Kernel Smoothing and Mean Shift Theories with Applications to Cosmic Web Detection

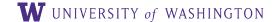
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Joint work with Yen-Chi Chen* and Rafael S. de Souzat

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What Is Cosmic Web?

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- Large scale: $1 \, \mathrm{Mpc} \approx 3.26 \, \mathrm{light}$ -years.
- **Cause**: the anisotropic collapse of matter in gravitational instability scenarios at the early stage of the Universe (Zel'Dovich, 1970).

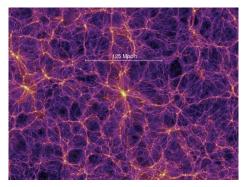


Figure: Visualization of *Cosmic Web* (credited to the millennium simulation project (Springel et al., 2005)).

Key Characteristics of Cosmic Web

Cosmic web consists of four distinct components (Libeskind et al., 2018):

- Massive galaxy clusters (or nodes),
- Interconnected **filaments**,
- Two-dimensional tenuous *sheets/walls*,

around • Vast and near-empty *voids*.

on which matter concentrates.

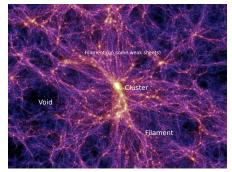


Figure: Characteristics of *Cosmic Web* (credited to the millennium simulation).

Significance of Cosmic Filaments

We will focus on detecting the (one-dimensional) cosmic filaments, because

- They connect complexes of super-clusters (Lynden-Bell et al., 1988).
- They contain information about the global cosmology and the nature of dark matter (Zhang et al., 2009; Tempel et al., 2014).

Significance of Cosmic Filaments

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- They connect complexes of super-clusters (Lynden-Bell et al., 1988).
- They contain information about the global cosmology and the nature of dark matter (Zhang et al., 2009; Tempel et al., 2014).
- The trajectory of cosmic microwave background light can be distorted due to cosmic filaments, creating the weak lensing effect.

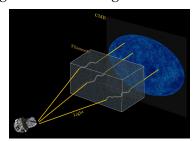


Figure: Illustration of the bending trajectory of CMB lights (credit to Siyu He, Shadab Alam, Wei Chen, and Planck/ESA; see He et al. (2018) for details).

Challenges in Detecting Cosmic Filaments

- The filamentary structures are overwhelmingly complex (Cautun et al., 2013):
 - Lack of structural symmetries,
 - Uncertainty in measuring its connectivity,
 - Intrinsic multi-scale nature, etc.

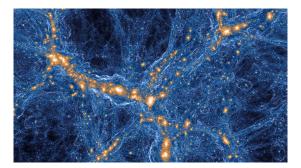


Figure: A view of the present-day cosmic web 300 million light-years across, as modeled by IllustrisTNG (Vogelsberger et al., 2014).

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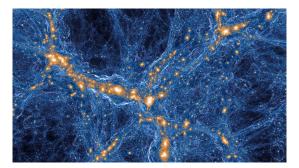


Figure: A view of the present-day cosmic web 300 million light-years across, as modeled by IllustrisTNG (Vogelsberger et al., 2014).

▶ There are no universal and mathematically rigorous definitions of cosmic filament!

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- Oiscuss directional density ridges from both statistical and computational perspectives:
 - Establish the statistical consistency of estimating the true density ridges with directional kernel density estimator (KDE).
 - Estimate the directional density ridges via our proposed *Directional Subspace Constrained Mean Shift* (DirSCMS) algorithm.
 - Establish the linear convergence properties of our DirSCMS algorithm.

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 - Establish the linear convergence properties of our DirSCMS algorithm.
- Apply our DirSCMS algorithm to the galaxy observations in the Sloan Digital Sky Survey (SDSS-IV; Ahumada et al. 2020) and construct a cosmic web catalog.

Previous Works on Cosmic Filament Detection



Observational Data for Filament Detection

In astronomical survey data, the observed objects (or galaxies) are recorded as:

$$\{(\alpha_1,\delta_1,Z_1),...,(\alpha_n,\delta_n,Z_n)\},$$

where, for i = 1, ..., n,

- $\alpha_i \in [0, 360^\circ)$ is the *right ascension* (RA), i.e., celestial longitude,
- $\eta_i \in [-90^\circ, 90^\circ]$ is the *declination* (DEC), i.e., celestial latitude,
- $Z_i \in (0, \infty)$ is the *redshift* value, i.e., measuring its distance to the Earth.

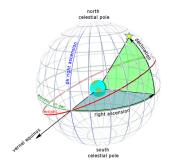


Figure: Illustration of RA and DEC (Image Courtesy of Wikipedia).

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• **3D methods:** Convert $\{(\alpha_i, \delta_i, Z_i)\}_{i=1}^n$ to their Cartesian coordinates as

$$X_i = d(Z_i)\cos\alpha_i\cos\delta_i, \quad Y_i = d(Z_i)\sin\alpha_i\cos\delta_i, \quad Z_i = d(Z_i)\sin\delta_i,$$

where $d(\cdot)$ is a distance transforming function; see Tempel et al. (2014) for details.

• **2D methods:** Slice the Universe into thin redshift slices (Chen et al., 2015b; Duque et al., 2022).

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- **2D methods:** Slice the Universe into thin redshift slices (Chen et al., 2015b; Duque et al., 2022).
- ▶ Note: Our method can easily switch between the above two categories.

2D Methods: Slicing the Universe

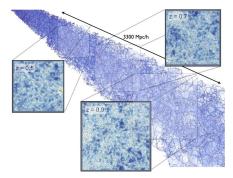


Figure: Illustration of slicing the Universe (credit to Laigle et al. 2018).

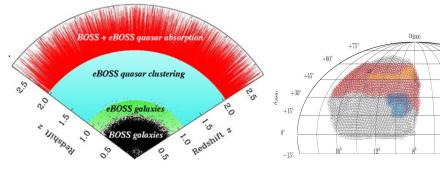
The tomographic filament detection has its own advantages over 3D methods:

- It controls the redshift distortions along the line-of-sight direction (i.e., the *finger-of-god* effect).
- The measurement error in one slice will not propagate to other slices.
- It helps reduce computational cost...

Caveats of Slicing the Universe

The slices ($\Delta Z = 0.005$) in the survey data are not some flat 2D planes, but some **spherical shells**, which have a *nonlinear* curvature!

Recall that the locations of astronomical objects in a slice are recorded by $\{(\alpha_i, \delta_i)\}_{i=1}^n$ on a celestial sphere $\Omega_2 = \{x \in \mathbb{R}^3 : ||x||_2 = 1\}$.



(a) Planned eBOSS coverage of the Universe (credit to M. Blanton and SDSS)

(b) BOSS/eBOSS Spectroscopic Footprint as of DR16 (credit to SDSS)

∩ BOSS

O eBOSS ELG

Why can't we ignore the spherical geometry?

Setup: Suppose that we want to recover the true ring/filament structure across the North and South pole of a unit sphere given some noisy data points from it.

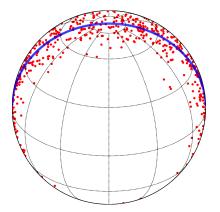
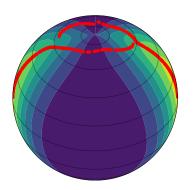


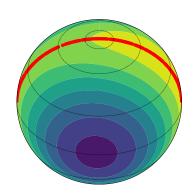
Figure: Noisy observations (red points) and the underlying true ring/filament structure (blue line).

Why can't we ignore the spherical geometry?

The background contour plots are kernel density estimators on the flat plane $[-90^\circ, 90^\circ] \times [0^\circ, 360^\circ)$ and unit sphere $\Omega_2 = \left\{x \in \mathbb{R}^3 : ||x||_2 = 1\right\}$, respectively.



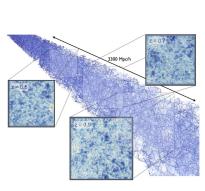
(a) Euclidean SCMS Method (ignoring the spherical geometry).



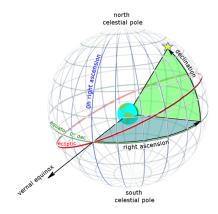
(b) Directional SCMS Method.

* SCMS: subspace constrained mean shift (Ozertem and Erdogmus, 2011).

Importance of Modeling Cosmic Web Under Spherical Geometry



(a) Slicing the Universe.



(b) Positioning of the observed galaxy.

▶ Research Question: How do we model and estimate the cosmic filaments based on the observed galaxies in each (redshift) spherical slice?

Cosmic Filament Model: Directional Density Ridges



Our Filament Model: Directional Density Ridges

► Fact: The cosmic filaments are 1D curves tracing over the high-density regions of matter (or galaxy) density field.

Our Filament Model: Directional Density Ridges

- ▶ Fact: The cosmic filaments are 1D curves tracing over the high-density regions of matter (or galaxy) density field.
- ▶ Our Model: (Directional) density ridges are generalized local maxima (within some subspaces) of the underlying density function (on $\Omega_q = \{x \in \mathbb{R}^{q+1} : ||x||_2 = 1\}$).

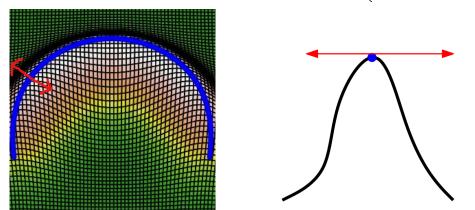


Figure: Density ridge (lifted onto the underlying density function; Chen et al. 2015a)

Definition of Directional Density Ridges

▶ Local Modes/Maxima of f on $\Omega_q = \{x \in \mathbb{R}^{q+1} : ||x||_2 = 1\}$:

$$\mathcal{M} \equiv \mathtt{Mode}(f) = \{x \in \Omega_q : \mathtt{grad}f(x) = \mathbf{0}, \lambda_1(x) < 0\}$$
.

- grad f(x) is the Riemannian gradient and $\mathcal{H}f(x)$ is the Riemannian Hessian on Ω_q .
- $\lambda_1(x) \ge \cdots \ge \lambda_q(x)$ are (descending) eigenvalues of $\mathcal{H}f(x)$ associated with eigenvectors $v_1(x), ..., v_q(x)$ that lies within the tangent space T_x .

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▶ Density ridge on Ω_q (or directional density ridge) of f:

$$\mathcal{R}_d \equiv ext{Ridge}(f) = \left\{ oldsymbol{x} \in \Omega_q : V_d(oldsymbol{x}) V_d(oldsymbol{x})^T ext{grad} f(oldsymbol{x}) = oldsymbol{0}, \lambda_{d+1}(oldsymbol{x}) < 0
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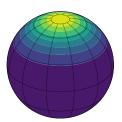
where $V_d(x) = [v_{d+1}(x), ..., v_q(x)] \in \mathbb{R}^{(q+1)\times(q-d)}$ consists of the last q-d eigenvectors of $\mathcal{H}f(x)$ within T_r .

Estimation of Directional Density Ridges

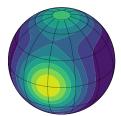
We first estimate the density function f on Ω_q via the directional KDE (Hall et al., 1987; Bai et al., 1988; García-Portugués, 2013) as:

$$\widehat{f}_h(\mathbf{x}) = \frac{C_{L,q}(h)}{n} \sum_{i=1}^n L\left(\frac{1-\mathbf{x}^T \mathbf{X}_i}{h^2}\right),$$

- $L: [0, \infty) \to [0, \infty)$ is a directional kernel, *i.e.*, a rapidly decaying nonnegative function. (Example: von Mises kernel $L(r) = e^{-r}$.)
- h > 0 is the bandwidth parameter, and $C_{L,q}(h)$ is a normalizing term.



(a) $f_{\text{VMF},2}(x; \boldsymbol{\mu}, \nu)$ with $\boldsymbol{\mu} = (0, 0, 1)$ and $\nu = 4.0$.



(b) $\frac{2}{5} \cdot f_{\text{vMF},2}(x; \boldsymbol{\mu}_1, 5) + \frac{3}{5} \cdot f_{\text{vMF},2}(x; \boldsymbol{\mu}_2, 5)$ with $\boldsymbol{\mu}_1 = (0, 0, 1), \boldsymbol{\mu}_2 = (1, 0, 0).$

Statistical Consistency of Directional Density Ridge Estimation

The directional KDE \hat{f}_h is useful because its plug-in estimators

$$\widehat{\mathcal{M}} = \left\{x \in \Omega_q : \operatorname{grad} \widehat{f}_h(x) = \mathbf{0}, \widehat{\lambda}_1(x) < 0
ight\}$$

and

$$\widehat{\mathcal{R}}_d = \left\{ \boldsymbol{x} \in \Omega_q : \widehat{V}_d(\boldsymbol{x}) \widehat{V}_d(\boldsymbol{x})^T \mathrm{grad} \widehat{f}_h(\boldsymbol{x}) = \boldsymbol{0}, \widehat{\lambda}_{d+1}(\boldsymbol{x}) < 0 \right\}$$

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approach \mathcal{M} and \mathcal{R}_d in a statistically consistent way (Theorem 6 in Zhang and Chen 2021 and Theorem 4.1 in Zhang and Chen 2022):

- Haus $(\mathcal{M},\widehat{\mathcal{M}})=O(h^2)+O_P\left(\sqrt{\frac{1}{nh^{q+2}}}\right)$, as h o 0 and $nh^{q+2} o \infty$,
- Haus $\left(\mathcal{R}_d,\widehat{\mathcal{R}}_d\right)=O(h^2)+O_P\left(\sqrt{\frac{|\log h|}{nh^{q+4}}}\right)$, as $h\to 0$ and $\frac{nh^{q+6}}{|\log h|}\to \infty$,

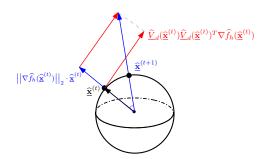
where
$$\operatorname{Haus}(A,B) = \max \left\{ r > 0 : \sup_{\boldsymbol{x} \in A} d(\boldsymbol{x},B), \sup_{\boldsymbol{y} \in B} d(\boldsymbol{y},A) \right\}.$$

Algorithmic Estimation of Directional Density Ridges

We generalize the traditional subspace constrained mean shift algorithm Ozertem and Erdogmus (2011) in \mathbb{R}^D to estimate $\widehat{\mathcal{R}}_d$ in practice as the **directional subspace** constrained mean shift (DirSCMS) algorithm (Section 4.2 in Zhang and Chen 2022):

$$\widehat{\boldsymbol{x}}^{(t+1)} \leftarrow \widehat{\boldsymbol{x}}^{(t)} + \widehat{V}_d(\widehat{\boldsymbol{x}}^{(t)}) \widehat{V}_d(\widehat{\boldsymbol{x}}^{(t)})^T \cdot \frac{\nabla \widehat{f}_h(\widehat{\boldsymbol{x}}^{(t)})}{\left|\left|\nabla \widehat{f}_h(\widehat{\boldsymbol{x}}^{(t)})\right|\right|_2} \quad \text{and} \quad \widehat{\boldsymbol{x}}^{(t+1)} \leftarrow \frac{\widehat{\boldsymbol{x}}^{(t+1)}}{\left|\left|\widehat{\boldsymbol{x}}^{(t+1)}\right|\right|_2},$$

for t = 0, 1,



Essentially, this is a subspace constrained gradient ascent algorithm on Ω_q , for which we establish the linear convergence results in Section 4.3 of Zhang and Chen (2022).

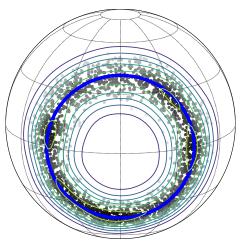


Figure: The underlying circle (blue curve) and sampled points (gray dots) on Ω_2 .

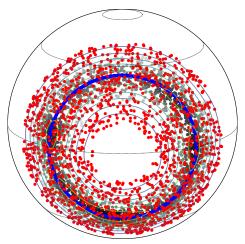


Figure: Directional SCMS at Step 0.

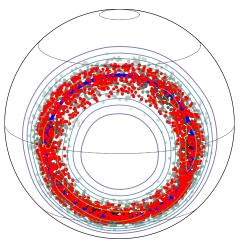


Figure: Directional SCMS at Step 1.

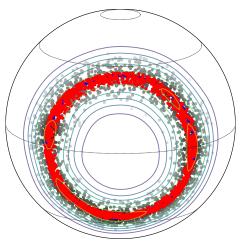


Figure: Directional SCMS at Step 2.

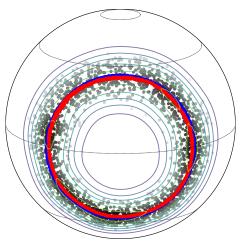


Figure: Directional SCMS at Step 4.

DirSCMS Algorithm: Simulation Study

We simulate 2000 data points from a circle on Ω_2 with additive Gaussian noises $\mathcal{N}(0, 0.1^2)$ on their Cartesian coordinates and L_2 normalization.

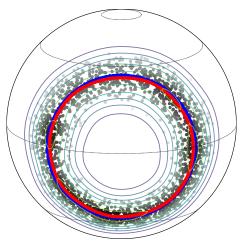


Figure: Directional SCMS at Step 8.

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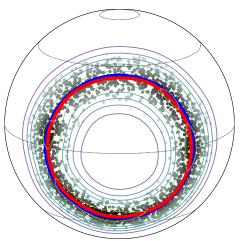


Figure: Directional SCMS at Step 24 (converged).

An Extension to Directional-Linear Product Spaces

The observed galactic data $\{(\phi_i, \eta_i, z_i)\}_{i=1}^n \subset \Omega_2 \times \mathbb{R}^+$ are directional-linear, and the density ridges in $\Omega_2 \times \mathbb{R}^+$ (Zhang and Chen, 2025) can also be estimated as:

Density estimation at $(x, z) \in \Omega_q \times \mathbb{R}$ (García-Portugués et al., 2015):

$$\widehat{f}_h(x,z) = \frac{C_L(h_1)}{nh_2} \sum_{i=1}^n L\left(\frac{1-x^T X_i}{h_1^2}\right) K\left(\frac{z-Z_i}{h_2}\right).$$

Ridge-Finding via SCMS algorithm on $\mathbf{y}^{(t)} = (\mathbf{x}^{(t)}, \mathbf{z}^{(t)})$ as:

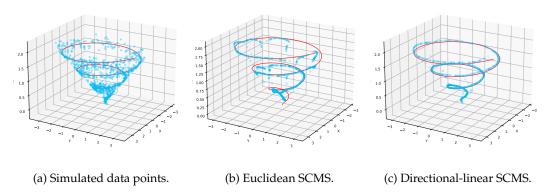
$$\mathbf{y}^{(t+1)} \leftarrow \mathbf{y}^{(t)} + \eta \cdot \widehat{V}_d(\mathbf{y}^{(t)}) \widehat{V}_d(\mathbf{y}^{(t)})^T \mathbf{H}^{-1} \Xi(\mathbf{y}^{(t)})$$
 with

$$\Xi(y) = (\Xi_{x}(x,z),\Xi_{z}(x,z))^{T} = \begin{pmatrix} \sum_{i=1}^{n} \mathbf{X}_{i} L^{i} \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ \sum_{i=1}^{n} L^{i} \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{2}} \right) \\ - \mathbf{x}, \quad \sum_{i=1}^{n} L \left(\frac{1 - \mathbf{X}_{i}^{T} \mathbf{x}^{(t)}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z_{i}}{h_{1}^{2}} \right) K^{i} \left(\frac{z^{(t)} - Z$$

▶ Note: A naive generalization of SCMS algorithm $z^{(t+1)} \leftarrow z^{(t)} + \widehat{V}_d(z^{(t)})\widehat{V}_d(z^{(t)})^T \Xi(z^{(t)})$ plus standardization as with pure Euclidean/directional data does not work (Zhang and Chen, 2025)!

Filament Detection in the Directional-Linear Space

We sample 1000 observations on a spiral curve with additive Gaussian noises $\mathcal{N}(0, 0.2^2)$ to their angular-linear coordinates.



▶ Our directional-linear SCMS algorithm is stabler than its Euclidean prototype.

Python Implementation: SCONCE-SCMS

All of our proposed methods are encapsulated in a Python package called **SCONCE-SCMS** (Spherical and **CON**ic Cosmic wEb finder with the extended **SCMS** algorithms; Zhang et al. 2022).



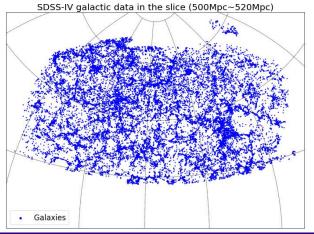
- Python Package Index: https://pypi.org/project/sconce-scms/.
- Documentation: https://sconce-scms.readthedocs.io/en/latest/.

SDSS-IV Cosmic Web Catalog



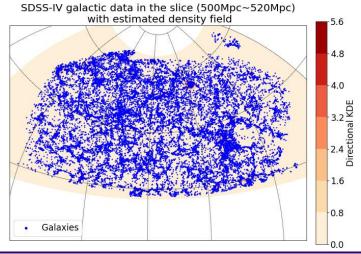
Step 1 (Slicing the Universe): Partition the redshift range into 325 spherical slices based on the comoving distance $\Delta L = 20 \,\mathrm{Mpc}$.

• Within each slice, we consider the redshifts of galaxies to be the same so that the galaxies are located on Ω_2 .



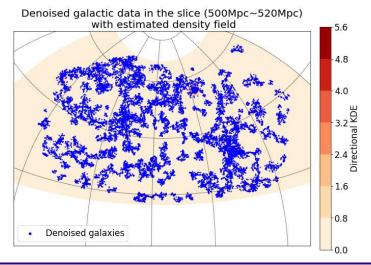
Step 2 (Density Estimation): Estimate the galaxy density field within each spherical slice by directional KDE.

• The bandwidth parameter is selected via a data-adaptive approach.

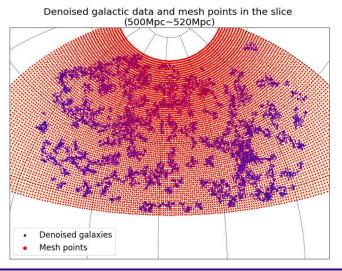


Step 3 (Denoising): Remove the observations with low-density values.

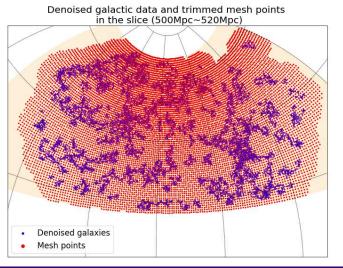
• We keep at least 80% of the original galaxy data in the slice.



Step 4 (Laying Down the Mesh Points): We place a set of dense mesh points on the interested region, which are the initial points of our DirSCMS iterations.



Step 5 (Thresholding the Mesh Points): We discard those mesh points with low-density values and keep 85% of the original mesh points.



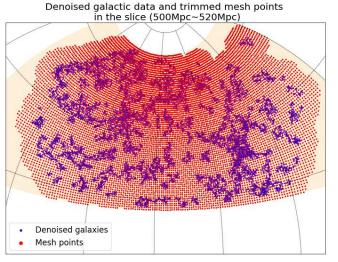


Figure: DirSCMS Iterations (Step 0).

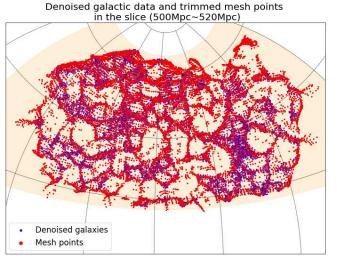


Figure: DirSCMS Iterations (Step 1).

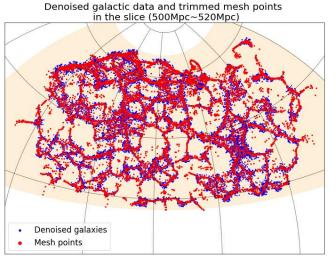


Figure: DirSCMS Iterations (Step 2).

Step 6 (DirSCMS Iterations): We iterate our DirSCMS algorithm on each remaining mesh point until convergence.

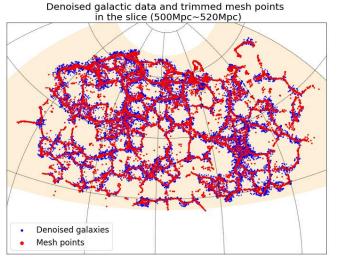


Figure: DirSCMS Iterations (Step 3).

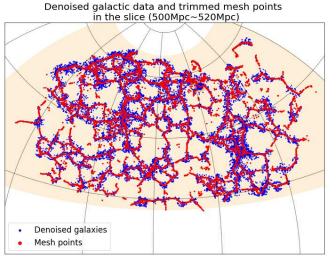


Figure: DirSCMS Iterations (Step 5).

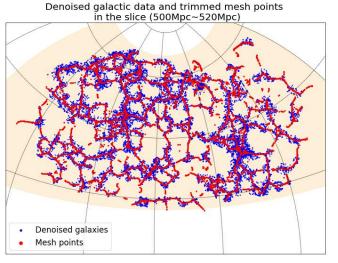


Figure: DirSCMS Iterations (Step 8).

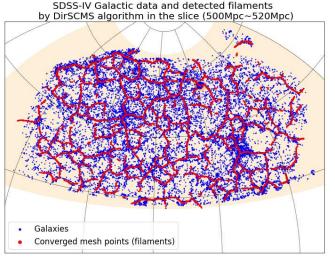


Figure: DirSCMS Iterations (Final).

Step 7 (Mode and Knot Estimation): We seek out the local modes and knots on the filaments as cosmic nodes.

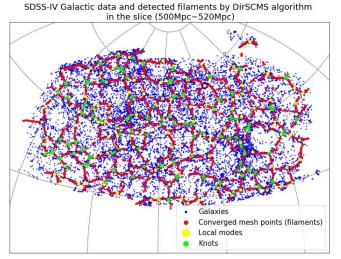
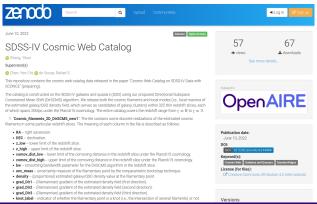


Figure: Nodes on the detected filaments.

Final Cosmic Web Catalog on SDSS-IV Data

- The input data incorporate not only galaxy but also quasar (QSO) observations so as to dive deeper into the Universe.
- We compute the uncertainty measure and other features for each detected filamentary point.
- The final catalog is available at https://doi.org/10.5281/zenodo.6244866.



Conclusion and Future Works



In this talk, we discuss our method for estimating cosmic filament structures from observed galactic data and its statistical theory.

• The cosmic filaments are modeled by directional density ridges, which can be consistently estimated by directional KDE.

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- We design an efficient algorithm (DirSCMS) to find the directional density ridges in practical applications.

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- 6 The cosmic web catalog based on our proposed method is publicly available.

Future Work: Cosmic Void Detection

Along this line of research, we are planning to

 Leverage our cosmic filament catalog to identify cosmic voids and infer the precise cosmology (Sánchez et al., 2016).

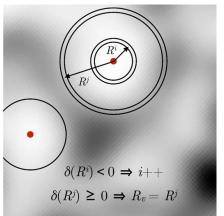
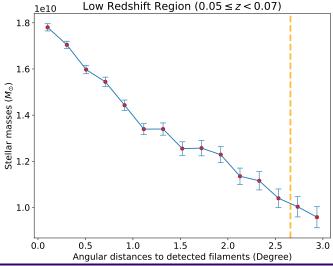


Figure: Simple void-finding algorithm (Sánchez et al., 2016).

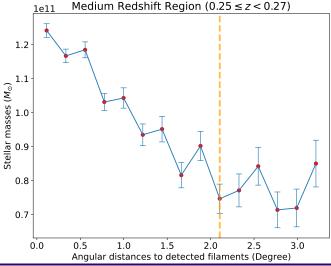
Future Work: Filament Effects of Galaxy Properties

 Analyze if galaxy properties, such as stellar mass, color, and star formation rate, are correlated with our detected cosmic web structures (Chen et al., 2017; Kotecha, 2020)...



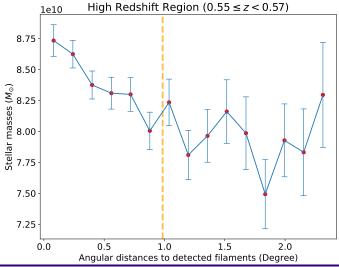
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Future Work: Filament Effects of Galaxy Properties

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Thank you!

More details can be found in

[1] Y. Zhang and Y.-C. Chen. Kernel Smoothing, Mean Shift, and Their Learning Theory with Directional Data. *Journal of Machine Learning Research*, 22(154):1–92, 2021.

https://arxiv.org/abs/2010.13523

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https://arxiv.org/abs/2104.14977

[4] Y. Zhang and Y.-C. Chen. Mode and Ridge Estimation in Euclidean and Directional Product Spaces: A Mean Shift Approach. *Journal of Computational and Graphical Statistics*, (just-accepted): 1-20, 2025.

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[5] Y. Zhang, R. S. de Souza, and Y.-C. Chen. SCONCE: A Cosmic Web Finder for Spherical and Conic Geometries. *Monthly Notices of the Royal Astronomical Society*, 517(1): 1197-1217, 2022.

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Riemannian Gradient and Hessian on Ω_q

Assume tentatively that the directional function f is well-defined and smooth in $\mathbb{R}^{q+1} \setminus \{\mathbf{0}\}$ (or at least in an open neighborhood $U \supset \Omega_q$).

• Riemannian gradient grad f(x) on Ω_q :

$$\operatorname{grad} f(x) = \left(I_{q+1} - xx^T \right) \nabla f(x),$$

where I_{q+1} is the identity matrix in $\mathbb{R}^{(q+1)\times(q+1)}$.

• *Riemannian Hessian* $\mathcal{H}f(x)$ on Ω_q (Zhang and Chen, 2021):

$$\mathcal{H}f(x) = (\mathbf{I}_{q+1} - xx^T) \left[\nabla \nabla f(x) - \nabla f(x)^T x \cdot \mathbf{I}_{q+1} \right] (\mathbf{I}_{q+1} - xx^T).$$

Here, I_{q+1} is the identity matrix in $\mathbb{R}^{(q+1)\times(q+1)}$, while $\nabla f(x)$ and $\nabla \nabla f(x)$ are total gradient and Hessian in \mathbb{R}^{q+1} .

Detailed Procedures of DirSCMS Algorithm

Input:

- A directional data sample $X_1, ..., X_n \sim f(x)$ on Ω_q
- The order d of the directional ridge, smoothing bandwidth h > 0, and tolerance level $\epsilon > 0$.
- A suitable mesh $\mathcal{M}_D \subset \Omega_q$ of initial points.

Step 1: Compute the directional KDE
$$\widehat{f}_h(x) = \frac{c_{L,q}(h)}{n} \sum_{i=1}^n L\left(\frac{1-x^TX_i}{h^2}\right)$$
 on the mesh \mathcal{M}_D .

Step 2: For each $\hat{x}^{(0)} \in \mathcal{M}_D$, iterate the following DirSCMS update until convergence:

while
$$\left\|\sum_{i=1}^n \widehat{V}_d(\widehat{\mathbf{x}}^{(0)})\widehat{V}_d(\widehat{\mathbf{x}}^{(0)})^T X_i \cdot L'\left(\frac{1-X_i^T\widehat{\mathbf{x}}^{(0)}}{h^2}\right)\right\|_2 > \epsilon$$
 do:

Detailed Procedures of DirSCMS Algorithm

• **Step 2-1**: Compute the scaled version of the estimated Hessian matrix as:

$$\begin{split} \frac{nh^2}{c_{L,q}(h)}\mathcal{H}\widehat{f}_h(\widehat{\boldsymbol{x}}^{(t)}) &= \left[\boldsymbol{I}_{q+1} - \widehat{\boldsymbol{x}}^{(t)} \left(\widehat{\boldsymbol{x}}^{(t)}\right)^T\right] \left[\frac{1}{h^2} \sum_{i=1}^n \boldsymbol{X}_i \boldsymbol{X}_i^T \cdot L'' \left(\frac{1 - \boldsymbol{X}_i^T \widehat{\boldsymbol{x}}^{(t)}}{h^2}\right) \right. \\ &+ \left. \sum_{i=1}^n \boldsymbol{X}_i^T \widehat{\boldsymbol{x}}^{(t)} \boldsymbol{I}_{q+1} \cdot L' \left(\frac{1 - \boldsymbol{X}_i^T \widehat{\boldsymbol{x}}^{(t)}}{h^2}\right)\right] \left[\boldsymbol{I}_{q+1} - \widehat{\boldsymbol{x}}^{(t)} \left(\widehat{\boldsymbol{x}}^{(t)}\right)^T\right]. \end{split}$$

- **Step 2-2**: Perform the spectral decomposition on $\frac{nh^2}{c_{L,q}(h)}\mathcal{H}\widehat{f}_h\left(\widehat{x}^{(t)}\right)$ and compute $\widehat{V}_d(\widehat{x}^{(t)}) = \left[v_{d+1}(\widehat{x}^{(t)}), ..., v_q(\widehat{x}^{(t)})\right]$, whose columns are orthonormal eigenvectors corresponding to the smallest q-d eigenvalues inside the tangent space $T_{\widehat{x}^{(t)}}$.
- Step 2-3: Update

$$\widehat{m{x}}^{(t+1)} \leftarrow \widehat{m{x}}^{(t)} - \widehat{V}_d(\widehat{m{x}}^{(t)})\widehat{V}_d(\widehat{m{x}}^{(t)})^T \left| rac{\sum_{i=1}^n m{X}_i L'\left(rac{1-m{X}_i^T m{x}^{(t)}}{h^2}
ight)}{\sum_{i=1}^n m{X}_i L'\left(rac{1-m{X}_i^T m{x}^{(t)}}{h^2}
ight)}
ight|.$$

Detailed Procedures of DirSCMS Algorithm

• Step 2-4: Standardize $\widehat{x}^{(t+1)}$ as $\widehat{x}^{(t+1)} \leftarrow \frac{\widehat{x}^{(t+1)}}{\|\widehat{x}^{(t+1)}\|_2}$.

Output: An estimated directional *d*-ridge $\widehat{\mathcal{R}}_d$ represented by the collection of resulting points.

Linear Convergence of Subspace Constrained Gradient Ascent on Ω_q

Under some regularity conditions, we prove the following (Theorem 4.6 in Zhang and Chen 2022):

R-Linear convergence of $d(x^{(k)}, \mathcal{R}_d)$ **with** f. When the step size $\underline{\eta} > 0$ is sufficiently small and the initial point $x^{(0)}$ lies within a small neighborhood of its limiting point x^* in \mathcal{R}_d ,

$$d\left(x^{(k)},\mathcal{R}_{d}\right)\leq\underline{\Upsilon}^{k}\cdot d\left(x^{(0)},x^{*}\right) \quad ext{ with } \quad \underline{\Upsilon}=\sqrt{1-rac{\underline{\Upsilon}oldsymbol{eta}_{0}}{4}},$$

where $\beta_0 > 0$ is the eigengap between the *d*-th and (d + 1)-th eigenvalues of $\mathcal{H}f(x)$.

R-Linear convergence of $d(\widehat{x}^{(k)}, \mathcal{R}_d)$ **with** \widehat{f}_h . When the step size $\underline{\eta} > 0$ is sufficiently small and the initial point $\widehat{x}^{(0)}$ lies within a small neighborhood of x^* in \mathcal{R}_d ,

$$d\left(oldsymbol{x}^{(k)}, \mathcal{R}_d
ight) \leq \underline{\Upsilon}^k \cdot d\left(oldsymbol{x}^{(0)}, oldsymbol{x}^*
ight) + O(h^2) + O_P\left(\sqrt{rac{|\log h|}{nh^{q+4}}}
ight)$$

with probability tending to 1, as $h \to 0$ and $\frac{nh^{q+4}}{|\log h|} \to 0$.

Linear Convergence of Mean Shift and SCMS Algorithms

- The linear convergence results can also be proved for the subspace constrained gradient ascent method but under some stricter conditions (Zhang and Chen, 2022).
- The (directional) mean shift and SCMS algorithms can be viewed as variants of the (subspace constrained) gradient ascent methods (on Ω_q) but with adaptive step sizes.
- The step sizes can be made sufficiently small as the bandwidth *h* is small and the sample size *n* is large, but also universally bounded away from 0 with respect to the iteration number *t*.

Application of DirLinSCMS to SDSS-IV Galaxy Data

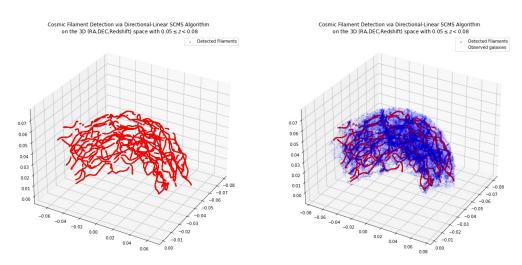


Figure: Cosmic filament detection in the 3D (RA,DEC,Redshift) space with our directional-linear SCMS algorithm.

Drawback of 3D Methods

There are some potential drawbacks of detecting filaments with survey data in the 3D space:

- The determination of $d(\cdot)$ relies on complex cosmological models.
- The galaxy distribution is distorted along the line of sight due to the peculiar velocities of galaxies (i.e., the so-called *finger-of-god* (Sargent and Turner, 1977) and *Kaiser* (Kaiser, 1987) effects).

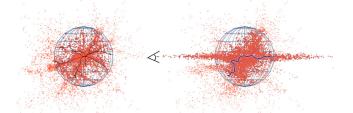


Figure: Redshift distortions along the line of sight (Kuchner et al., 2021).

• The number of galaxies varies across different redshift values, so applying 3D approaches will be computationally intensive.