountains

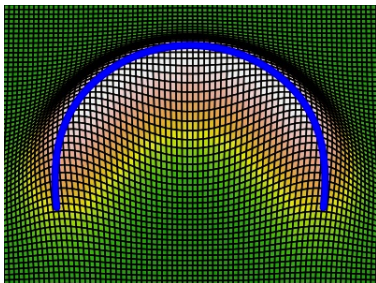
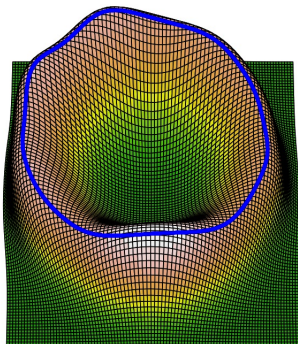


Credit: Google

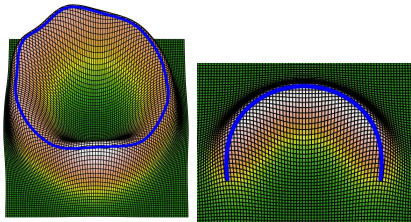
Example: Ridges in Smooth Functions



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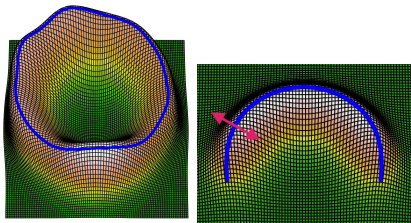


Ridges: Local Modes in Subspace



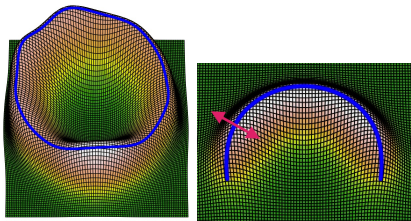
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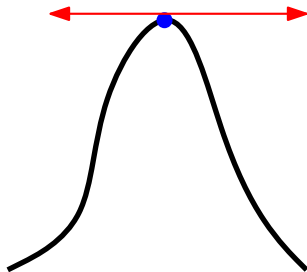


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Formal Definition of Density Ridges

- $p(x)$: the density function.

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Estimator and Algorithm

We use the plug-in estimate:

$$\hat{R}_n = \text{Ridge}(\hat{p}_n),$$

where $\hat{p}_n = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{x-X_i}{h}\right)$ is the KDE.

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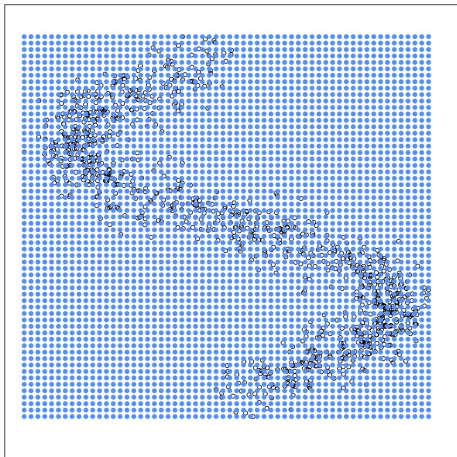
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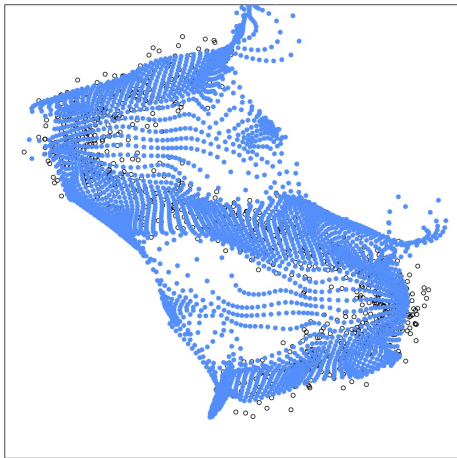
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- The Subspace Constraint Mean Shift (SCMS; Ozertem2011) algorithm allows us to find \hat{R}_n , ridges of the KDE.

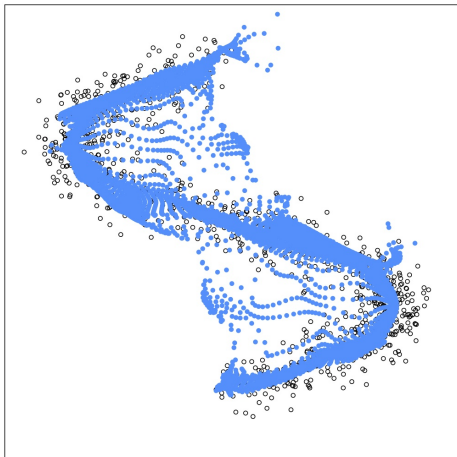
SCMS: Ridge Recovery Algorithm



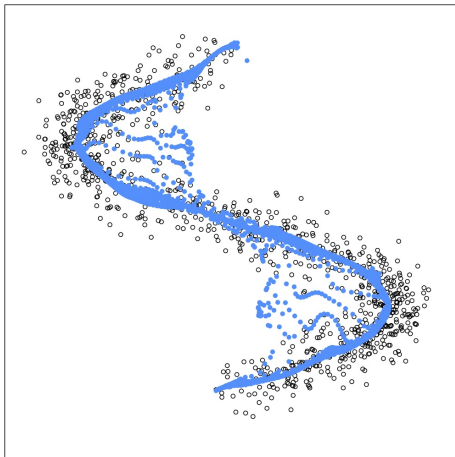
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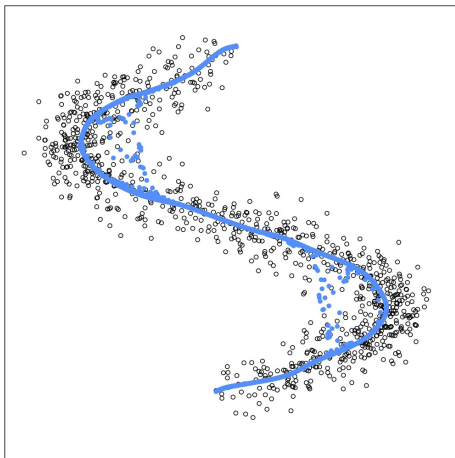
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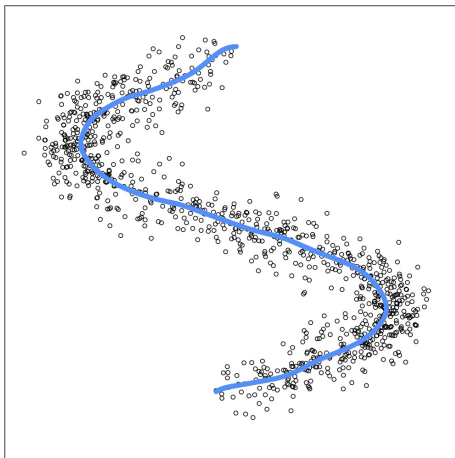
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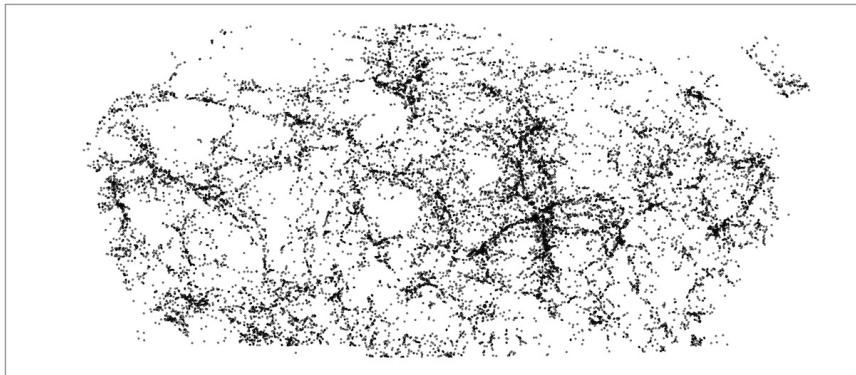
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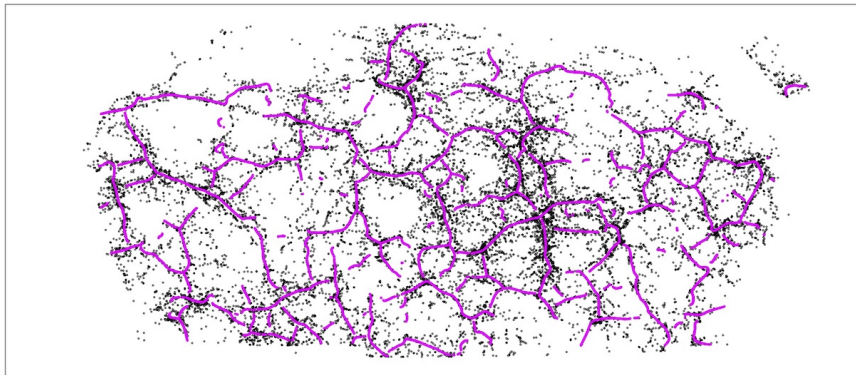
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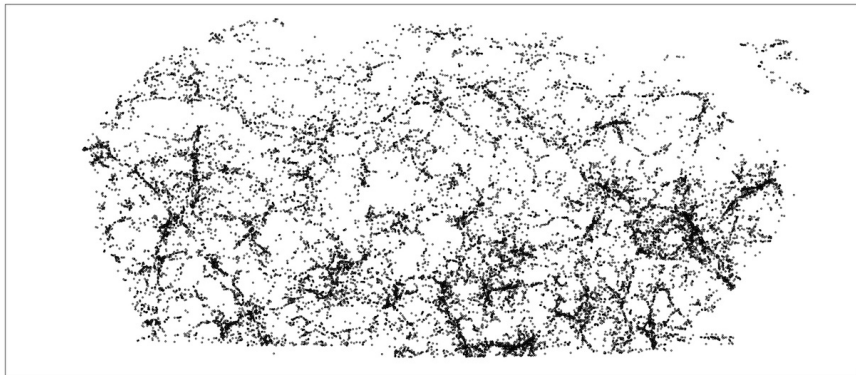
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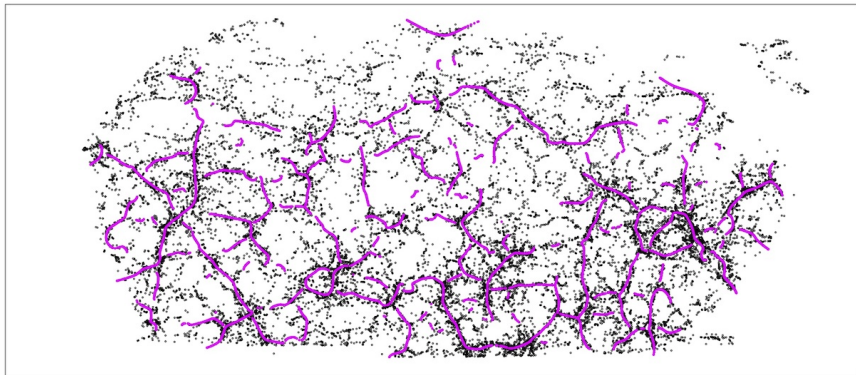
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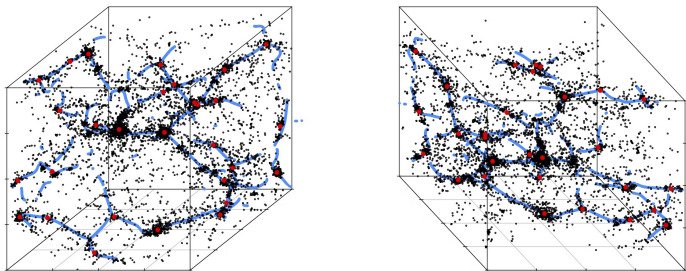
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3D Example for Estimated Ridges



Blue curves: density ridges.

Red points: density local modes.

Statistical Inference: Confidence Sets

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In what follows, we ignore the bias for estimating R and focus only on the stochastic variation of \hat{R}_n .

Useful Metric: Hausdorff Distance

We introduce a useful metric—the *Hausdorff distance* for sets:

$$\text{Haus}(A, B) = \max \left\{ \sup_{x \in A} d(x, B), \sup_{x \in B} d(x, A) \right\},$$

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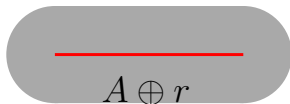
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- Haus is an \mathcal{L}_∞ metric for sets.
- Consistency: $\text{Haus}(\hat{R}_n, R) = o_{\mathbb{P}}(1)$.

The \oplus Operation

We define $A \oplus r = \{x : d(x, A) \leq r\}$.



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Then we have the following inclusion property:

$$A \subset B \oplus \text{Haus}(A, B), \quad B \subset A \oplus \text{Haus}(A, B).$$

Hausdorff Distance and Confidence Sets

We can use Hausdorff distance and \oplus operation to construct confidence sets.

Let F_n be the CDF for $\text{Haus}(\widehat{R}_n, R)$ and $t_{1-\alpha} = F_n^{-1}(1 - \alpha)$ be the $1 - \alpha$ quantile.

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- It can be shown that

$$\mathbb{P}\left(R \subset \widehat{R}_n \oplus t_{1-\alpha}\right) \geq 1 - \alpha.$$

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- We need to find the distribution F_n .

Asymptotic Theory

Key observation:

$$\begin{aligned}\sqrt{nh^{d+2}}\text{Haus}(\hat{R}_n, R) &\approx \sqrt{nh^{d+2}} \sup_{x \in R} d(x, \hat{R}_n) \\ &\approx \sup \{ \text{Empirical process on } R \} \\ &\approx \sup \{ \text{Gaussian process on } R \}.\end{aligned}$$

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Theorem

Under regularity conditions and $\frac{\log n}{nh^{d+6}} \rightarrow 0$, there exists a tight Gaussian process \mathbb{B} defined on a certain function space \mathcal{F} such that

$$\begin{aligned}\sup_t \left| \mathbb{P} \left(\sqrt{nh^{d+2}}\text{Haus}(\widehat{R}_n, R) < t \right) - \mathbb{P} \left(\sup_{f \in \mathcal{F}} |\mathbb{B}(f)| < t \right) \right| \\ = O \left(\left(\frac{\log^7 n}{nh^{d+2}} \right)^{1/8} \right).\end{aligned}$$

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 - Bad news: the asymptotic behavior is complicated.
- A solution: the bootstrap.

The Bootstrap Consistency

- Bootstrap sample \implies bootstrap ridges \widehat{R}_n^* .
- Compute $\text{Haus}(\widehat{R}_n^*, \widehat{R}_n)$ to get a CDF estimator \widehat{F}_n .
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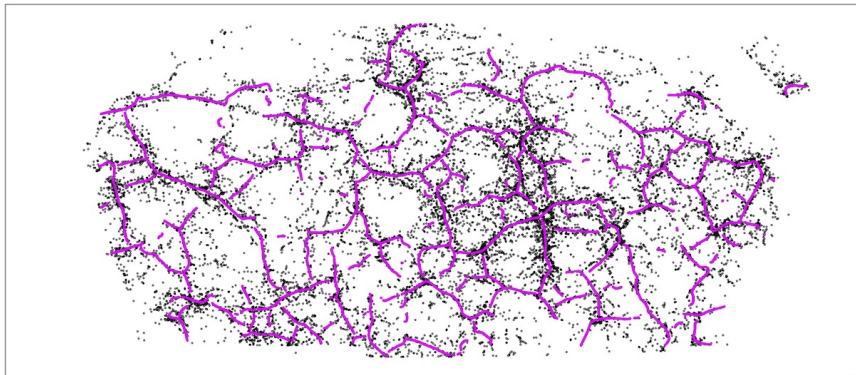
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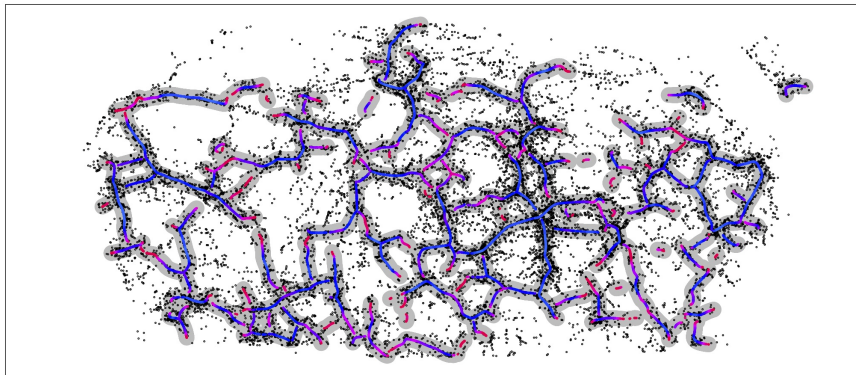
Under regularity conditions and $\frac{\log n}{nh^{d+6}} \rightarrow 0$,

$$\mathbb{P}\left(R \subset \widehat{R}_n \oplus \widehat{t}_{1-\alpha}\right) = 1 - \alpha + O\left(\left(\frac{\log^7 n}{nh^{d+2}}\right)^{1/8}\right).$$

Example for Confidence Sets



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Concluding Remarks

Density ridges are very cool objects because

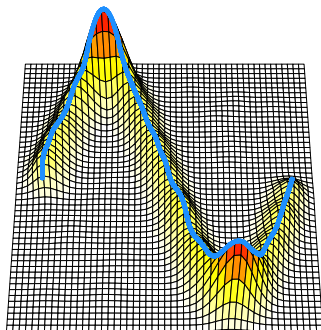
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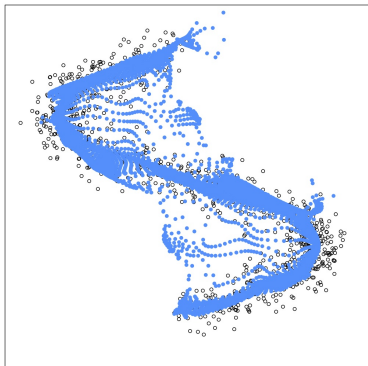
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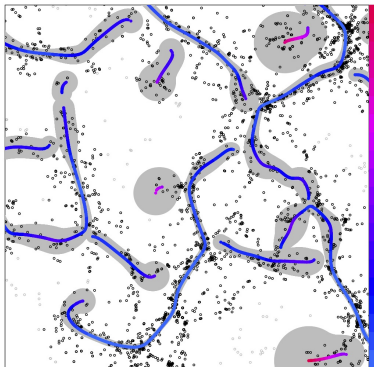
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Density ridges are very cool objects because

- 1 they have cosmological applications,
- 2 they are well-defined objects,
- 3 there is a fast algorithm to compute them,
- 4 their statistical properties are well-studied.



Thank you!

More details can be found in: <http://www.stat.cmu.edu/~yenchic/>

References

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Regularity Conditions

- (K1) The kernel function K is \mathbf{BC}^4 and integrable.
- (K2) K satisfies the VC-type class condition.
- (P1) The density p is in \mathbf{BC}^4 .
- (P2) The eigengap $\lambda_1(x) - \lambda_2(x) \geq \beta_0 > 0$ for points around ridges.
- (P3) The orientation of each ridge point is close to the gradient.

Regularity Conditions on Kernel Functions

(K1) The kernel K is in \mathbf{BC}^4 and $\|K\|_{\infty,4}^* < \infty$.

(K2) Let

$$\mathcal{K}_r = \left\{ y \mapsto K^{(\alpha)} \left(\frac{x-y}{h} \right) : x \in \mathbb{R}^d, |\alpha| = r \right\},$$

where $K^{(\alpha)}$ is the α -th derivative and let $\mathcal{K}_4^* = \bigcup_{r=0}^4 \mathcal{K}_r$. We assume that \mathcal{K}_4^* is a VC-type class. i.e. there exists constants A, ν and a constant envelope b_0 such that

$$\sup_Q N(\mathcal{K}_4^*, \mathcal{L}^2(Q), b_0 \epsilon) \leq \left(\frac{A}{\epsilon} \right)^\nu, \quad (1)$$

where $N(T, d_T, \epsilon)$ is the ϵ -covering number for a semi-metric set T with metric d_T and $\mathcal{L}^2(Q)$ is the L_2 norm with respect to the probability measure Q .

Regularity Conditions on Distributions

- (P1) The density p is in \mathbf{BC}^4 .
- (P2) There exists constants $\beta_0, \beta_1, \beta_2, \delta_0 > 0$ such that

$$\begin{aligned}\lambda_2(x) &\leq -\beta_1 \\ \lambda_1(x) &\geq \beta_0 - \beta_1 \\ \|g(x)\| \max_{|\alpha|=3} |p^{(\alpha)}(x)| &\leq \beta_0(\beta_1 - \beta_2)\end{aligned}\tag{2}$$

for all $x \in R \oplus \delta_0$.

- (P3) For each $x \in R$, $|e(x)^T g(x)|^2 \geq \frac{\lambda_1(x)}{\lambda_1(x) - \lambda_2(x)}$ where $e(x)$ is the direction of R at point $x \in R$.

Smoothed Density Ridges

In particular, we focus on making inference for the smoothed version of the density, denoted as p_h :

$$p_h(x) = p \otimes K_h(x) = \mathbb{E}(\hat{p}_n(x)), \quad K_h(x) = \frac{1}{h^d} K\left(\frac{x}{h}\right),$$

where \otimes denotes the convolution.

- We define $R_h = \text{Ridge}(p_h)$.

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where \otimes denotes the convolution.

- We define $R_h = \text{Ridge}(p_h)$.
- The advantages for focusing on R_h :
 - Always well-defined.
 - Topologically similar.
 - Asymptotically the same.
 - Fast rate of convergence.

Smoothed Density Ridges

In particular, we focus on making inference for the smoothed version of the density, denoted as p_h :

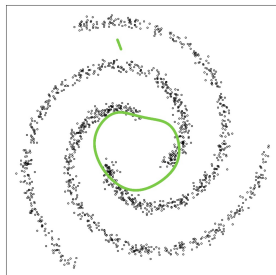
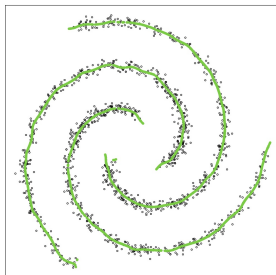
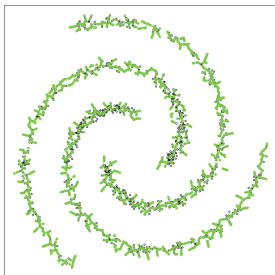
$$p_h(x) = p \otimes K_h(x) = \mathbb{E}(\hat{p}_n(x)), \quad K_h(x) = \frac{1}{h^d} K\left(\frac{x}{h}\right),$$

where \otimes denotes the convolution.

- We define $R_h = \text{Ridge}(p_h)$.
- The advantages for focusing on R_h :
 - Always well-defined.
 - Topologically similar.
 - Asymptotically the same.
 - Fast rate of convergence.
- One can always slightly undersmooth so that inference for R_h is asymptotically valid for R .

Bandwidth Selection for Density Ridges

Effect of Smoothing Bandwidth



Risk for Ridges

Let R and \hat{R}_n be the density ridges and their estimators.

Let

$$U_R \sim \text{Unif}(R), \quad U_{\hat{R}_n} \sim \text{Unif}(\hat{R}_n).$$

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Define

$$W_n = d(U_R, \hat{R}_n), \quad \tilde{W}_n = d(U_{\hat{R}_n}, R)$$

be the projected distance of U_R onto \hat{R}_n and $U_{\hat{R}_n}$ onto R .

We define L_2 risk as

$$\text{Risk}_{2,n} = \frac{1}{2} \mathbb{E}(W_n^2 + \tilde{W}_n^2).$$

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- This is a generalized mean integrated square errors.
- Similarly, one can define $\text{Risk}_{1,n}$ using L_1 loss.

Estimating Risks

We can use bootstrap or data splitting to estimate the risk $\text{Risk}_{2,n}$.
Let \widehat{R}_n^* be the bootstrap version of \widehat{R}_n . Let

$$W_n^* = d(U_{\widehat{R}_n}, \widehat{R}_n^*), \quad \widetilde{W}_n^* = d(U_{\widehat{R}_n^*}, \widehat{R}_n)$$

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$$\widehat{\text{Risk}}_{2,n} = \frac{1}{2} \mathbb{E}(W_n^{*2} + \widetilde{W}_n^{*2} | X_1, \dots, X_n).$$

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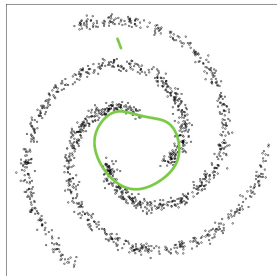
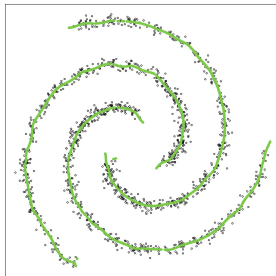
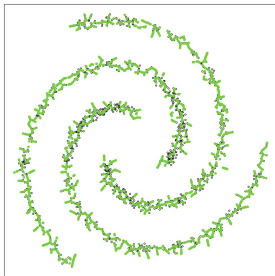
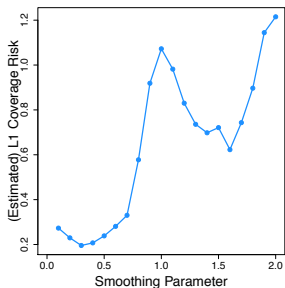
$$\widehat{\text{Risk}}_{2,n} = \frac{1}{2} \mathbb{E}(W_n^{*2} + \widetilde{W}_n^{*2} | X_1, \dots, X_n).$$

Theorem

Under regularity conditions,

$$\frac{\widehat{\text{Risk}}_{2,n}}{\text{Risk}_{2,n}} \xrightarrow{P} 1, \quad \frac{\widehat{\text{Risk}}_{1,n}}{\text{Risk}_{1,n}} \xrightarrow{P} 1.$$

Bandwidth Selection via Risk Minimization



Application to Cosmology Dataset

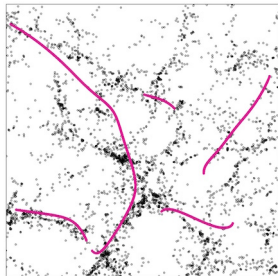
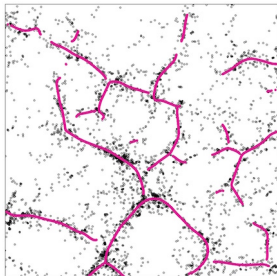
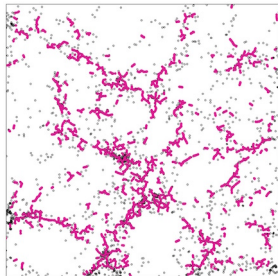
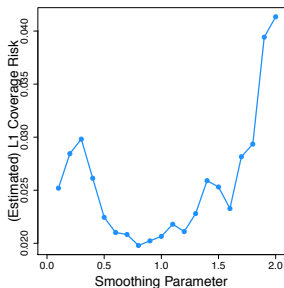
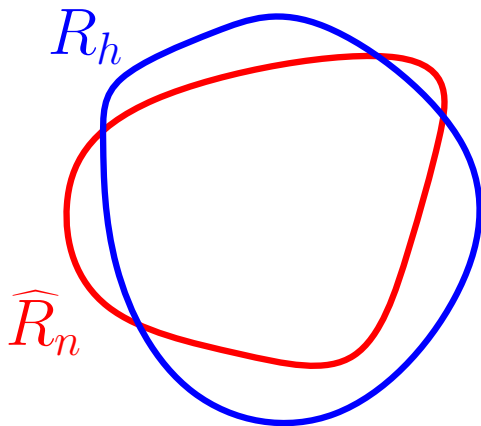
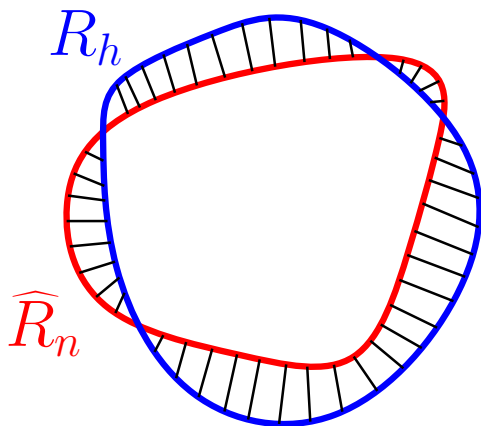
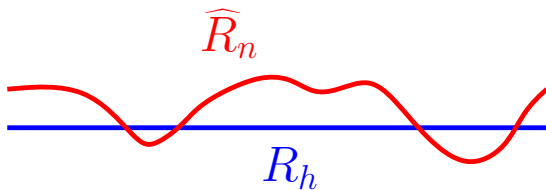


Illustration for Asymptotic Theory

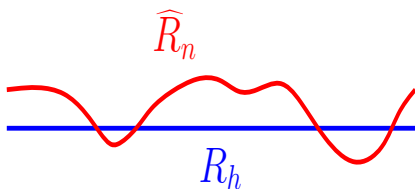






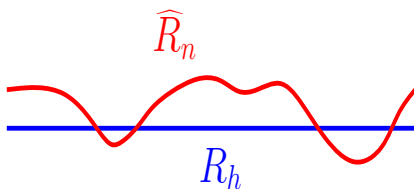
Asymptotic Theory

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- 2 This stochastic process \approx empirical process.



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- 2 This stochastic process \approx empirical process.
- 3 $\text{Haus}(\widehat{D}_n, D_h) = \sup\{\text{projection distance}\} \approx \sup\{\text{Empirical process}\}.$

