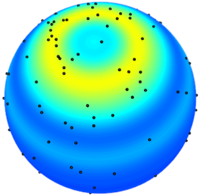

Smoothing-based inference with directional data

Eduardo García-Portugués (edgarcia@est-econ.uc3m.es)

Department of Statistics
Universidad Carlos III de Madrid

EAFIT, September 15, 2017

Directional data: what, why, where?

- Directional data are vectors whose support is the hypersphere

$$\Omega_q = \left\{\mathbf{x} \in \mathbb{R}^{q+1} : ||\mathbf{x}|| = 1\right\}$$

- Particular cases are the circle ($q = 1$) and the sphere ($q = 2$)
- Statistical methods must account for the special nature of directional data
- Present in different applied fields: corner stone in bioinformatics, used in text mining

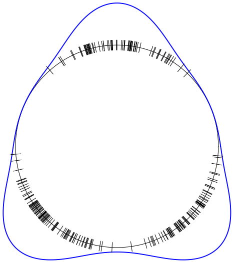

Figure: Circular density

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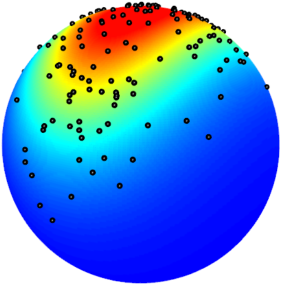

Figure: Spherical density

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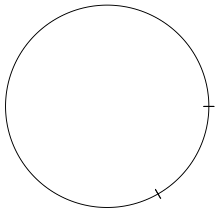

Figure: Circular mean

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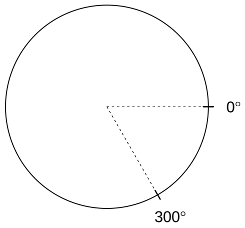

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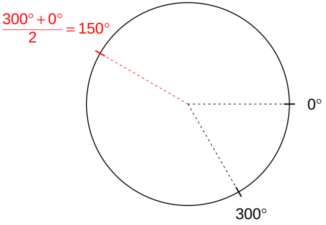

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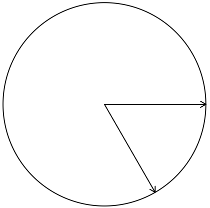

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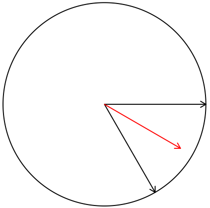

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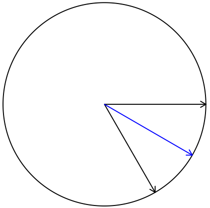

Figure: Circular mean

Literature overview

- **Mardia, K. V. (1972).** *Statistics of Directional Data.* Academic Press.
- **Batschelet, E. (1981).** *Circular Statistics in Biology.* Academic Press.
- **Watson, G. S. (1983).** *Statistics on Spheres.* John Wiley & Sons.
- **Fisher, N. I. (1993).** *Statistical Analysis of Circular Data.* Cambridge University Press.
- **Fisher, N. I., Lewis, T. and Embleton, B. J. J. (1993).** *Statistical Analysis of Spherical Data.* Cambridge University Press.
- **Mardia, K. V. and Jupp, P. E. (2000).** *Directional Statistics.* John Wiley & Sons.
- **Hamelryck, T. and Mardia, K. V. and Ferkinghoff-Borg, J. (2012).** *Bayesian Methods in Structural Bioinformatics.* Springer.
- **Pewsey, A., Neuhäuser, M. and Ruxton, G. D. (2013).** *Circular Statistics in R.* Oxford University Press.
- **Ley, C. and Verdebout, T. (2017).** *Modern Directional Statistics.* Chapman and Hall/CRC.
- **Ley, C. and Verdebout, T. (2018+).** *Applied Directional Statistics: Modern Methods and Case Studies.* Chapman and Hall/CRC.

Protein structure modelling

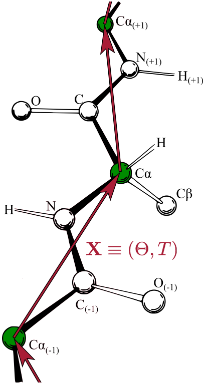

Figure: Backbone and C_α representation

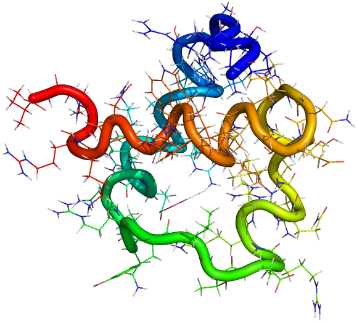

Figure: Cartoon view of a protein

Boomsma, W., Mardia, K. V., Taylor, C. C., Ferkinghoff-Borg, J., Krogh, A. and Hamelryck, T. A generative, probabilistic model of local protein structure. *PNAS*, 105(26):8932-8937

Text mining

- Document d (Ronald Fisher, 1938):

  > "To call in the statistician after the experiment is done may be no more than asking him to perform a post-mortem examination: he may be able to say what the experiment died of."

- Preprocessing of d:
  1. Lowercase conversion, remove punctuation, remove format, ...
  2. Pruning (remove stop words and too common or uncommon words)
  3. Stemming ("statistician" $\rightarrow$ "statistic")
- **Vector Space Model**:
  1. Set a dictionary as a basis for a collection of documents:
     $$D = \{\text{"hello"}, \text{"statistic"}, \text{"experi"}, \text{"examin"}, \text{"world"}\}$$
  2. Codify the document d as a frequency vector
     $$\mathbf{d} = (0, 1, 2, 1, 0).$$
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Von Mises-Fisher distribution

- The **von Mises-Fisher** (vMF) is the most well known directional density:

$$f_{\mathrm{vMF}}(\mathbf{x};\boldsymbol{\mu},\kappa)=C_q(\kappa)\exp\left\{\kappa\mathbf{x}^T\boldsymbol{\mu}\right\},\quad C_q(\kappa)=\frac{\kappa^{\frac{q-1}{2}}}{(2\pi)^{\frac{q+1}{2}}\mathcal{I}_{\frac{q-1}{2}}(\kappa)}$$

  parametrized by a mean $\boldsymbol{\mu}\in\Omega_q$ and a concentration $\kappa\geq 0$

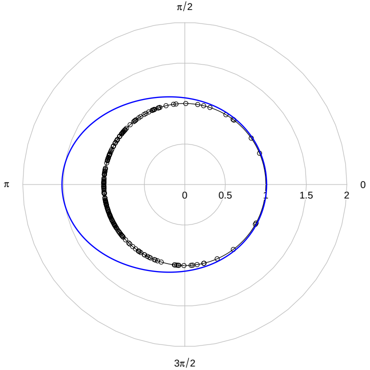
- Density wrt the Lebesgue measure ω_q in Ω_q. ω_q denotes also the area surface of Ω_q:

$$\omega_q\equiv\omega_q(\Omega_q)=2\pi^{\frac{q+1}{2}}/\Gamma\left(\frac{q+1}{2}\right)$$

- (Isotropic) **Gaussian analogue**:
  1. Same MLE characterization property
  2. If $\mathbf{X}\sim\mathcal{N}_{q+1}\left(\boldsymbol{\mu},\sigma^2\mathbf{I}_{q+1}\right)$, then

$$\mathbf{X}\,\Big|\,||\mathbf{X}||=1\sim\mathrm{vMF}\left(\frac{\boldsymbol{\mu}}{||\boldsymbol{\mu}||},\frac{||\boldsymbol{\mu}||}{\sigma^2}\right)$$

Von Mises distribution



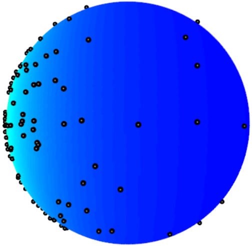


Figure: $\mathrm{vM}(\boldsymbol{\mu}, \kappa)$ density in the circle and the sphere, with $\boldsymbol{\mu} = (\mathbf{0}_q, 1)$ and $\kappa = 2$.

Von Mises distribution

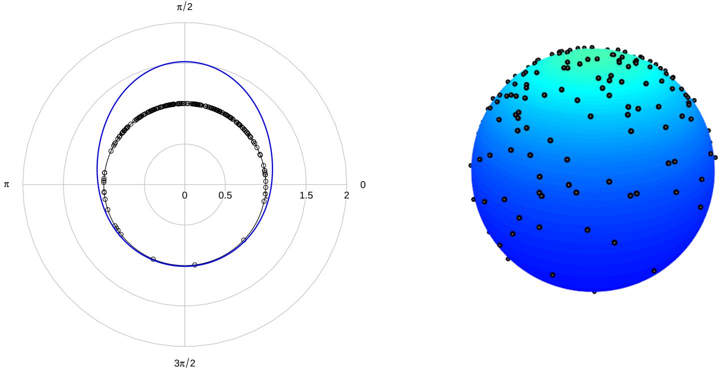
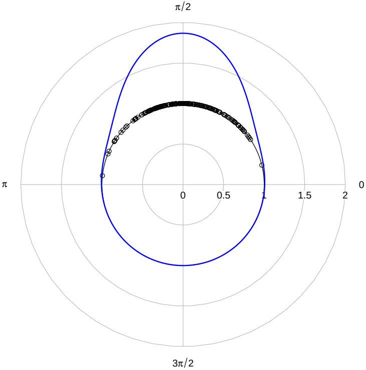


Figure: $\mathrm{vM}(\boldsymbol{\mu}, \kappa)$ density in the circle and the sphere, with $\boldsymbol{\mu} = (-1, \mathbf{0}_q)$ and $\kappa = 2$.

Von Mises distribution



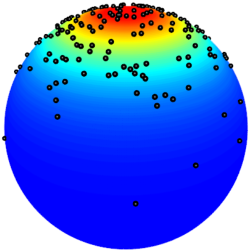
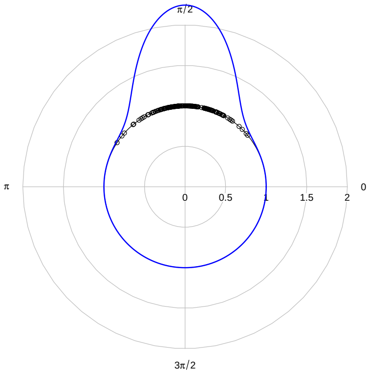


Figure: $\mathrm{vM}(\boldsymbol{\mu}, \kappa)$ density in the circle and the sphere, with $\boldsymbol{\mu} = (\mathbf{0}_q, 1)$ and $\kappa = 5$.

Von Mises distribution



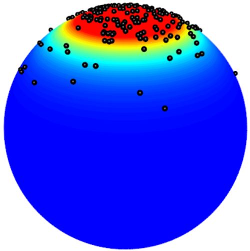
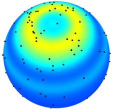


Figure: $\mathrm{vM}(\boldsymbol{\mu}, \kappa)$ density in the circle and the sphere, with $\boldsymbol{\mu} = (\mathbf{0}_q, 1)$ and $\kappa = 10$.

Contents of the talk

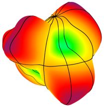
1. **Part I**. Kernel **density** estimation with directional data under rotational symmetry

- Present a KDE under **rotational symmetry**
- Study its main **asymptotic properties**
- Illustrate **empirical performance** through simulations



2. **Part II**. Estimation and testing in linear-directional **regression**

- Present a **local linear estimator** with directional predictor
- Build a **goodness-of-fit** test for regression models
- Apply both to test a common assumption in **bioinformatics**



Part I

Kernel density estimation with directional data under rotational symmetry

García-Portugués, E., Ley, C., Verdebout, T. (2017). Kernel density estimation for directional data under rotational symmetry. *Work in progress.*

Contents of Part I

KDE with directional data

- For a sample $\mathbf{X}_1, \ldots, \mathbf{X}_n \sim f$, the Kernel Density Estimator (KDE) for directional data is

$$\hat{f}_h(\mathbf{x}) = \frac{c_{h,q}(L)}{n} \sum_{i=1}^{n} L\left(\frac{1 - \mathbf{x}^T \mathbf{X}_i}{h^2}\right) = \frac{1}{n} \sum_{i=1}^{n} L_h\left(\mathbf{x}, \mathbf{X}_i\right), \quad \mathbf{x} \in \Omega_q$$

Bai, Z. D., Rao, C. R. and Zhao, L. C. (1988). Kernel estimators of density function of directional data. *J. Multivariate Anal.*, 27:24–39

- Note the h^2 because $2(1 - \mathbf{x}^T \mathbf{X}_i) = ||\mathbf{x} - \mathbf{X}_i||^2$
- Normalizing constant $c_{h,q}(L)^{-1} = \lambda_q(L) h^q (1 + o(1))$ with

$$\lambda_q(L) = 2^{\frac{q}{2}-1} \omega_{q-1} \int_0^\infty L(r) r^{\frac{q}{2}-1}\, dr$$

- "Second moment" of L: $b_q(L) = \int_0^\infty L(r) r^{\frac{q}{2}}\, dr \big/ \int_0^\infty L(r) r^{\frac{q}{2}-1}\, dr$
- If $L(r) = e^{-r}$, the *vMF kernel*, $c_{h,q}(L) = e^{1/h^2} C_q(1/h^2)$

Circular case

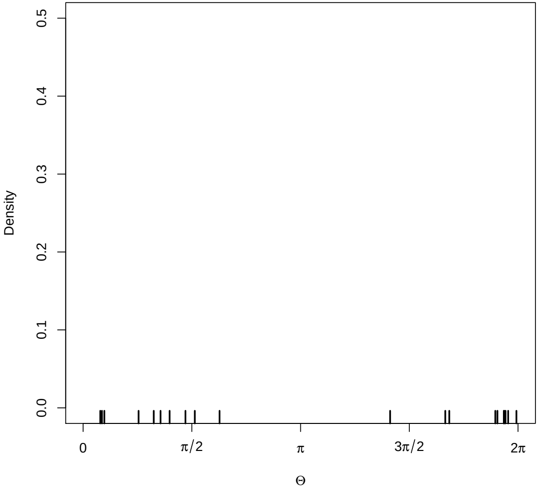
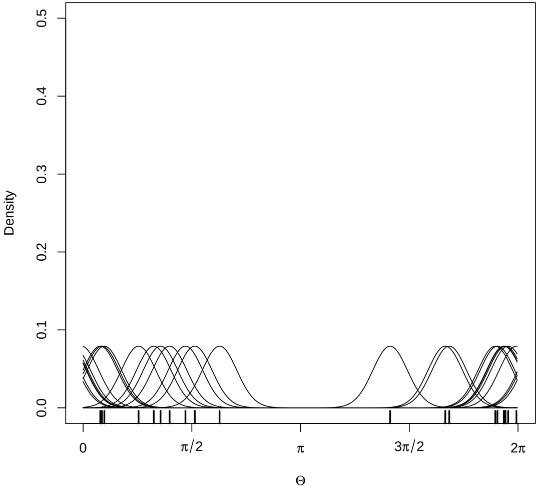


Figure: Construction of the kernel density estimator with $n = 20$.

Circular case



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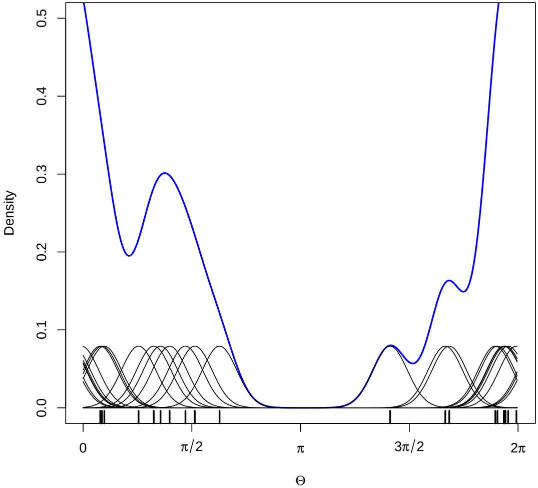

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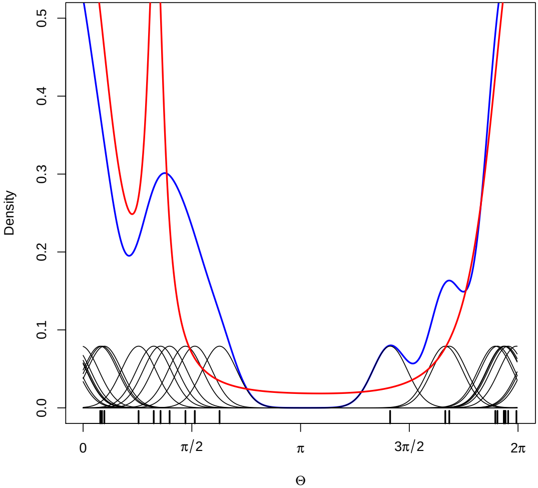

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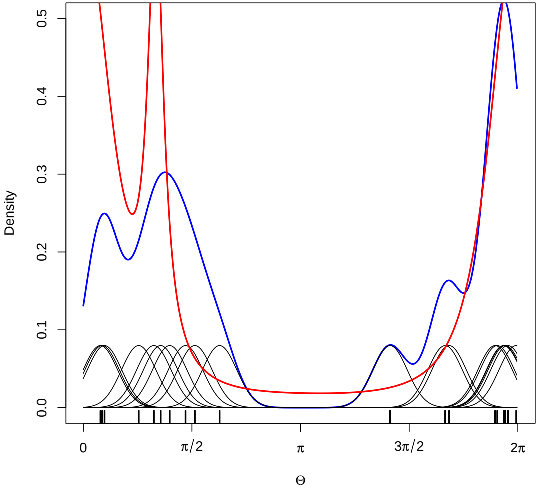

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KDE construction: spherical case

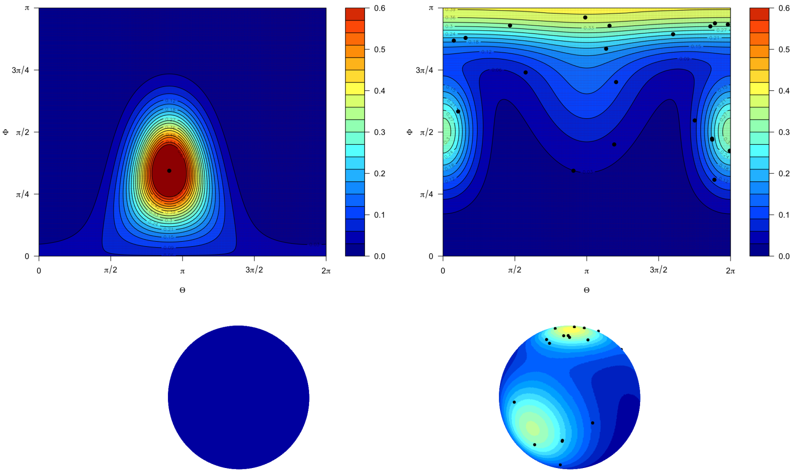


Figure: Left: KDE with $n = 1$. Right: true density

KDE construction: spherical case

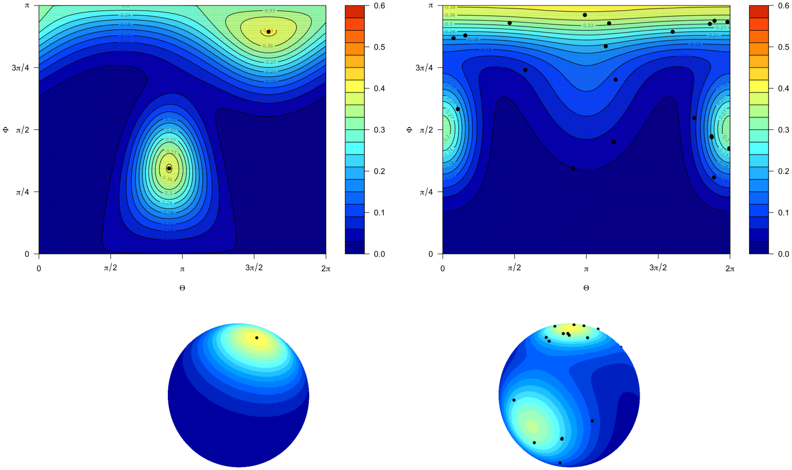


Figure: Left: KDE with $n = 2$. Right: true density

KDE construction: spherical case

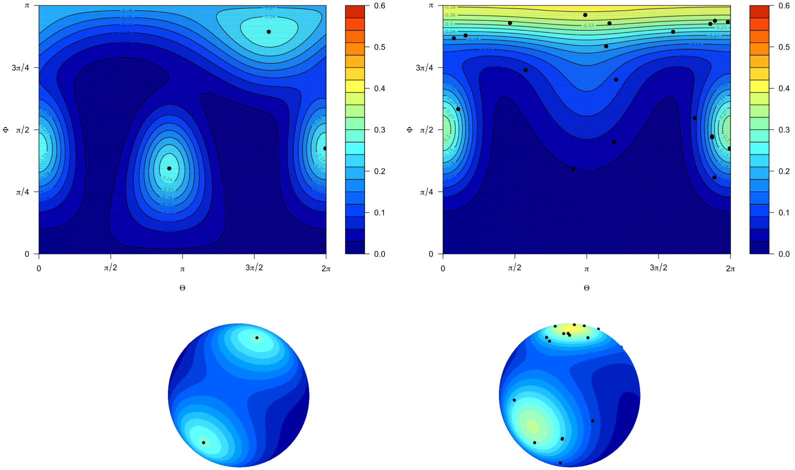


Figure: Left: KDE with $n = 3$. Right: true density

KDE construction: spherical case

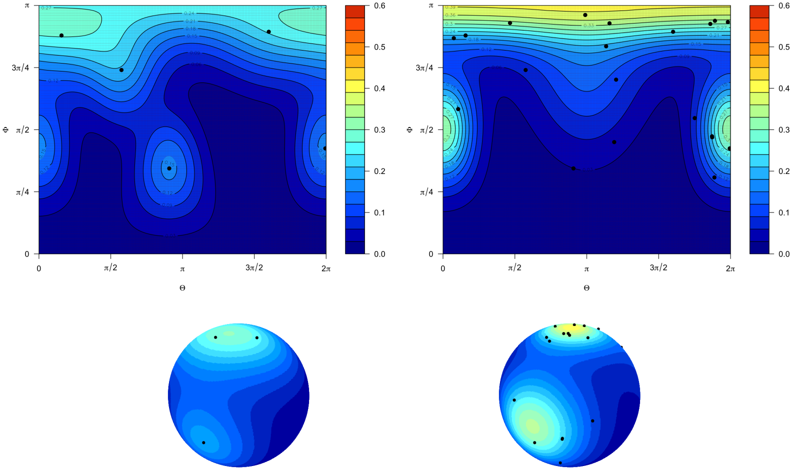


Figure: Left: KDE with $n = 5$. Right: true density

KDE construction: spherical case

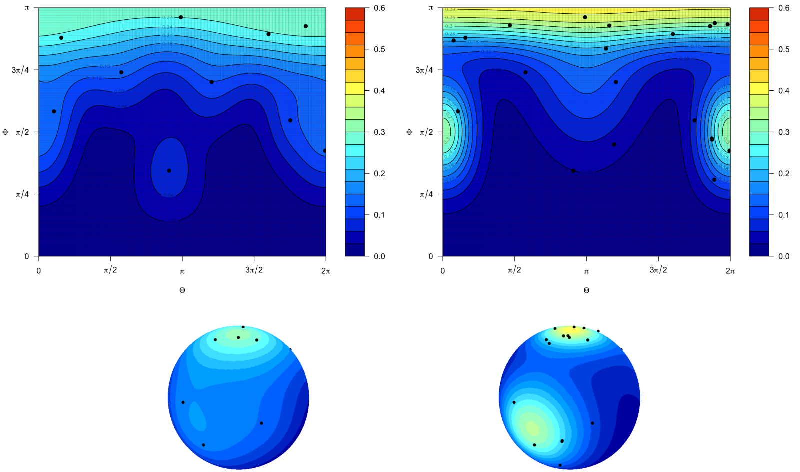


Figure: Left: KDE with $n = 10$. Right: true density

KDE construction: spherical case

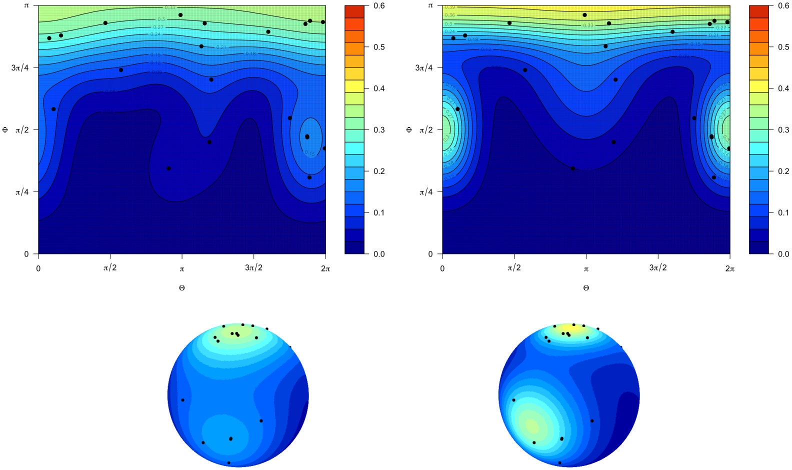
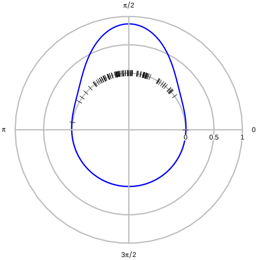


Figure: Left: KDE with $n = 20$. Right: true density

Rotasymmetry I

- Recurrent assumption: $\mathbf{X}$ is **rotational symmetric** (or **rotasymmetric**) about some direction $\boldsymbol{\theta} \in \Omega_q$
- Circular case: rotasymmetry is **reflective symmetry**
- High-dimensional situation: rotasymmetry is behind many **celebrated distributions**



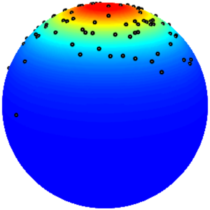


Figure: Rotasymmetry in the circular and spherical cases

Rotasymmetry II

Proposition (Rotasymmetry characterization)

Let $\mathbf{X}$ *a directional rv with density* f. *These statements are equivalent:*

1. $\mathbf{X} \stackrel{d}{=} \mathbf{O}\mathbf{X}$, *where* $\mathbf{O} = \boldsymbol\theta\boldsymbol\theta^T + \sum_{i=1}^q \mathbf{b}_i\mathbf{b}_i^T$ *is a rotation matrix on* $\mathbb{R}^{q+1}$ *that fixes* $\boldsymbol\theta \in \Omega_q$
2. $f(\mathbf{x}) = g\left(\mathbf{x}^T\boldsymbol\theta\right)$, $\forall \mathbf{x} \in \Omega_q$, *where* $g : [-1,1] \longrightarrow \mathbb{R}^+$ *is a* ***link*** *such that*

$$f^*(t) = \omega_{q-1} g(t)(1-t^2)^{\frac{q}{2}-1} \text{ is a density in } [-1,1]$$

- Rotasymmetry is related with the **tangent-normal decomposition**:

$$\mathbf{x} = t\boldsymbol\theta + (1-t^2)^{\frac{1}{2}}\mathbf{B}_{\boldsymbol\theta}\boldsymbol\xi$$

  with $t = \mathbf{x}^T\boldsymbol\theta \in [-1,1]$, $\boldsymbol\xi \in \Omega_{q-1}$ and $\mathbf{B}_{\boldsymbol\theta} = (\mathbf{b}_1, \ldots, \mathbf{b}_q)_{(q+1)\times q}$ such that $\mathbf{B}_{\boldsymbol\theta}^T\mathbf{B}_{\boldsymbol\theta} = \mathbf{I}_q$ and $\mathbf{B}_{\boldsymbol\theta}\mathbf{B}_{\boldsymbol\theta}^T = \mathbf{I}_{q+1} - \boldsymbol\theta\boldsymbol\theta^T$
- **No monotonicity** required in g, axial variables are covered as well

The rotasymmetrizer

Definition (Rotasymmetrizer)

The ***rotasymmetrizer*** *around* $\boldsymbol{\theta}$, $R_{\boldsymbol{\theta}}$, *transforms a function* $f : \Omega_q \longrightarrow \mathbb{R}$ *into*

$$R_{\boldsymbol{\theta}} f(\mathbf{x}) := \frac{1}{\omega_{q-1}} \int_{\Omega_{q-1}} f(\mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi}})\, \omega_{q-1}(d\boldsymbol{\xi}),$$

with $\mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi}} = (\mathbf{x}^T\boldsymbol{\theta})\boldsymbol{\theta} + (1 - (\mathbf{x}^T\boldsymbol{\theta})^2)^{\frac{1}{2}} \mathbf{B}_{\boldsymbol{\theta}}\boldsymbol{\xi}$

- For point $\mathbf{x} \in \Omega_q$, the operator **averages out** the density along the points sharing the same **colatitude** (wrt $\boldsymbol{\theta}$)
- Intuitively: parallel redistribution of probability mass

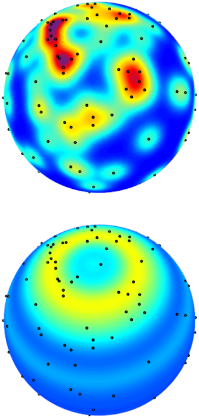


Figure: Input and output of $R_{\boldsymbol{\theta}}$ with $\boldsymbol{\theta} = (0, 0, 1)$

Properties

Proposition (Rotasymmetrizer properties)

Let be $f, f_1, f_2 : \Omega_q \longrightarrow \mathbb{R}^+$ *directional densities and* $\boldsymbol{\theta} \in \Omega_q$.

1. ***Invariance*** *from different matrices* $\mathbf{B}_{\boldsymbol{\theta}}$:
$$\int_{\Omega_{q-1}} f\left(\mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi},1}\right) \omega_{q-1}(d\boldsymbol{\xi}) = \int_{\Omega_{q-1}} f\left(\mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi},2}\right) \omega_{q-1}(d\boldsymbol{\xi}),$$
with $\mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi},k} = (\mathbf{x}^T\boldsymbol{\theta})\boldsymbol{\theta} + (1-(\mathbf{x}^T\boldsymbol{\theta})^2)^{\frac{1}{2}}\mathbf{B}_{\boldsymbol{\theta},k}\boldsymbol{\xi}$, $k = 1, 2$
2. ***Linearity***: $R_{\boldsymbol{\theta}}(\lambda_1 f_1 + \lambda_2 f_2)(\mathbf{x}) = \lambda_1 R_{\boldsymbol{\theta}} f_1(\mathbf{x}) + \lambda_2 R_{\boldsymbol{\theta}} f_2(\mathbf{x})$
3. ***Density preservation***: $R_{\boldsymbol{\theta}} f$ *is a density*
4. ***Characterization***: $R_{\boldsymbol{\theta}} f = f \iff f$ *is rotasymmetric around* $\boldsymbol{\theta}$
5. *Explicit expression for the* ***vMF density***:
$$R_{\boldsymbol{\theta}} f_{\mathrm{vMF}}(\mathbf{x}; \boldsymbol{\mu}, \kappa) = \frac{C_q(\kappa) \exp\left\{\kappa \mathbf{x}^T\boldsymbol{\theta}\boldsymbol{\mu}^T\boldsymbol{\theta}\right\}}{\omega_{q-1} C_{q-1}\left(\kappa\left[(1-(\mathbf{x}^T\boldsymbol{\theta})^2)(1-(\boldsymbol{\mu}^T\boldsymbol{\theta})^2)\right]^{\frac{1}{2}}\right)}$$

Rotasymmetric KDE

- **Goal: estimate semiparametrically f under rotasymmetry**

Definition (Rotasymmetric KDE)

The ***rotasymmetric KDE (RKDE)*** *is the application of the rotasymmetrizer to the usual KDE:*

$$\hat{f}_{h,\boldsymbol{\theta}}(\mathbf{x}) := R_{\boldsymbol{\theta}} \hat{f}_h(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} L_{h,\boldsymbol{\theta}}(\mathbf{x}, \mathbf{X}_i),$$

with $L_{h,\boldsymbol{\theta}}(\mathbf{x}, \mathbf{X}_i) = \frac{c_{h,q}(L)}{\omega_{q-1}} \int_{\Omega_{q-1}} L\left(\frac{1 - \mathbf{x}_{\boldsymbol{\theta},\boldsymbol{\xi}}^T \mathbf{X}_i}{h^2}\right) \omega_{q-1}(d\boldsymbol{\xi})$

- The rotasymmetric vMF kernel has an explicit expression:

$$L_{h,\boldsymbol{\theta}}(\mathbf{x}, \mathbf{X}_i) = \frac{C_q(1/h^2) \exp\left\{\mathbf{x}^T \boldsymbol{\theta} \mathbf{X}_i^T \boldsymbol{\theta} / h^2\right\}}{\omega_{q-1} C_{q-1}\left(\left[(1 - (\mathbf{x}^T \boldsymbol{\theta})^2)(1 - (\mathbf{X}_i^T \boldsymbol{\theta})^2)\right]^{\frac{1}{2}} / h^2\right)}$$

- The order of the normalizing constant is $\mathcal{O}\left(h^{-1}\right)$

Comparison of kernels

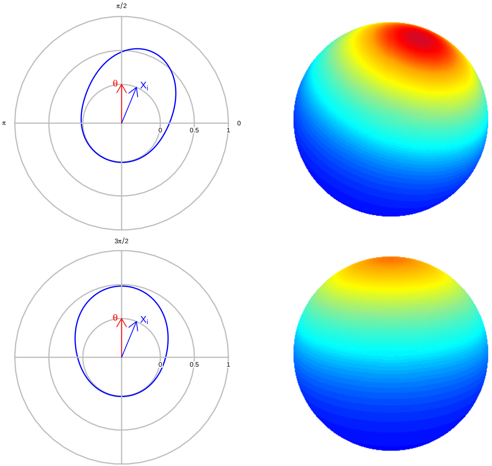
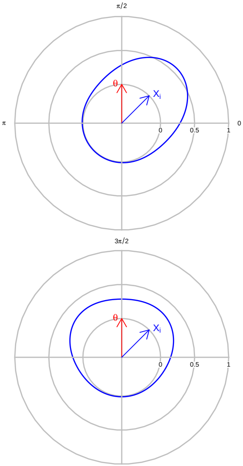


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Comparison of kernels



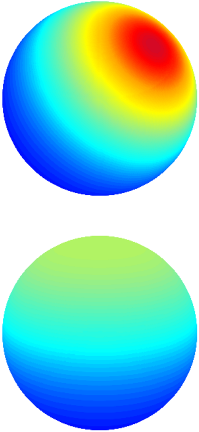


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Comparison of kernels

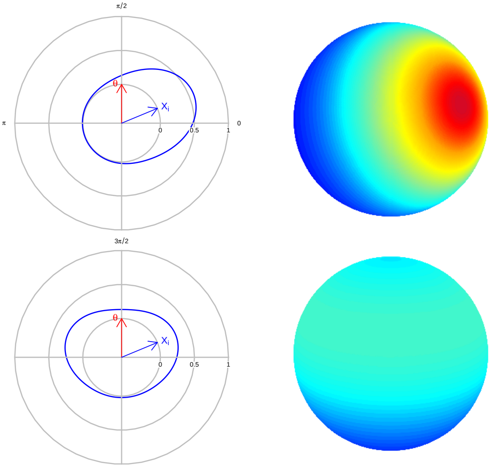


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Comparison of kernels

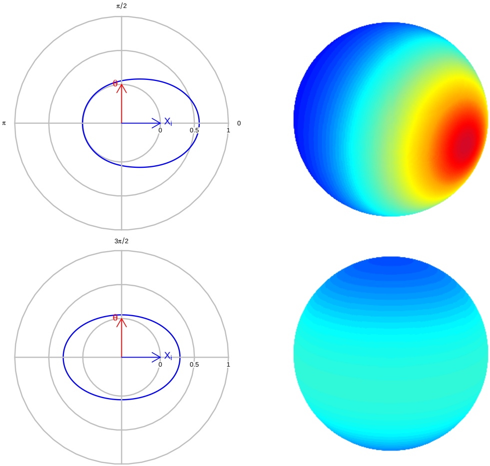
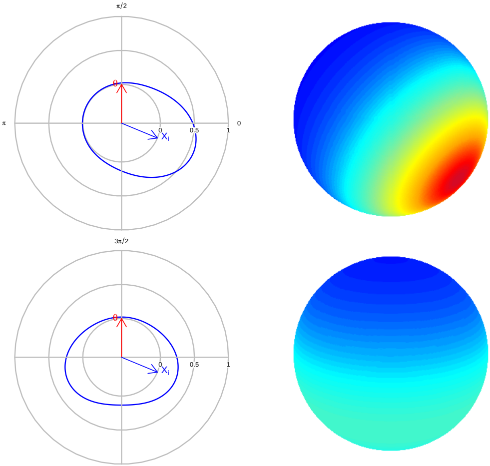


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Comparison of kernels



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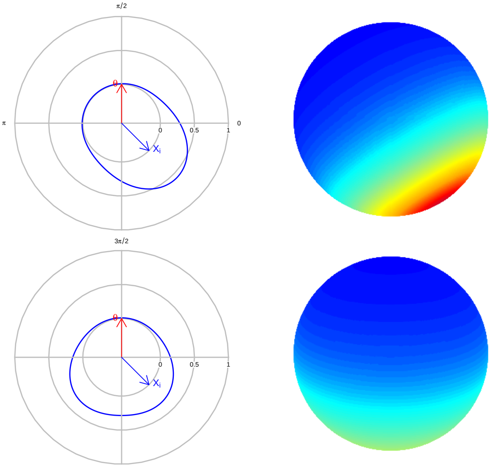
Comparison of kernels



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Comparison of kernels

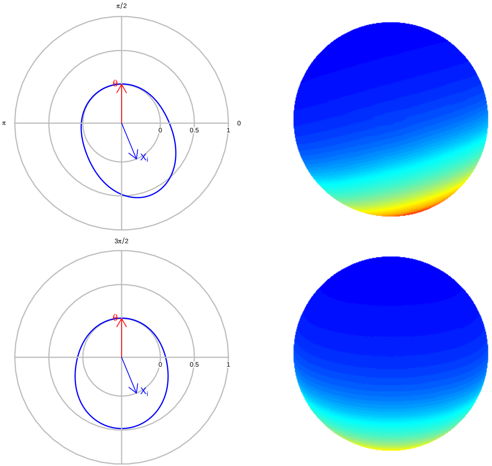


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Comparison of kernels

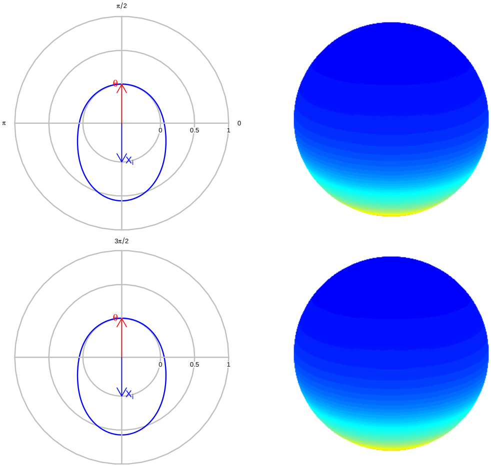


Figure: Kernels for the KDE (upper row) and their RKDE counterparts (lower), with $\boldsymbol{\theta} = (\mathbf{0}_q, 1)$. The kernels have the same bandwidth

Connections with KDE in $[-1, 1]$

- The RKDE kernels **only** depend on the **projected sample** $T_i = \mathbf{X}_i^T \boldsymbol{\theta}$ and the **projected point** $t = \mathbf{x}^T \boldsymbol{\theta}$
- RKDE is equivalent to KDE on $[-1, 1]$ with bounded kernels adapted to capture the spikes of $f^*(t) = \omega_{q-1} g(t)(1 - t^2)^{\frac{q}{2}-1}$
- Boundary bias is $\mathcal{O}\left(h^2\right)$ without any corrections

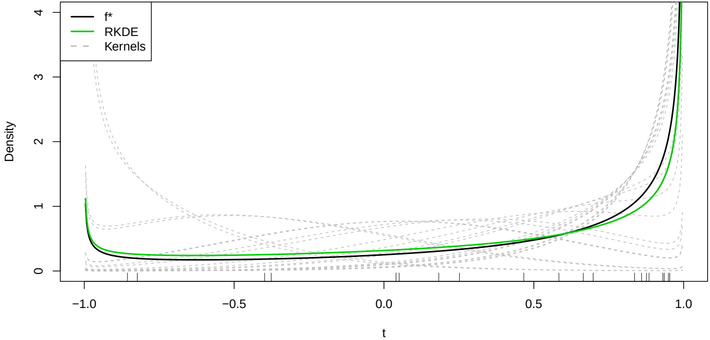


Figure: KDE of f^* with $g(t) = C_q(\kappa) \exp\{\kappa t\}$, $\kappa = 1$ and $q = 1$

Connections with KDE in $[-1,1]$

- The RKDE kernels **only** depend on the **projected sample** $T_i = \mathbf{X}_i^T\boldsymbol{\theta}$ and the **projected point** $t = \mathbf{x}^T\boldsymbol{\theta}$
- RKDE is equivalent to KDE on $[-1,1]$ with bounded kernels adapted to capture the spikes of $f^*(t) = \omega_{q-1}g(t)(1-t^2)^{\frac{q}{2}-1}$
- Boundary bias is $\mathcal{O}\left(h^2\right)$ without any corrections

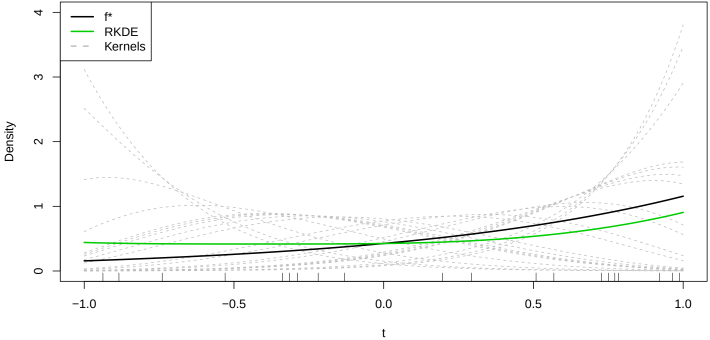


Figure: KDE of f^* with $g(t) = C_q(\kappa)\exp\{\kappa t\}$, $\kappa = 1$ and $q = 2$

Connections with KDE in $[-1,1]$

- The RKDE kernels **only** depend on the **projected sample** $T_i = \mathbf{X}_i^T\boldsymbol{\theta}$ and the **projected point** $t = \mathbf{x}^T\boldsymbol{\theta}$
- RKDE is equivalent to KDE on $[-1,1]$ with bounded kernels adapted to capture the spikes of $f^*(t) = \omega_{q-1}g(t)(1-t^2)^{\frac{q}{2}-1}$
- Boundary bias is $\mathcal{O}\left(h^2\right)$ without any corrections

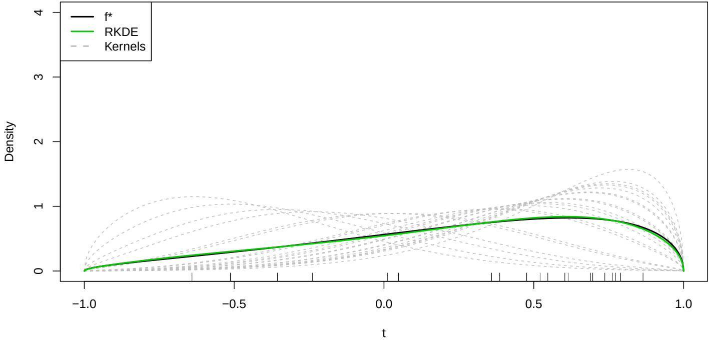


Figure: KDE of f^* with $g(t) = C_q(\kappa)\exp\{\kappa t\}$, $\kappa = 1$ and $q = 3$

Connections with KDE in $[-1, 1]$

- The RKDE kernels **only** depend on the **projected sample** $T_i = \mathbf{X}_i^T \boldsymbol{\theta}$ and the **projected point** $t = \mathbf{x}^T \boldsymbol{\theta}$
- RKDE is equivalent to KDE on $[-1, 1]$ with bounded kernels adapted to capture the spikes of $f^*(t) = \omega_{q-1} g(t)(1-t^2)^{\frac{q}{2}-1}$
- Boundary bias is $\mathcal{O}\left(h^2\right)$ without any corrections

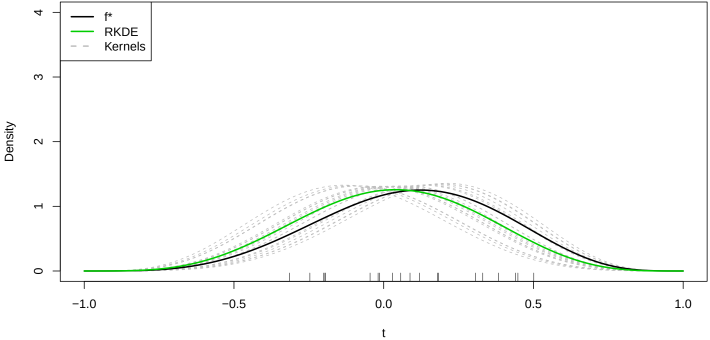


Figure: KDE of f^* with $g(t) = C_q(\kappa) \exp\{\kappa t\}$, $\kappa = 1$ and $q = 10$

Connections with KDE in $[-1, 1]$

- The RKDE kernels **only** depend on the **projected sample** $T_i = \mathbf{X}_i^T \boldsymbol{\theta}$ and the **projected point** $t = \mathbf{x}^T \boldsymbol{\theta}$
- RKDE is equivalent to KDE on $[-1, 1]$ with bounded kernels adapted to capture the spikes of $f^*(t) = \omega_{q-1} g(t)(1 - t^2)^{\frac{q}{2}-1}$
- Boundary bias is $\mathcal{O}\left(h^2\right)$ without any corrections

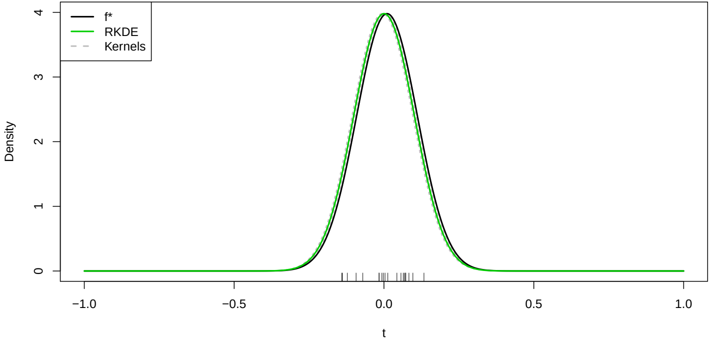


Figure: KDE of f^* with $g(t) = C_q(\kappa) \exp\{\kappa t\}$, $\kappa = 1$ and $q = 100$

Bias (θ known)

- **Assumptions:**

  A1 f is extended by $f(\mathbf{x}/\|\mathbf{x}\|)$ and is twice continuously differentiable
  A2 $L : \mathbb{R}^+ \to \mathbb{R}^+$ is continuous, bounded and has exponential decay
  A3-1 The sequence $h = h_n$ satisfies $h \to 0$ and $nh \to \infty$
  A3-q The sequence $h = h_n$ satisfies $h \to 0$ and $nh^q \to \infty$

- **A3**-q is required for consistency at $\mathbf{x} = \pm\boldsymbol{\theta}$ (note **A3**-$q \Rightarrow$ **A3**-1)

Proposition (Bias, $\boldsymbol{\theta}$ known)

*Under **A1–A3**-1 and uniformly in $\mathbf{x} \in \Omega_q$,*

$$\mathbb{E}\left[\hat{f}_{h,\boldsymbol{\theta}}(\mathbf{x})\right] = R_{\boldsymbol{\theta}} f(\mathbf{x}) + \frac{b_q(L)}{q} \mathrm{tr}\left[R_{\boldsymbol{\theta}} \boldsymbol{\mathcal{H}} f(\mathbf{x})\right] h^2 + o\left(h^2\right)$$

If rotasymmetry holds, then $R_{\boldsymbol{\theta}} f = f$ and the bias is KDE's one

Variance (θ known)

Proposition (Variance, θ known)

Under ***A1–A2***, ***A3*** *if* $(\mathbf{x}^T\boldsymbol{\theta})^2 < 1$ *and* ***A4*** *otherwise,*

$$\mathbb{V}\mathrm{ar}\left[\hat{f}_{h,\boldsymbol{\theta}}(\mathbf{x})\right] = C_{\mathbf{x}^T\boldsymbol{\theta},q,L}(h)\frac{R_{\boldsymbol{\theta}} f(\mathbf{x})}{n}(1+o(1)) - \frac{(R_{\boldsymbol{\theta}} f(\mathbf{x}))^2}{n}$$

uniformly in $\mathbf{x} \in \Omega_q$, *where*

$$C_{\mathbf{x}^T\boldsymbol{\theta},q,L}(h) \propto \begin{cases} \dfrac{\lambda_q(L^2)\lambda_q(L)^{-2}}{h^q}, & (\mathbf{x}^T\boldsymbol{\theta})^2 = 1,\ q \geq 1, \\ \dfrac{\lambda_1(L^2)\lambda_1(L)^{-2}}{2h}, & (\mathbf{x}^T\boldsymbol{\theta})^2 < 1,\ q = 1, \\ \dfrac{\lambda_q(L)^2\lambda_{q-1}(L)^{-2}}{\omega_{q-1}\left(1-(\mathbf{x}^T\boldsymbol{\theta})^2\right)^{\frac{1}{2}} h}, & (\mathbf{x}^T\boldsymbol{\theta})^2 < 1,\ q \geq 2 \end{cases}$$

- The asymptotic constant of the variance increases with $q \to \infty$ since $\omega_{q-1} \to 0$! (but slowly than KDE's)

Spherical area surface

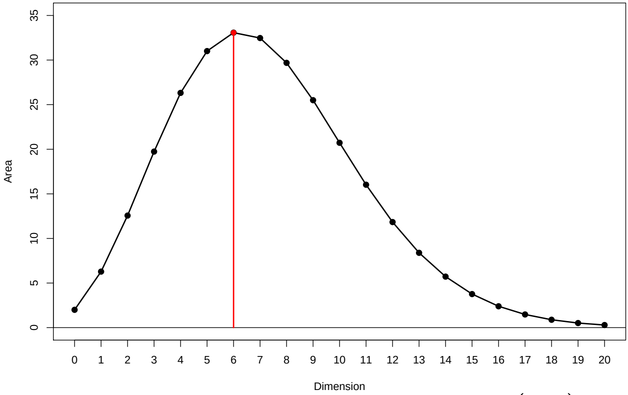


Figure: Spherical surface $\omega_q = 2\pi^{\frac{q+1}{2}} / \Gamma\left(\frac{q+1}{2}\right)$

- The area of Ω_q tends to zero, but not monotonically
- *Weird* maximum at dimension $q = 6$
- $[-1, 1]^q$ touches Ω_q in 2^q points, yet its area tends to infinity!

Key orders & asymptotic normality

Concept	KDE ($\checkmark/\times$ rotasym.)	RKDE ($\checkmark$ rotasym.)	RKDE ($\times$ rotasym.)
Bias	$\mathcal{O}\left(h^2\right)$	$\mathcal{O}\left(h^2\right)$	$\mathcal{O}\left(R_{\boldsymbol\theta} f(\mathbf{x}) - f(\mathbf{x})\right)$
Variance	$\mathcal{O}\left((nh^q)^{-1}\right)$	$\mathcal{O}\left((nh)^{-1}\right)$	$\mathcal{O}\left((nh)^{-1}\right)$
Optimal AMISE	$\mathcal{O}\left(n^{-\frac{4}{4+q}}\right)$	$\mathcal{O}\left(n^{-\frac{4}{5}}\right)$	$\mathcal{O}\left(\int (R_{\boldsymbol\theta} f - f)^2\right)$

Table: Summary of the KDE and RKDE key orders

Corollary (Pointwise asymptotic normality, $\boldsymbol\theta$ known)

Under ***A1–A2***, ***A3*** *if* $(\mathbf{x}^T\boldsymbol\theta)^2 < 1$ *and* ***A4*** *otherwise,*

$$a_n\left(\hat f_{h,\boldsymbol\theta}(\mathbf{x}) - f(\mathbf{x})\right) \xrightarrow{d} \mathcal{N}\left(R_{\boldsymbol\theta} f(\mathbf{x}) - f(\mathbf{x}), C_{\mathbf{x}^T\boldsymbol\theta,q,L}(1)\right),$$

where $a_n = \sqrt{nh}$ *if* $(\mathbf{x}^T\boldsymbol\theta)^2 < 1$ *and* $a_n = \sqrt{nh^q}$ *otherwise*

Simulation study

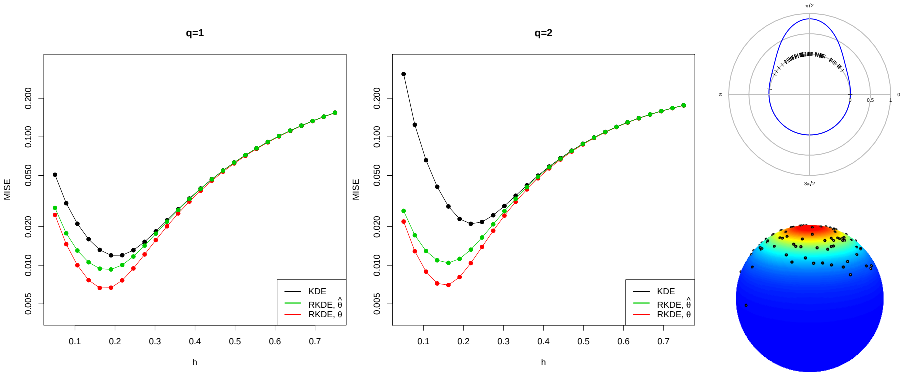


Figure: Performance of the three kernel estimators with $q = 1$ (left) and $q = 2$ (right), with $n = 100$

Ratios optimal MISEs	$q = 1$	$q = 2$	$q = 3$	$q = 4$	$q = 5$	$q = 6$
KDE/RKDE, θ	1.796	2.999	4.065	5.643	5.871	8.019
KDE/RKDE, $\hat{\theta}$	1.289	2.014	2.537	3.035	3.207	3.467

Simulation study

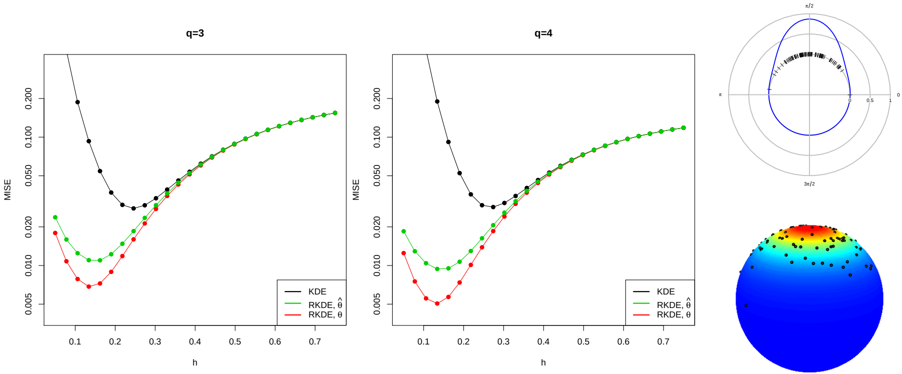


Figure: Performance of the three kernel estimators with $q = 3$ (left) and $q = 4$ (right), with $n = 100$

Ratios optimal MISEs	$q = 1$	$q = 2$	$q = 3$	$q = 4$	$q = 5$	$q = 6$
KDE/RKDE, θ	1.796	2.999	4.065	5.643	5.871	8.019
KDE/RKDE, $\hat{\theta}$	1.289	2.014	2.537	3.035	3.207	3.467

Simulation study

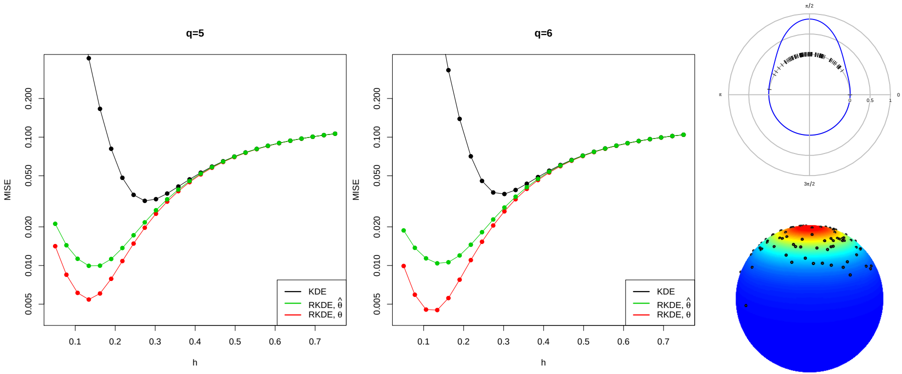


Figure: Performance of the three kernel estimators with $q = 5$ (left) and $q = 6$ (right), with $n = 100$

Ratios optimal MISEs	$q = 1$	$q = 2$	$q = 3$	$q = 4$	$q = 5$	$q = 6$
KDE/RKDE, θ	1.796	2.999	4.065	5.643	5.871	8.019
KDE/RKDE, $\hat{\theta}$	1.289	2.014	2.537	3.035	3.207	3.467

Part II

Estimation and testing in linear-directional regression

García-Portugués, E., Van Keilegom, I., Crujeiras, R. and González-Manteiga, W. (2016). Testing parametric models in linear-directional regression. *Scand. J. Stat.*, 43(4):1178–1191.

Contents of Part II

Regression with directional data

- Let $(\mathbf{X}, Y)$ be a rv with support in $\Omega_q \times \mathbb{R}$ and $\mathbf{X}$ having density f
- Consider the location-scale regression model

$$Y = m(\mathbf{X}) + \sigma(\mathbf{X})\varepsilon \quad \text{with} \quad \begin{cases} m(\mathbf{x}) = \mathbb{E}\left[Y|\mathbf{X}=\mathbf{x}\right], \\ \sigma^2(\mathbf{x}) = \mathbb{V}\mathrm{ar}\left[Y|\mathbf{X}=\mathbf{x}\right], \end{cases}$$

with $\mathbb{E}\left[\varepsilon|\mathbf{X}\right] = 0$, $\mathbb{E}\left[\varepsilon^2|\mathbf{X}\right] = 1$ and $\mathbb{E}\left[|\varepsilon|^3|\mathbf{X}\right]$ and $\mathbb{E}\left[\varepsilon^4|\mathbf{X}\right]$ bounded rv's

- **Goal: estimate m nonparametrically from $\{(\mathbf{X}_i, Y_i)\}_{i=1}^n$**
- Taylor expansions are required, so the first condition is:

  A1 m and f are extended as $m\left(\mathbf{x}/\left|\left|\mathbf{x}\right|\right|\right)$ and $f\left(\mathbf{x}/\left|\left|\mathbf{x}\right|\right|\right)$. m is third and f is twice continuously differentiable and f is bounded away from zero

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$m(\mathbf{X}_i) = m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T(\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(||\mathbf{X}_i - \mathbf{x}||^2\right)$$

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$m(\mathbf{X}_i) = m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T \left(\mathbf{I}_{q+1} - \mathbf{x}\mathbf{x}^T\right)(\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(||\mathbf{X}_i - \mathbf{x}||^2\right)$$

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$m(\mathbf{X}_i) = m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T \mathbf{B_x} \mathbf{B_x}^T (\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(||\mathbf{X}_i - \mathbf{x}||^2 \right)$$

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$
\begin{aligned}
m(\mathbf{X}_i) &= m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T \mathbf{B}_\mathbf{x} \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(||\mathbf{X}_i - \mathbf{x}||^2 \right) \\
&\approx \beta_0 + (\beta_1, \ldots, \beta_q)^T \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}),
\end{aligned}
$$

  with $\mathbf{B}_\mathbf{x} = (\mathbf{b}_1, \ldots, \mathbf{b}_q)_{(q+1)\times q}$ such that $\mathbf{B}_\mathbf{x}\mathbf{B}_\mathbf{x}^T = \mathbf{I}_{q+1} - \mathbf{x}\mathbf{x}^T$,
  $\beta_0 = m(\mathbf{x})$ and $(\beta_1, \ldots, \beta_q) = \mathbf{B}_\mathbf{x}^T \boldsymbol{\nabla} m(\mathbf{x})$

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$\begin{aligned} m(\mathbf{X}_i) &= m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T \mathbf{B}_\mathbf{x} \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(\|\mathbf{X}_i - \mathbf{x}\|^2\right) \\ &\approx \beta_0 + (\beta_1, \ldots, \beta_q)^T \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}), \end{aligned}$$

  with $\mathbf{B}_\mathbf{x} = (\mathbf{b}_1, \ldots, \mathbf{b}_q)_{(q+1)\times q}$ such that $\mathbf{B}_\mathbf{x}\mathbf{B}_\mathbf{x}^T = \mathbf{I}_{q+1} - \mathbf{x}\mathbf{x}^T$, $\beta_0 = m(\mathbf{x})$ and $(\beta_1, \ldots, \beta_q) = \mathbf{B}_\mathbf{x}^T \boldsymbol{\nabla} m(\mathbf{x})$

- Weighted minimum least squares problem:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^{q+1}} \sum_{i=1}^n \left(Y_i - \beta_0 - \delta_{p,1} (\beta_1, \ldots, \beta_q)^T \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}) \right)^2 L_h(\mathbf{x}, \mathbf{X}_i)$$

Estimator

- Let $\mathbf{x}, \mathbf{X}_i \in \Omega_q$. The one term Taylor expansion of m is:

$$\begin{aligned} m(\mathbf{X}_i) &= m(\mathbf{x}) + \boldsymbol{\nabla} m(\mathbf{x})^T \mathbf{B}_\mathbf{x} \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}) + \mathcal{O}\left(||\mathbf{X}_i - \mathbf{x}||^2\right) \\ &\approx \beta_0 + (\beta_1, \ldots, \beta_q)^T \, \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x}), \end{aligned}$$

  with $\mathbf{B}_\mathbf{x} = (\mathbf{b}_1, \ldots, \mathbf{b}_q)_{(q+1)\times q}$ such that $\mathbf{B}_\mathbf{x}\mathbf{B}_\mathbf{x}^T = \mathbf{I}_{q+1} - \mathbf{x}\mathbf{x}^T$, $\beta_0 = m(\mathbf{x})$ and $(\beta_1, \ldots, \beta_q) = \mathbf{B}_\mathbf{x}^T \boldsymbol{\nabla} m(\mathbf{x})$

- Weighted minimum least squares problem:

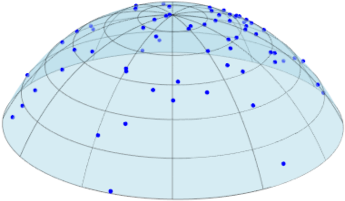
$$\min_{\boldsymbol{\beta} \in \mathbb{R}^{q+1}} \sum_{i=1}^n \left(Y_i - \beta_0 - \delta_{p,1} \, (\beta_1, \ldots, \beta_q)^T \, \mathbf{B}_\mathbf{x}^T (\mathbf{X}_i - \mathbf{x})\right)^2 L_h(\mathbf{x}, \mathbf{X}_i)$$

- The solution is given by

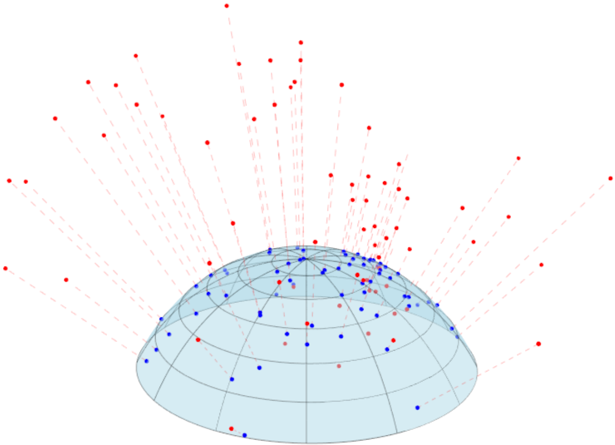
$$\hat{m}_{h,p}(\mathbf{x}) = \mathbf{e}_{1,p}^T \left(\boldsymbol{\mathcal{X}}_{\mathbf{x},p}^T \boldsymbol{\mathcal{W}}_\mathbf{x} \boldsymbol{\mathcal{X}}_{\mathbf{x},p}\right)^{-1} \boldsymbol{\mathcal{X}}_{\mathbf{x},p}^T \boldsymbol{\mathcal{W}}_\mathbf{x} \mathbf{Y} = \sum_{i=1}^n W_p^n \left(\mathbf{x}, \mathbf{X}_i\right) Y_i,$$

$$\boldsymbol{\mathcal{X}}_{\mathbf{x},1} = \begin{pmatrix} 1 & (\mathbf{X}_1 - \mathbf{x})^T \mathbf{B}_\mathbf{x} \\ \vdots & \vdots \\ 1 & (\mathbf{X}_n - \mathbf{x})^T \mathbf{B}_\mathbf{x} \end{pmatrix}, \quad \boldsymbol{\mathcal{W}}_\mathbf{x} = \mathrm{diag}\left(L_h(\mathbf{x}, \mathbf{X}_1), \ldots, L_h(\mathbf{x}, \mathbf{X}_n)\right)$$

How does it work?



How does it work?



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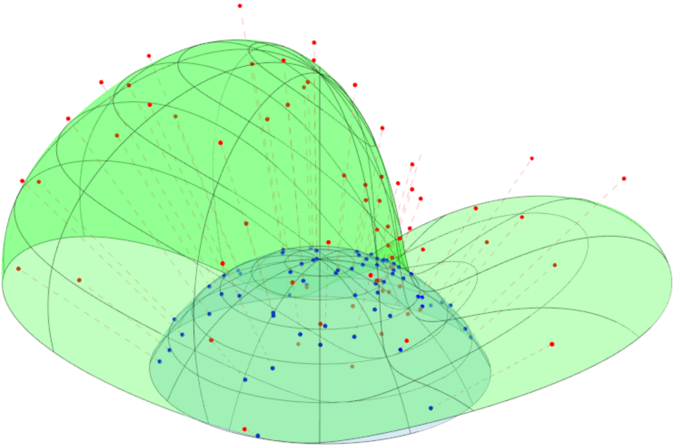

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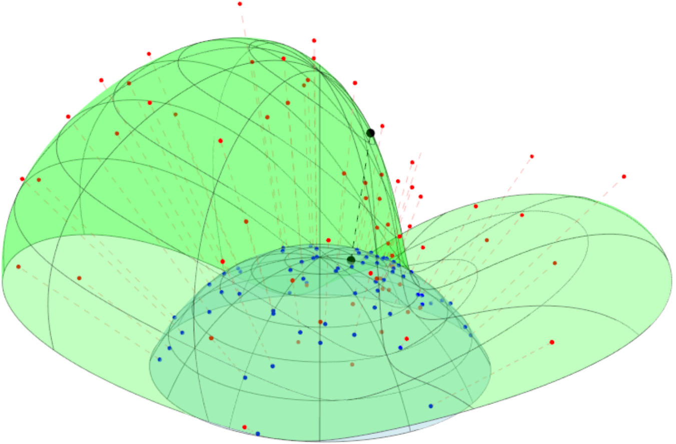
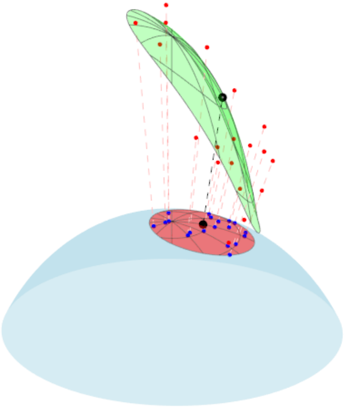
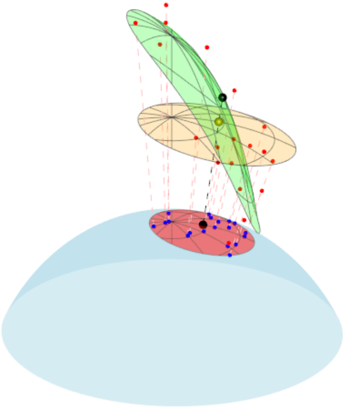


How does it work?



How does it work?



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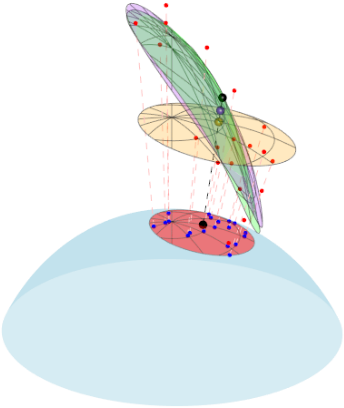

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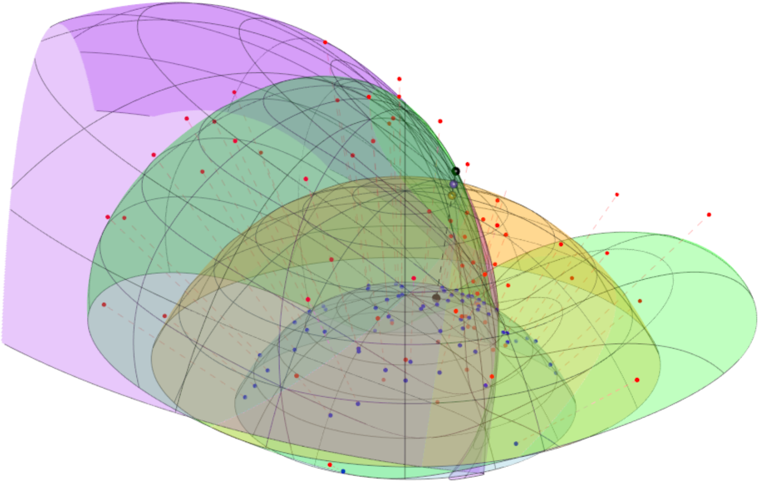


Output

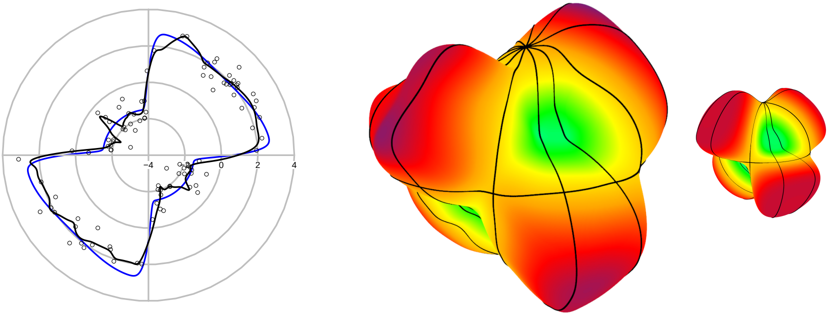


Figure: Local linear estimator with $n = 100$ for the circle and the sphere

Testing a parametric model

- **Goal: check nonparametrically** $H_0 : m \in \mathcal{M}_\Theta = \{m_{\boldsymbol{\theta}} : \boldsymbol{\theta} \in \Theta \subset \mathbb{R}^s\}$
- The statistic is the weighted L^2-distance between $\hat{m}_{h,p}$ and the smoothed $m_{\hat{\boldsymbol{\theta}}}$:

$$T_n = \int_{\Omega_q} \left(\hat{m}_{h,p}(\mathbf{x}) - \mathcal{L}_{h,p} m_{\hat{\boldsymbol{\theta}}}(\mathbf{x})\right)^2 \hat{f}_h(\mathbf{x}) w(\mathbf{x})\, \omega_q(d\mathbf{x}),$$

with $\mathcal{L}_{h,p} m_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \sum_{i=1}^n W_n^p(\mathbf{x}, \mathbf{X}_i)\, m_{\hat{\boldsymbol{\theta}}}(\mathbf{X}_i)$ the smoothing operator and $w : \Omega_q \to \mathbb{R}^+$ a weight function (useful for removing possible boundary effects)

Alcalá, J. T., Cristóbal, J. A., and González-Manteiga, W. (1999). Goodness-of-fit test for linear models based on local polynomials. *Statist. Probab. Lett.*, 42(1):39–46

Härdle, W. and Mammen, E. (1993). Comparing nonparametric versus parametric regression fits. *Ann. Statist.*, 21(4):1926–1947

Asymptotic distribution

Theorem (Goodness-of-fit for linear-directional models)

Under A1–A6 and $H_0 : m \in \mathcal{M}_\Theta$ (i.e., $m = m_{\boldsymbol{\theta}_0}$),

$$nh^{\frac{q}{2}}\left(T_n - \frac{\lambda_q(L^2)\lambda_q(L)^{-2}}{nh^q}\int_{\Omega_q}\sigma^2_{\boldsymbol{\theta}_0}(\mathbf{x})w(\mathbf{x})\,\omega_q(d\mathbf{x})\right) \xrightarrow{d} \mathcal{N}\left(0, 2\nu^2_{\boldsymbol{\theta}_0}\right),$$

where $\sigma^2_{\boldsymbol{\theta}_0}(\mathbf{x}) = \mathbb{E}\left[(Y - m_{\boldsymbol{\theta}_0}(\mathbf{X}))^2|\mathbf{X} = \mathbf{x}\right]$ *and*

$$\nu^2_{\boldsymbol{\theta}_0} = \int_{\Omega_q}\sigma^4_{\boldsymbol{\theta}_0}(\mathbf{x})w(\mathbf{x})^2\,\omega_q(d\mathbf{x})$$
$$\times\,\gamma_q\lambda_q(L)^{-4}\int_0^\infty r^{\frac{q}{2}-1}\left\{\int_0^\infty \rho^{\frac{q}{2}-1}L(\rho)\varphi_q(r,\rho)\,d\rho\right\}^2 dr$$

- Conditions:
  - A5 $\hat{\boldsymbol{\theta}}$ is such that $\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_1 = \mathcal{O}_{\mathbb{P}}\left(n^{-\frac{1}{2}}\right)$, with $\boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$ if H_0 holds
  - A6 $m_{\boldsymbol{\theta}}$ is continuously differentiable as a function of $\boldsymbol{\theta}$, being this derivative also continuous for $\mathbf{x} \in \Omega_q$
- If L is the von Mises kernel, $\nu^2_{\boldsymbol{\theta}_0} = \int_{\Omega_q}\sigma^4_{\boldsymbol{\theta}_0}(\mathbf{x})w(\mathbf{x})^2\,\omega_q(d\mathbf{x}) \times (8\pi)^{-\frac{q}{2}}$

Empirical evidence

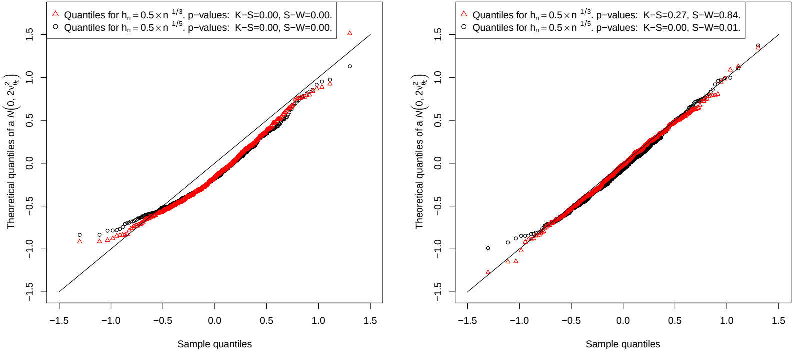


Figure: QQ-plot comparing the quantiles of the asymptotic distribution with the sample quantiles for $\left\{nh^{\frac{1}{2}}\left(T_n^j - \frac{\sqrt{\pi}}{4}nh\right)\right\}_{j=1}^{500}$ with $n = 10^2$ (left) and $n = 5 \times 10^5$ (right)

Calibration in practice

Algorithm (Calibration in practice)

To test $H_0 : m \in \mathcal{M}_{\boldsymbol{\Theta}}$ *from the sample* $\{(\mathbf{X}_i, Y_i)\}_{i=1}^n$:

1. *Obtain* $\hat{\boldsymbol{\theta}}$, *set* $\hat{\varepsilon}_i = Y_i - m_{\hat{\boldsymbol{\theta}}}(\mathbf{X}_i)$, $i = 1, \ldots, n$ *and compute* T_n
2. *Bootstrap resampling. For* $b = 1, \ldots, B$:
   - *Set* $Y_i^* = m_{\hat{\boldsymbol{\theta}}}(\mathbf{X}_i) + \hat{\varepsilon}_i V_i^*$, *where* V_i^* *are iid rv's such that* $\mathbb{E}^*[V_i^*] = 0$ *and* $\mathbb{E}^*[(V_i^*)^2] = 1$, $i = 1, \ldots, n$
   - *Compute* $\hat{\boldsymbol{\theta}}^*$ *from* $\{(\mathbf{X}_i, Y_i^*)\}_{i=1}^n$ *and* T_n^{*b}
3. *Estimate the p-value by* $\frac{1}{B}\sum_{b=1}^B \mathbf{1}_{\{T_n \leq T_n^{*b}\}}$

Theorem (Bootstrap consistency)

Under A1–A4, A5–A6 and A9, conditionally on the sample,

$$nh^{\frac{q}{2}}\left(T_n^* - \frac{\lambda_q(L^2)\lambda_q(L)^{-2}}{nh^q}\int_{\Omega_q}\sigma^2_{\boldsymbol{\theta}_1}(\mathbf{x})w(\mathbf{x})\,\omega_q(d\mathbf{x})\right) \xrightarrow{d} \mathcal{N}\left(0, 2\nu^2_{\boldsymbol{\theta}_1}\right)$$

in probability. If H_0 *holds, then* $\boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$ *and* $T_n^* \stackrel{d}{=} T_n$ *asymptotically*

Protein structure modelling

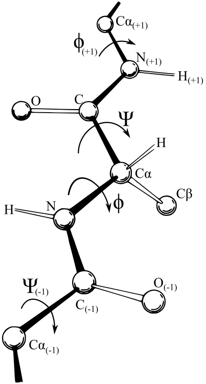


Figure: Backbone and C_α representation

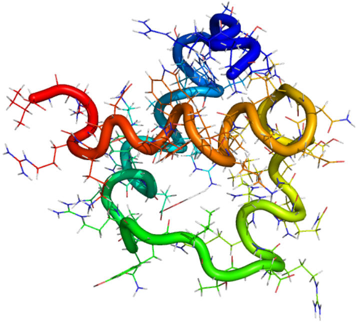
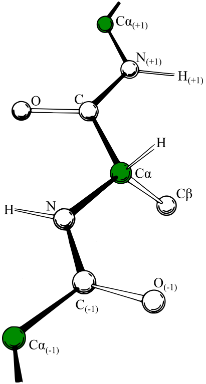


Figure: Cartoon view of a protein

Boomsma, W., Mardia, K. V., Taylor, C. C., Ferkinghoff-Borg, J., Krogh, A. and Hamelryck, T. A generative, probabilistic model of local protein structure. *PNAS*, 105(26):8932-8937

Protein structure modelling



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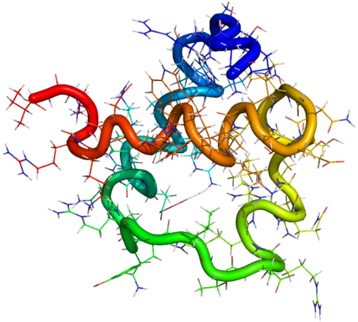

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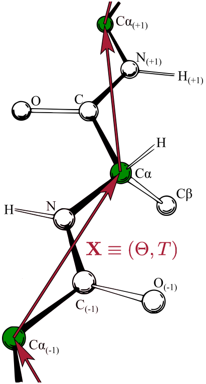

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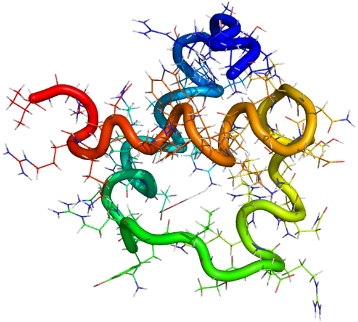

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Testing in the C_α representation

- **Goal: test the constant pseudo--bond length assumption**:

$$H_0 : m(\mathbf{x}) = c,\ c \in \mathbb{R}$$

- Data: $n = 18030$ pseudo-angles ($\mathbf{X} \equiv (\Theta, T)$) and pseudo-lengths ($Y$) extracted from 100 high precision protein structures
- Grid of 10 bandwidths, $B = 1000$ bootstrap replicates and weight $w(\theta, \tau) = \mathbf{1}_{\left\{80 \leq \frac{180}{\pi}\theta \leq 150\right\}}$
- **Emphatically rejection of H_0**
- Exploration of $m(\theta, \tau)$ by local linear estimator $\hat{m}_{h_{\mathrm{CV}},1}(\theta, \tau)$

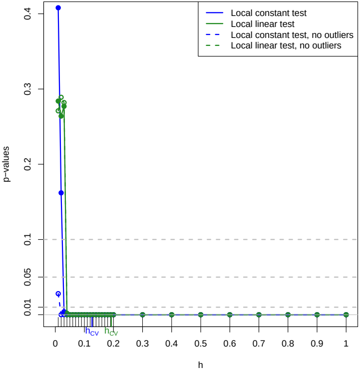

Figure: Significance trace of the goodness-of-fit tests

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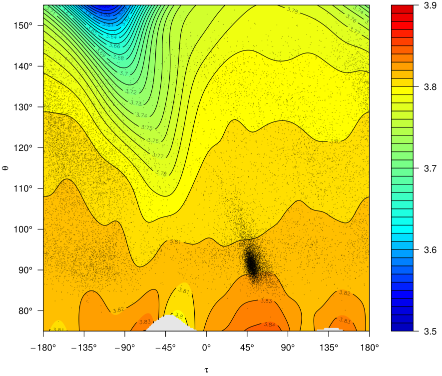
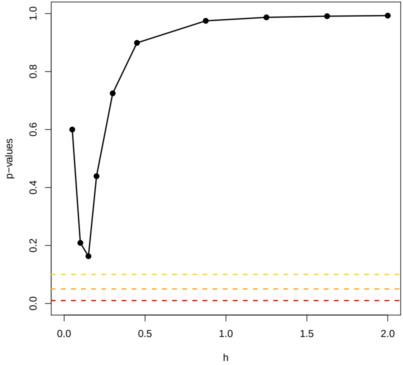


Figure: Contourplot of $\hat{m}_{h_{\mathrm{CV}},1}(\theta,\tau)$ and pseudo-angles sample

Text mining application

- Data: 8121 news published in `slashdot.org` in 2013
- Complex data acquisition and treatment
- News: $\mathbf{X} \in \Omega_{1508-1}$. Log-number of comments: $Y \in \mathbb{R}$
- $H_0 : m(\mathbf{x}) = c + \boldsymbol{\eta}^T \mathbf{x}$ such that only $d = 77$ coefficients are non-zero. d chosen using overpenalized LASSO
- Grid of 10 bandwidths with $B = 1000$ bootstrap replicates
- No evidence to reject the model



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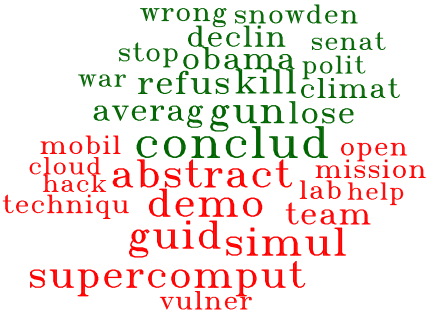

Figure: Most influential coefficients (significances of the d coefficients are < 0.002)

Thanks for your attention!