STATISTICAL INFERENCE USING GEOMETRIC FEATURES

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Statistics



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Statistics



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Ryan Tibshirani

Collaborators

Astronomy



Shirley Ho



Peter Freeman



Rachel Mandelbaum





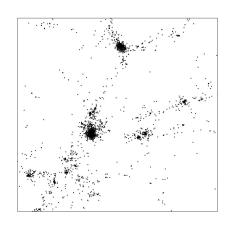
Ran Kafri (University of Toronto)



Miriam Ginzberg (Harvard)



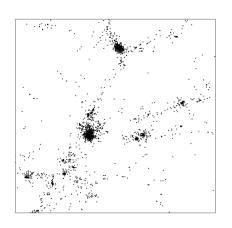
Shixuan Liu (University of Toronto)



The data can be viewed as

$$X_1, \cdots, X_n \sim p$$
,

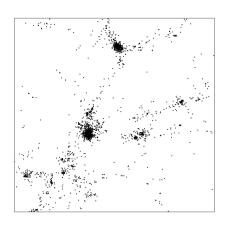
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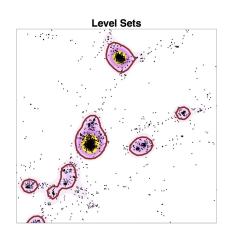
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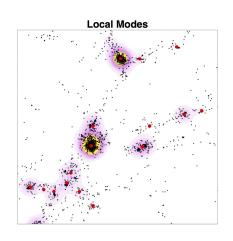
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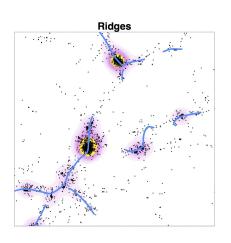
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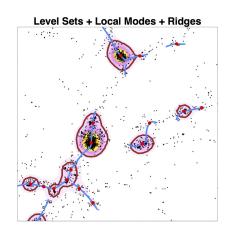
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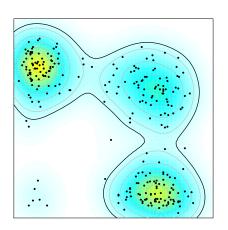
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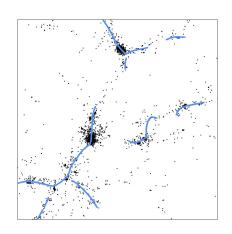


Geometric features I have studied include:

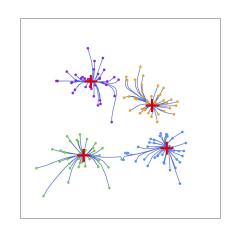
• Level Sets



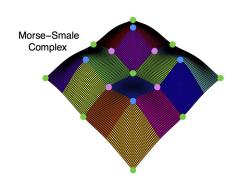
- Level Sets
- Ridges



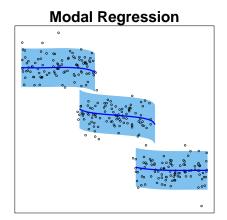
- Level Sets
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- Level Sets
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- Morse-Smale Complex



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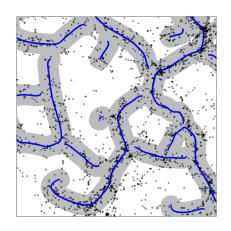


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- Level Sets
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- Modal Regression

With applications in

Astronomy



List of Papers

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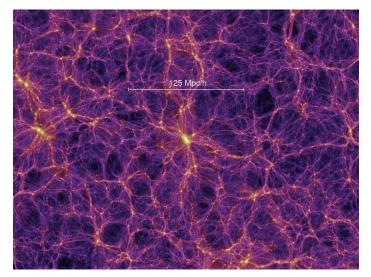
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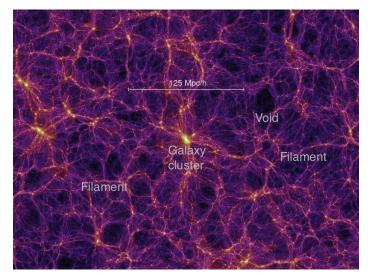
DENSITY RIDGES

Example: Cosmology



Credit: Millennium Simulation

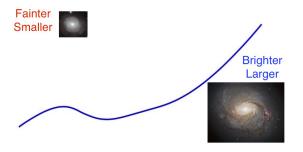
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The Importance of Filaments

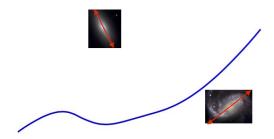
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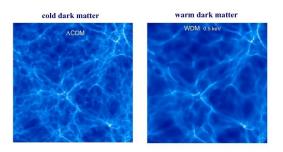
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The Importance of Filaments

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



• Credit: Kavli Institute for Cosmology, Cambridge

Density Ridges

We formalize the notion of filaments as *density ridges*.

Early work on ridges is in image analysis (Eberly 1996, Damon 1999).

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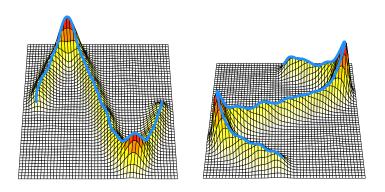
→In our work, we derive the asymptotic theory for ridge estimators and propose methods for constructing confidence sets.

Example: Ridges in Mountains

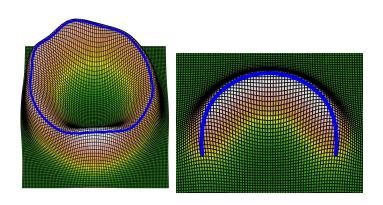


Credit: Google

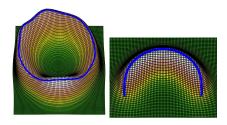
Example: Ridges in Smooth Functions



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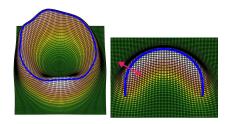


Ridges: Local Modes in Subspace



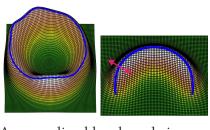
A generalized local mode in a specific 'subspace'.

Ridges: Local Modes in Subspace

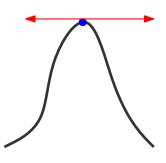


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Ridges: Local Modes in Subspace



A generalized local mode in a specific 'subspace'.



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- o Ridges:

$$R = \text{Ridge}(p) = \{x : V(x)V(x)^T \nabla p(x) = 0, \lambda_2(x) < 0\}.$$

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Local modes:

Mode(
$$p$$
) = { $x : \nabla p(x) = 0, \lambda_1(x) < 0$ }.

Dimension of Ridges

The dimension of a ridge is 1.

This is because ridges are points satisfying $V(x)V(x)^T\nabla p(x) = 0$.

 $V(x)V(x)^T$ has rank d-1, so there are d-1 effective constraints.

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Note that there are higher dimensional ridges but in this talk, we will focus on 1 dimensional ridges.

Estimator and Algorithm

We use the plug-in estimate:

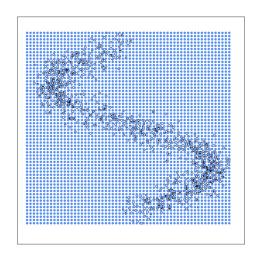
$$\widehat{R}_h = \operatorname{Ridge}(\widehat{p}_h),$$

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

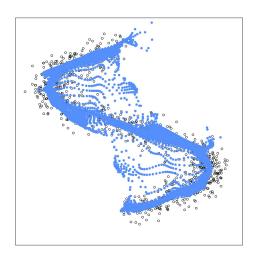
h is the smoothing bandwidth, which controls the amount of smoothing.

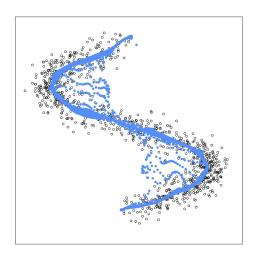
- In general, finding ridges from a given function is hard.
- The Subspace Constraint Mean Shift¹ (SCMS) algorithm allows us to find \widehat{R}_h , ridges of the KDE.

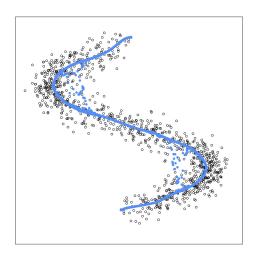
 $^{^1\}mbox{Ozertem}$, Umut, and Deniz Erdogmus. "Locally defined principal curves and surfaces." JMLR (2011).

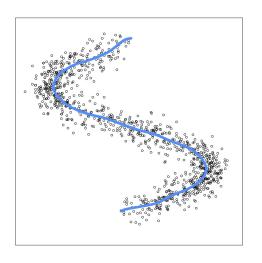


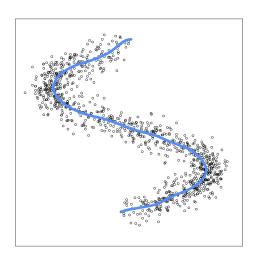




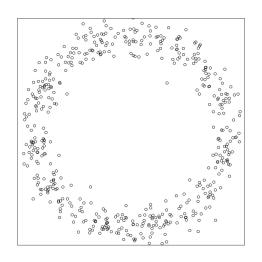


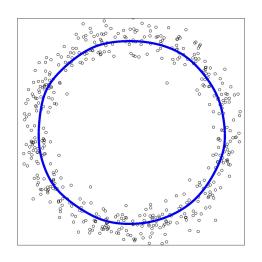


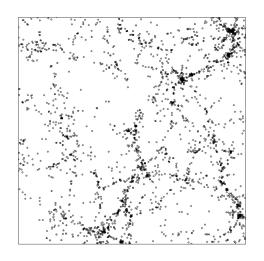


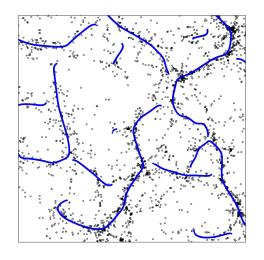


SCMS moves blue mesh points by gradient ascent and a projection.

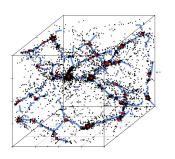


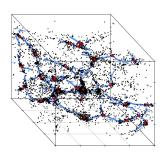






3D Example for Estimated Ridges





Blue curves: density ridges.

Red points: density local modes.

Statistical Inference: Confidence Sets

Having estimators is not enough for statistical inference.

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We need confidence sets for density ridges.

Namely, we want to find a set $C_{1-\alpha,n}$ from the data such that

$$\mathbb{P}\left(R\subset C_{1-\alpha,n}\right)\geq 1-\alpha.$$

Smoothed Density Ridges

In particular, we focus on making inference for the smoothed ridges $R_h = \text{Ridge}(p_h)$.

 p_h is the smoothed density function:

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

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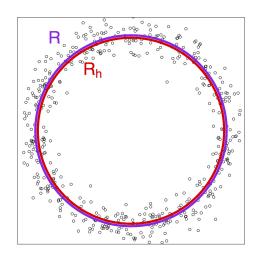
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where \otimes denotes the convolution.

- The advantages of R_h over R:
 - o Always well-defined.
 - Topologically similar.
 - We can undersmooth so that inference for R_h is also valid for R.

Ridges VS Smoothed Ridges



Useful Metric: Hausdorff Distance

We introduce a useful metric-the Hausdorff distance for sets:

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

where $d(x, A) = \inf_{y \in A} ||x - y||$ is the projection distance from point x to a set A.

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• Haus is an L_{∞} metric for sets.

The ⊕ Operation

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

A

 $A \oplus r$

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

 $A \longrightarrow A \longrightarrow A \oplus r$

Then we have the following inclusion property:

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

Confidence Sets

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

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

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

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• We need to find the distribution F_n .

Asymptotic Theory

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Key observation:

$$\sqrt{nh^{d+2}}$$
 Haus $(\widehat{R}_h, R_h) \approx \sqrt{nh^{d+2}} \sup_{x \in R_h} d(x, \widehat{R}_h)$
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Theorem (Chen, Genovese, and Wasserman (2015))

Under regularity conditions and $\frac{\log n}{nh^{d+8}} \to 0$, there exists a Gaussian process \mathbb{B}_n defined on a certain function space \mathcal{F} such that

 \approx sup {Gaussian process on R_h }.

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

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- o Good news: we have the limiting distribution.
- Bad news: the limiting distribution involves unknown quantities.

The Bootstrap

Theorem (Chen, Genovese, and Wasserman (2015))

Under regularity conditions and $\frac{\log n}{nh^{d+8}} \to 0$, there exists a Gaussian process \mathbb{B}_n defined on a certain function space \mathcal{F} such that

$$\sup_{t} \left| \mathbb{P}\left(\sqrt{nh^{d+2}} \operatorname{Haus}(\widehat{R}_{h}, R_{h}) < t\right) - \mathbb{P}\left(\sup_{f \in \mathscr{F}} \left|\mathbb{B}_{n}(f)\right| < t\right) \right| = O\left(\left(\frac{\log^{7} n}{nh^{d+2}}\right)^{1/8}\right).$$

- Good news: we have the limiting distribution.
- Bad news: the limiting distribution involves unknown quantities.
- \longrightarrow A solution: the bootstrap.

Bootstrap Confidence Set

- Bootstrap sample \Longrightarrow bootstrap ridges \widehat{R}_h^* .
- Repeat *B* times, we obtain *B* bootstrap ridges $\widehat{R}_h^{*(1)}, \dots, \widehat{R}_h^{*(B)}$.
- Compute the CDF estimator \widehat{F}_n by

$$\widehat{F}_n(t) = \frac{1}{B} \sum_{\ell=1}^{B} I\left(\mathsf{Haus}(\widehat{R}_h^{*(\ell)}, \widehat{R}_h) < t\right)$$

- Choose $\hat{t}_{1-\alpha}$ be the $1-\alpha$ quantile for \hat{F}_n .
- The confidence set is

$$C_{1-\alpha,n}=\widehat{R}_h\oplus \widehat{t}_{1-\alpha}$$

Bootstrap Consistency

We proved that

$$\sqrt{nh^{d+2}}$$
 Haus $(\widehat{R}_h^*, \widehat{R}_h) \approx \sup \{ \text{Gaussian process on } \widehat{R}_h \}$
 $\approx \sup \{ \text{Gaussian process on } R_h \}$
 $\approx \sqrt{nh^{d+2}}$ Haus (\widehat{R}_h, R_h) .

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This implies that $\widehat{t}_{1-\alpha}/t_{1-\alpha} \stackrel{P}{\to} 1$.

Bootstrap Consistency

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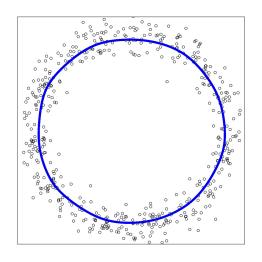
$$\begin{split} \sqrt{nh^{d+2}}\mathsf{Haus}(\widehat{R}_h^*,\widehat{R}_h) &\approx \sup \left\{ \mathsf{Gaussian} \ \mathsf{process} \ \mathsf{on} \ \widehat{R}_h \right\} \\ &\approx \sup \left\{ \mathsf{Gaussian} \ \mathsf{process} \ \mathsf{on} \ R_h \right\} \\ &\approx \sqrt{nh^{d+2}}\mathsf{Haus}(\widehat{R}_h,R_h). \end{split}$$

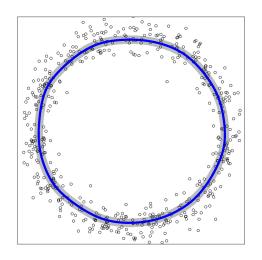
This implies that $\widehat{t}_{1-\alpha}/t_{1-\alpha} \stackrel{P}{\to} 1$.

Theorem (Chen, Genovese, and Wasserman (2015))

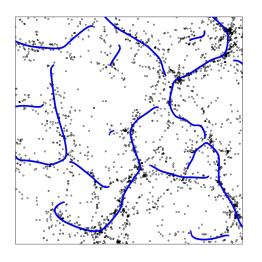
Under regularity conditions and $\frac{\log n}{nh^{d+8}} \rightarrow 0$,

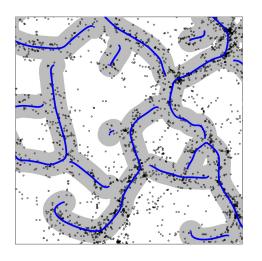
$$\mathbb{P}\left(R_h \subset \widehat{R}_h \oplus \widehat{t}_{1-\alpha}\right) = 1 - \alpha + O\left(\left(\frac{\log^7 n}{nh^{d+2}}\right)^{1/8}\right).$$



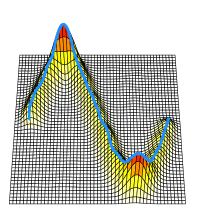


We have checked the coverage by simulation.

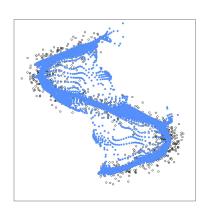




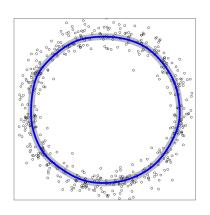
• Ridges of the density function.



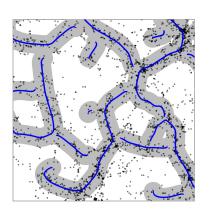
- Ridges of the density function.
- An algorithm for the estimator.



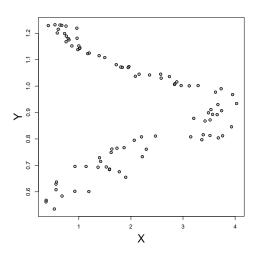
- Ridges of the density function.
- An algorithm for the estimator.
- Confidence sets.

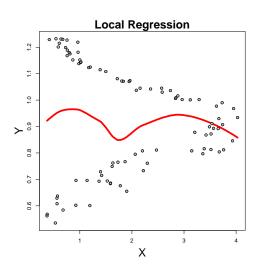


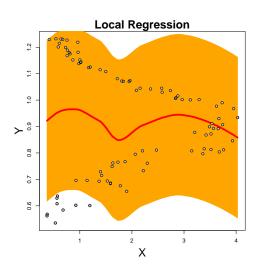
- Ridges of the density function.
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- Confidence sets.
- Applications in Astronomy.

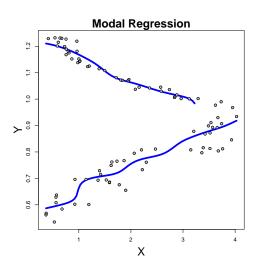


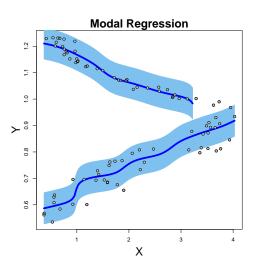


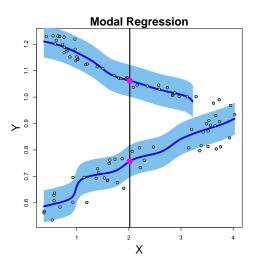












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In most of the above work, they consider the mode of the conditional density function.

 \longrightarrow In our work, we consider the multiple local modes of the conditional density function.

Definition for Modal Regression

We assume $x \in \mathbb{K} \subset \mathbb{R}^d$, where \mathbb{K} is a compact set.

• Modal function–the conditional (local) modes:

$$M(x) = \text{Mode}(Y|X = x) = \left\{ y : \frac{d}{dy} p(y|x) = 0, \frac{d^2}{dy^2} p(y|x) < 0 \right\}.$$

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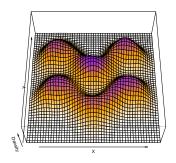
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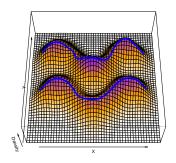
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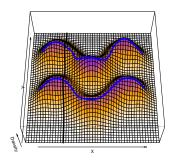
$$M(x) = \operatorname{Mode}(Y|X=x) = \left\{ y : \frac{d}{dy} p(y|x) = 0, \frac{d^2}{dy^2} p(y|x) < 0 \right\}.$$

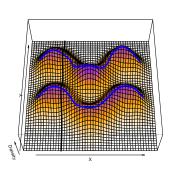
- M(x) is a multi-valued function.
- An equivalent expression:

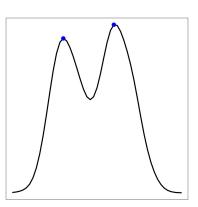
$$M(x) = \left\{ y : \frac{\partial}{\partial y} p(x, y) = 0, \frac{\partial^2}{\partial y^2} p(x, y) < 0 \right\}.$$











Estimator for Modal Regression

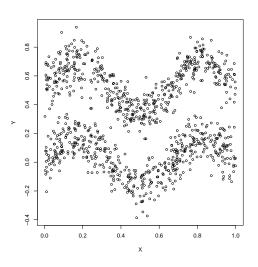
• Our estimator is the plug-in from the KDE:

$$\widehat{M}_n(x) = \left\{ y : \frac{\partial}{\partial y} \widehat{p}_n(x,y) = 0, \frac{\partial^2}{\partial y^2} \widehat{p}_n(x,y) < 0 \right\}.$$

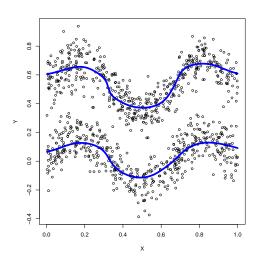
• Partial mean shift²: a simple algorithm for computing $\widehat{M}_n(x)$, the plug-in estimator of the KDE, from the data.

²Einbeck, Jochen, and Gerhard Tutz. "Modelling beyond regression functions: an application of multimodal regression to speed–flow data." JRSSC (2006)

Example for Modal Regression



Example for Modal Regression



Losses of Modal regression

To measure the errors, we consider the following two losses:

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• the *pointwise* loss

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Losses of Modal regression

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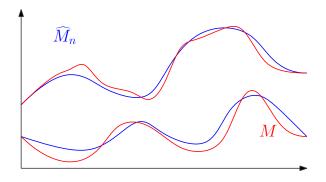
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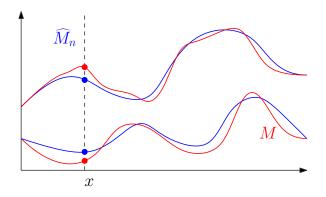
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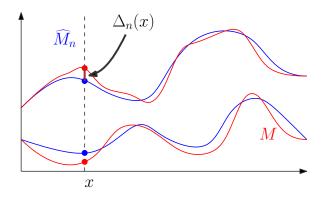
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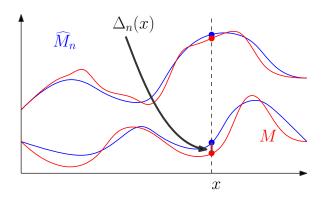
• the *uniform* loss

$$\Delta_n = \sup_x \Delta_n(x) = \sup_x \operatorname{Haus}(\widehat{M}_n(x), M(x)).$$









Rate of Convergence

Both the pointwise and the uniform losses obey the common nonparametric rate:

Theorem

Under regularity conditions and $\frac{\log n}{nh^{d+3}} \rightarrow 0$,

$$\Delta_n(x) = O(h^2) + O_P\left(\sqrt{\frac{1}{nh^{d+3}}}\right)$$
$$\Delta_n = O(h^2) + O_P\left(\sqrt{\frac{\log n}{nh^{d+3}}}\right).$$

Risk = Bias +
$$\sqrt{\text{Variance}}$$
.

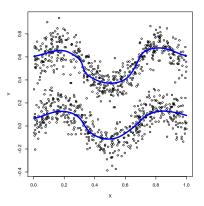
$$d + 3 = d + 1 + 2 = \dim(X) + \dim(Y) + \text{gradient}.$$

Confidence Sets

We can construct confidence sets using the uniform loss and the bootstrap.

Reason: the uniform loss Δ_n is an L_∞ metric for modal regression.

Bootstrap consistency follows in a similar way as density ridges.

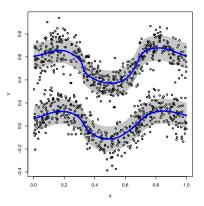


Confidence Sets

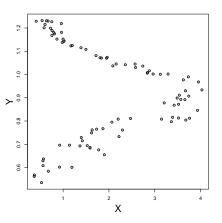
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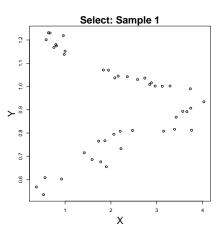
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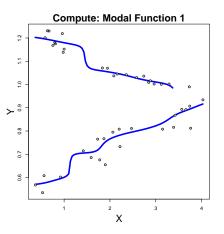
We can use modal regression to construct a prediction set.



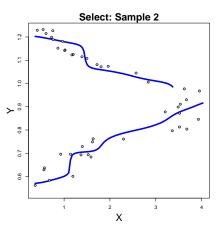
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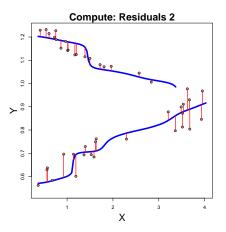
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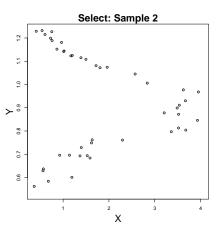
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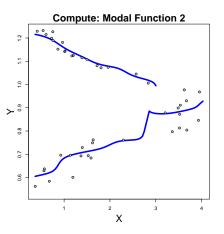
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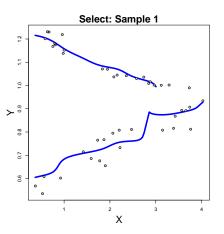
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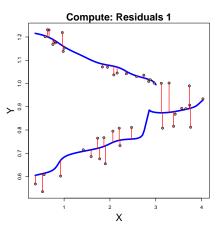
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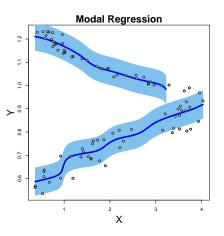
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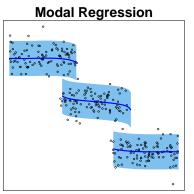
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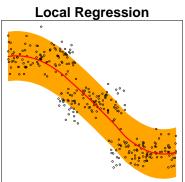


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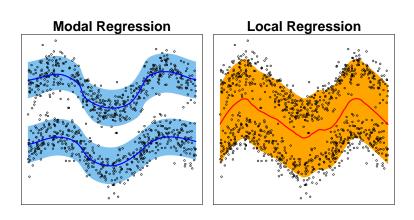


Examples of Prediction Sets





Examples of Prediction Sets



Bandwidth Selection

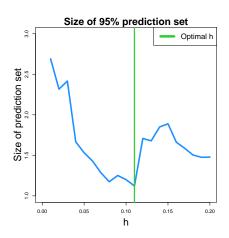
We can choose the smoothing parameter h via minimizing the size of the prediction set.

Namely, we choose

$$h^* = \underset{h>0}{\operatorname{argmin}} \operatorname{Vol}\left(\widehat{\mathcal{P}}_{1-\alpha}\right)$$
 ,

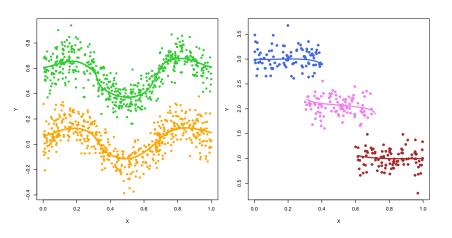
where $\widehat{\mathcal{P}}_{1-\alpha}$ is the prediction set.

Example: Bandwidth Selection



Regression Clustering

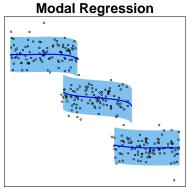
- Clustering based on the response Y.
- Clusters as functions of covariates *X*.

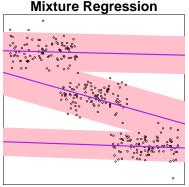


Modal Regression VS Mixture Regression

Modal regression and mixture regression are solving different problems.

Here is a case where modal regression gives a better result.





CONCLUDING REMARKS

List of Papers

Level Sets:

1. Chen, Genovese, and Wasserman. "Density Level Sets: Asymptotics, Inference, and Visualization." (2015).

o Ridges:

- 1. Chen, Genovese, and Wasserman. "Asymptotic theory for density ridges." The Annals of Statistics (2015).
- 2. Chen, Genovese, and Wasserman. "Generalized Mode and Ridge Estimation." (2014).
- Chen et al. "Optimal Ridge Detection using Coverage Risk." NIPS (2015).

Clustering:

- Chen, Genovese, and Wasserman. "A Comprehensive Approach to Mode Clustering." The Electronic Journal of Statistics (2016+).
- 2. Azizyan and Chen et al. "Risk Bounds for Mode Clustering." (2015).

o Modal Regression:

1. Chen et al. "Nonparametric Modal Regression." The Annals of Statistics (2016+).

Morse-Smale Complex:

1. Chen, Genovese, and Wasserman. "Statistical Inference Using the Morse-Smale Complex." (2015).

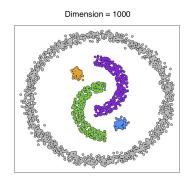
Astronomy:

- 1. Chen et al. "Detecting Effects of Filaments on Galaxy Properties in Sloan Digital Sky Survey III." (2015).
- 2. Chen et al. "Cosmic Web Reconstruction through Density Ridges: Catalogue." (2015).
- Chen et al. "Investigating Galaxy-Filament Alignment in Hydrodynamic Simulations using Density Ridges." Mon. Not. Roy. Astro. Soc. (2015).
- Chen et al. "Cosmic Web Reconstruction through Density Ridges: Method and Algorithm." Mon. Not. Roy. Astro. Soc. (2015).

Future Work

Some future directions:

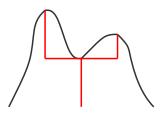
- More to do in geometric features.
- High-dimensional clustering.
- Influence for visualization tools.
- Interdisciplinary collaborations.



Future Work

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- More to do in geometric features.
- High-dimensional clustering.
- Influence for visualization tools.
- Interdisciplinary collaborations.



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

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Thank you!

References

- Chen, Yen-Chi, Christopher R. Genovese, and Larry Wasserman. "Density Level Sets: Asymptotics, Inference, and Visualization." Under review of the Journal of American Statistical Association. arXiv preprint arXiv:1504.05438 (2015).
- Chen, Yen-Chi, Christopher R. Genovese, and Larry Wasserman. "Asymptotic theory for density ridges." The Annals of Statistics 43, no. 5 (2015): 1896-1928.
- Chen, Yen-Chi, Christopher R. Genovese, Ryan J. Tibshirani, and Larry Wasserman. "Nonparametric Modal Regression."
 To appear in the Annals of Statistics. arXiv preprint arXiv:1412.1716 (2014).
- Chernozhukov, Victor, Denis Chetverikov, and Kengo Kato. "Gaussian approximation of suprema of empirical processes." The Annals of Statistics 42, no. 4 (2014): 1564-1597.
- Chernozhukov, Victor, Denis Chetverikov, and Kengo Kato. "Anti-concentration and honest, adaptive confidence bands."
 The Annals of Statistics 42, no. 5 (2014): 1787-1818.
- Einbeck, Jochen, and Gerhard Tutz. "Modelling beyond regression functions: an application of multimodal regression to speed-flow data." Journal of the Royal Statistical Society: Series C (Applied Statistics) 55, no. 4 (2006): 461-475.
- 7. Genovese, Christopher R., et al. "Nonparametric ridge estimation." The Annals of Statistics 42, no. 4 (2014): 1511-1545.
- Ozertem, Umut, and Deniz Erdogmus. "Locally defined principal curves and surfaces." The Journal of Machine Learning Research 12 (2011): 1249-1286.

4. Backups for Density Ridges	5. Backups for Modal Regression
4.1 Regularity Conditions	5.1 Regularity Conditions
4.2 Bandwidth Selection	5.2 3D Modal Regression
4.3 Local Uncertainty	5.3 Bifurcation and Merge
4.4 Why Smoothed Structures?	5.4 Comparisons
4.5 General Ridges	5.5 Theory for Prediction Sets
4.6 Illustration for Asymptotics	5.6 More about Confidence Sets



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 **BC**⁴.
- **(P2)** The eigengap $\lambda_1(x) \lambda_2(x) \ge \beta_0 > 0$ 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 **BC**⁴ and $||K||_{\infty}^*$ < ∞ .
- (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 $\mathcal{K}_l^* = \bigcup_{r=0}^l \mathcal{K}_r$. We assume that \mathcal{K}_4^* is a VC-type class. i.e. there exists constants A, v and a constant envelope b_0 such that

$$\sup_{Q} N(\mathcal{K}_{4}^{*}, \mathcal{L}^{2}(Q), b_{0}\epsilon) \leq \left(\frac{A}{\epsilon}\right)^{c}, \tag{1}$$

where $N(T, d_T, \epsilon)$ is the ϵ -covering number for an 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_h is in **BC**⁴.
- **(P2)** There exists constants β_0 , β_1 , β_2 , $\delta_0 > 0$ such that

$$\lambda_{2}(x) \leq -\beta_{1}$$

$$\lambda_{1}(x) \geq \beta_{0} - \beta_{1}$$

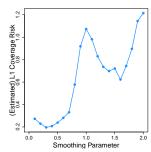
$$\|g_{h}(x)\| \max_{\|\alpha\|=3} |p_{h}^{(\alpha)}(x)| \leq \beta_{0}(\beta_{1} - \beta_{2})$$

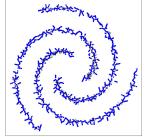
$$(2)$$

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

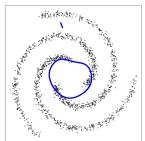
- **(P3)** For each $x \in R_h$, $|e(x)^T g_h(x)|^2 \ge \frac{\lambda_1(x)}{\lambda_1(x) \lambda_2(x)}$ where e(x) is the direction of R_h at point $x \in R_h$.
- **(P4)** The above assumptions hold for all sufficiently small h.

Bandwidth Selection

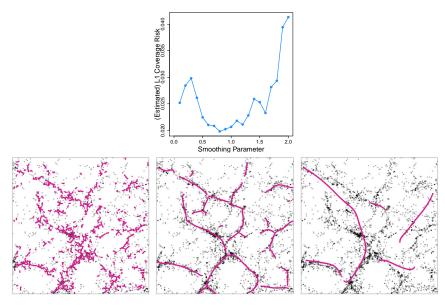




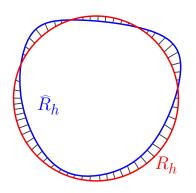




Bandwidth Selection



Bandwidth Selection

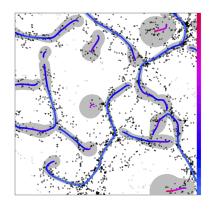


 L_1 distance are like the area of the shady regions.

We estimate this distance by data splitting or the bootstrap.

Reference: **Chen** et al. 'Optimal Ridge Detection using Coverage Risk' (NIPS 2015).

Local Uncertainty and Pointwise Confidence Sets

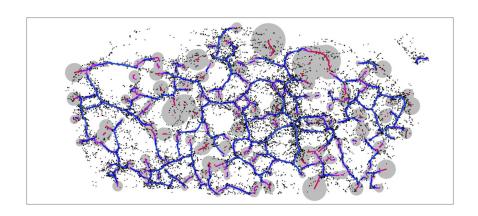


Color denotes the amount of uncertainty.

Red: unstable filaments.

Blue: stable filaments.

Local Uncertainty and Pointwise Confidence Sets



Color denotes the amount of uncertainty.

Red: unstable filaments.

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Why Smoothed Density? - Bias Consideration

We have the following decomposition:

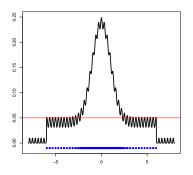
$$\mathsf{Haus}(\widehat{R}_h, R) \le \mathsf{Haus}(R_h, R) + \mathsf{Haus}(\widehat{R}_h, R)$$
$$= O(h^2) + O_P\left(\sqrt{\frac{\log n}{nh^{d+2}}}\right).$$

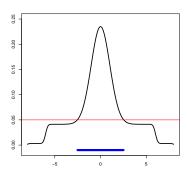
Bias + $\sqrt{\text{Variance}}$.

Work on smoothed ridges R_h allows us to avoid the problem of bias.

Optimal rate:
$$O_P\left(\left(\frac{\log n}{n}\right)^{\frac{2}{d+6}}\right)$$
 when we choose $h=O\left(\left(\frac{\log n}{n}\right)^{\frac{1}{d+6}}\right)$.

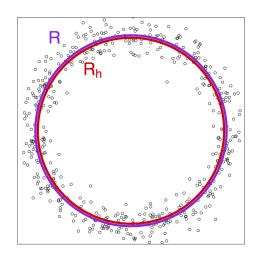
Why Smoothed Density? - A Level Set Example





Ridges VS Smoothed Ridges

Radius of ring: r = 1. Smoothing bandwidth: h = 0.25. Gaussian noise level: $\sigma = 0.1$



General Ridges

We can generalize ridges to higher dimensions. Pick

$$V_r(x) = [v_{r+1}(x), \cdots, v_d(x)].$$

We define

$$r$$
-Ridge $(p) = \{x : V_r(x)V_r(x)^T \nabla p(x) = 0, \lambda_{r+1}(x) < 0\}.$

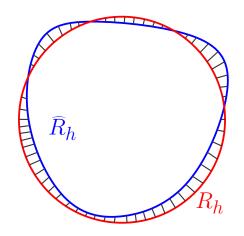
 $V_r(x)$ is a $d \times (d-r)$ matrix. There are d-r constraints.

By Implicit Function Theorem, *r*-ridges are *r*-manifolds.

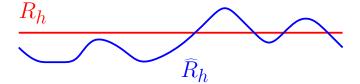
In Astronomy, r = 2 can be used to model 'Cosmic Sheets (Walls)'.

r = 0 coincides with the definition of local modes.

Asymptotic Theory



Asymptotic Theory





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 **BC**⁴.
- **(P2)** The second derivative along y axis is bounded away from 0 for points on M.
- **(P3)** *M* contains *L* well-separated, connected components.

Regularity Conditions on Kernel Functions

- **(K1)** The kernel *K* is in **BC**⁴ and $||K||_{\infty}^*$ < ∞ .
- (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 $\mathcal{K}_l^* = \bigcup_{r=0}^l \mathcal{K}_r$. We assume that \mathcal{K}_2^* is a VC-type class. i.e. there exists constants A, v and a constant envelope b_0 such that

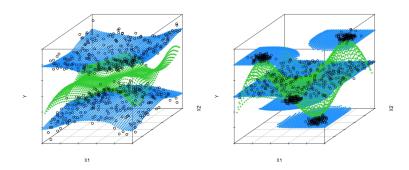
$$\sup_{Q} N(\mathcal{K}_{2}^{*}, \mathcal{L}^{2}(Q), b_{0}\epsilon) \leq \left(\frac{A}{\epsilon}\right)^{\nu}, \tag{3}$$

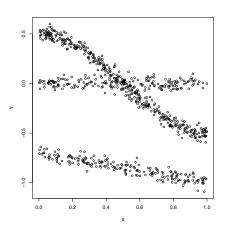
where $N(T, d_T, \epsilon)$ is the ϵ -covering number for an semi-metric set T with metric d_T and $\mathcal{L}^2(Q)$ is the L_2 norm with respect to the probability measure Q.

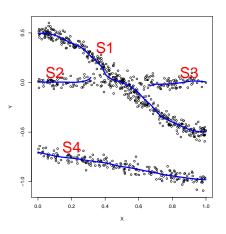
Regularity Conditions on Distributions

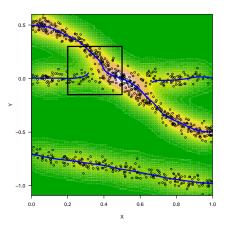
- **(P1)** The density p is in **BC**⁴.
- **(P2)** There exists constants $\lambda_0 > 0$ such that for any $(x, y) \in \mathbb{K} \times \mathbb{R}$ with $\frac{\partial}{\partial y} p(x, y) > 0$, the second derivative satisfies $\frac{\partial^2}{\partial^2 y} p(x, y) \leq -\lambda_0 < 0$.
- **(P3)** Modal function $M = \bigcup_{j=1}^{L} M_j$, where each M_j is a connected component with $M_j \cap M_i = \phi$ for $i \neq j$.

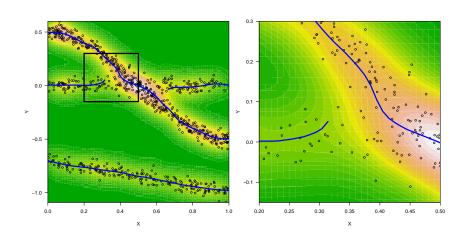
3D Modal Regression

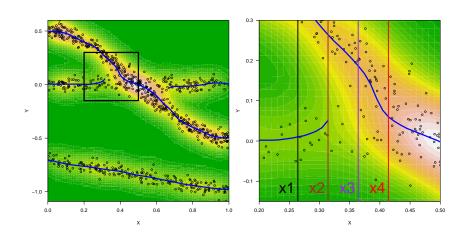


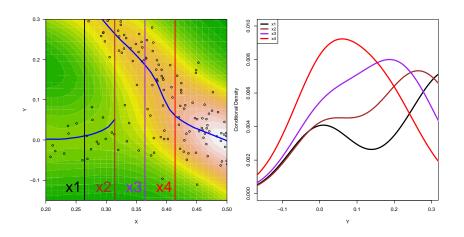


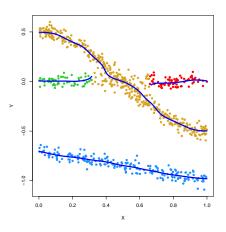












Comments on Mixture Regression

A general model for mixture regression:

$$p(y|x) = \sum_{j=1}^{K} \pi_{j}(x)\phi_{j}(y; \mu_{j}(x), \sigma_{j}^{2}(x)),$$

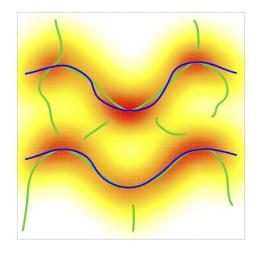
where each $\phi_j(y; \mu, \sigma^2)$ is a density function with mean μ and variance σ^2 .

Common assumptions:

- 1. $\pi_j(x) = \pi_j$.
- 2. $\mu_{j}(x) = \beta_{j}^{T} x$.
- 3. $\sigma_i^2(x) = \sigma_i^2$.
- 4. ϕ_j is a Gaussian.

Generally, we need to use EM algorithm to estimate the parameters.

Modal Regression VS Density Ridges

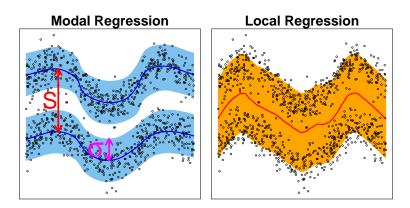


Mixture Inference versus Modal Inference

	Mixture-based	Mode-based
Density estimation	Gaussian mixture	Kernel density estimate
Clustering	K-means	Mean-shift clustering
Regression	Mixture regression	Modal regression
Algorithm	EM	Mean-shift
Complexity parameter	<i>K</i> (number of components)	h (smoothing bandwidth)
Туре	Parametric model	Nonparametric model

Table: Comparison for methods based on mixtures versus modes.

Theory for Prediction Sets



Theorem (Chen, Genovese, and Wasserman (2015))

When the signal-to-noise ratio S/σ is sufficiently large, the modal regression has a smaller prediction set than the nonparametric regression.

Confidence Sets

We can construct confidence sets using the uniform loss.

Reason: the uniform loss Δ_n is like an L_{∞} metric for modal regression.

Let $t_{1-\alpha}$ be the $1-\alpha$ quantile of F_n , the CDF of Δ_n .

 $\widehat{M}_n(x) \pm t_{1-\alpha}$ is a confidence set for M(x) uniformly for all x.

Problem: $t_{1-\alpha}$ cannot be computed.

Solution: the bootstrap.

The Bootstrap

- Bootstrap sample \Longrightarrow bootstrap modal function \widehat{M}_n^* .
- Repeat *B* times, we obtain *B* bootstrap modal functions $\widehat{M}_n^{*(1)}, \cdots, \widehat{M}_n^{*(B)}$.
- $\quad \text{Ompute } \widehat{\Delta}_n^{*(1)}, \cdots, \widehat{\Delta}_n^{*(B)} \text{ by } \widehat{\Delta}_n^{*(\ell)} = \sup_x \text{ Haus}(\widehat{M}_n^{*(\ell)}(x), \widehat{M}_n(x)).$
- Compute the CDF estimator \widehat{F}_n by

$$\widehat{F}_n(t) = \frac{1}{B} \sum_{\ell=1}^B I\left(\widehat{\Delta}_n^{*(\ell)} < t\right).$$

- Choose $\hat{t}_{1-\alpha}$ be the $1-\alpha$ quantile for \hat{F}_n .
- $\widehat{M}_n(x) \pm \widehat{t}_{1-\alpha}$ is an asymptotic confidence set uniformly for all x.

Bootstrap consistency follows in the similar way as ridges.

Pointwise Confidence Sets

