

Modeling and Estimation of Multivariate Densities

Modellierung und Schätzung von multivariaten Dichten

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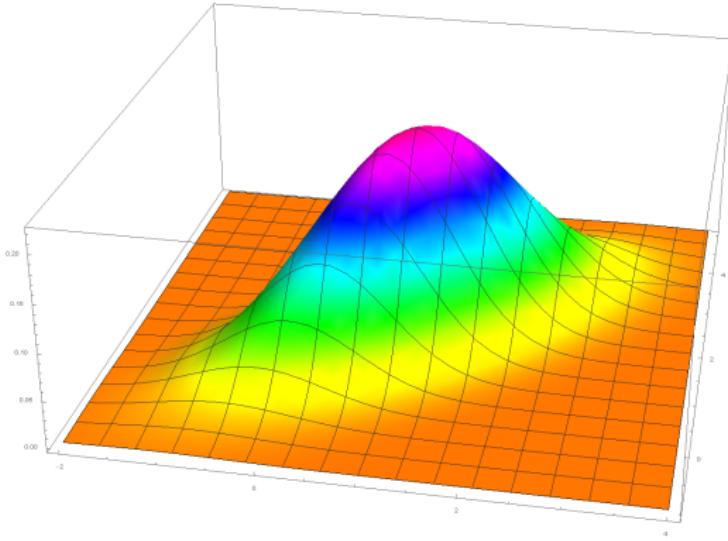
Outline

- ① Introduction
- ② Elliptical Distributions
- ③ Estimation of Elliptical Densities
- ④ Star-shaped Distributions
- ⑤ Estimation of Shar-shaped Densities
- ⑥ Summary

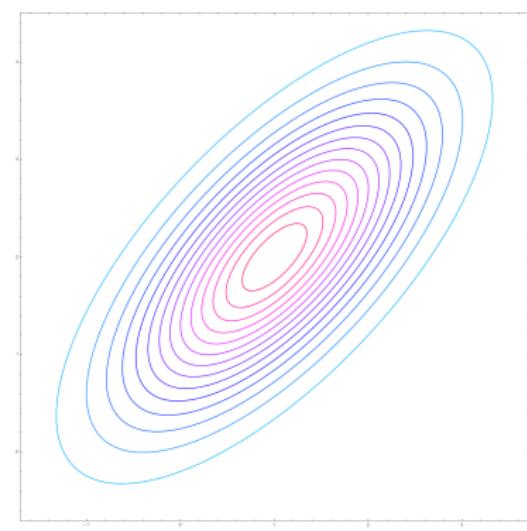
Multivariate Normal Distribution

(X, Y) normally distributed with $\mathbb{E}(X) = 1, \mathbb{E}(Y) = 2, \text{Var}(X) = 1,$
 $\text{Var}(Y) = 1, \text{corr}(X, Y) = 0.7$

bivariate density



contour plot



Modeling Multivariate Distributions

- elliptical distributions
- skewed normal distributions, mixture of normal distributions
- copulas
- star-shaped distributions

Fields of applications:

- methods of applied statistics: cluster analysis,...
- finance
- survival analysis - reliability
- time series analysis - multivariate time series
- Statistical Process Control

Spherical and Elliptical Densities

Random vector $X \in \mathbb{R}^p$ has a **continuous spherical distribution**

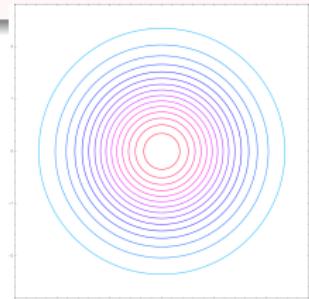
$SC_p(g_p)$, if the density exist and can be written as

$$g_p(t^T t) = g_p(t_1^2 + \dots + t_p^2) \text{ for } t \in \mathbb{R}^p$$

with a function $g_p : [0, \infty) \rightarrow [0, \infty)$, $X \sim SC_p(g_p)$.

$g_p \dots$ **density generator** for the dimension p

if $g_p \geq 0$, and $\int_0^\infty r^{p/2-1} g_p(r) dr = \frac{\Gamma(p/2)}{\pi^{p/2}}$ for $p \geq 1$.



Random vector $Y \in \mathbb{R}^p$ has a **continuous elliptical distribution** with

parameter $\mu \in \mathbb{R}^p$ and $\Sigma \in \mathbb{R}^{p,p}$, $\text{rank}(\Sigma) = p$, $\Sigma = AA^T$, in symbols

$Y \sim EC_p(\mu; \Sigma; g_p)$ if

$$Y \stackrel{d}{=} \mu + AZ, \quad Z \sim SC_p(g_p)$$

Elliptical Densities

- **density of the random vector** $X = (X^{(1)}, \dots, X^{(p)})^T$:

$$f_X(x) = \det(\Sigma)^{-1/2} g\left((x - \mu)^T \Sigma^{-1} (x - \mu)\right), \quad x \in \mathbb{R}^p,$$

generator fcn. $g : [0, +\infty) \rightarrow [0, +\infty)$,

location $\mu \in \mathbb{R}^d$, scaling matrix $\Sigma = AA^T$

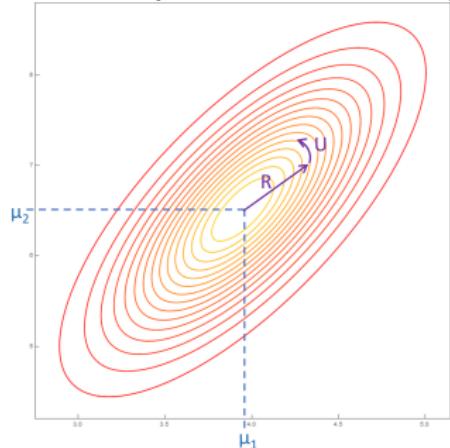
- Representation:

$$X \stackrel{d}{=} \mu + R AU$$

random vector $U \in \mathcal{S}_{p-1}$ uniform distribution

random variable $R \in [0, +\infty)$,
 R and U independent

contour plot of the density



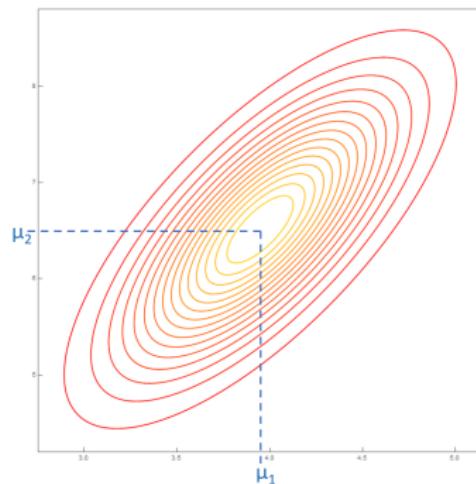
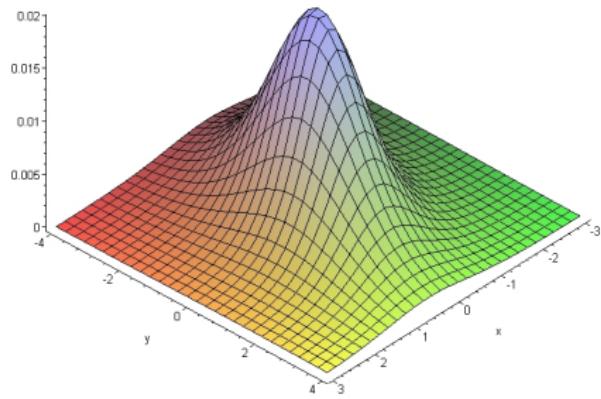
Elliptical Densities

- **density of the random vector** $X = (X^{(1)}, \dots, X^{(p)})^T \sim EC_p(\mu; \Sigma; g_p)$:

$$f_X(x) = \det(\Sigma)^{-1/2} g_p \left((x - \mu)^T \Sigma^{-1} (x - \mu) \right), \quad x \in \mathbb{R}^d,$$

location $\mu \in \mathbb{R}^d$, scaling matrix Σ

contour plot of the density



Fang/Zhang 1990, Fang/Kotz/Ng 1990, Bilodeau/Brenner 1999

Consistent Families of Generators

$$f_X(x) = \det(\Sigma)^{-1/2} g_p \left((x - \mu)^T \Sigma^{-1} (x - \mu) \right), \quad x \in \mathbb{R}^d,$$

$\{g_p\}_{p=1,2,\dots}$ family of density generators

This family is **consistent** : \iff

$$g_p(r) = 2 \int_0^\infty g_{p+1}(r + t^2) dt = \int_r^\infty \frac{1}{\sqrt{y-r}} g_{p+1}(y) dy$$

for $r \geq 0, 1 \leq p < p_0$. Then: $z \mapsto g_q(z_1^2 + \dots + z_q^2)$

$(z = (z_1, \dots, z_q)^T \in \mathbb{R}^q)$ is the q -dimensional marginal density of X for $q < p$.

Consistent Families of Generators

$\{g_p\}_{p=1,2,\dots}$ family of density generators

Theorem.

Assume that $g_1 : [0, \infty) \rightarrow [0, \infty)$ completely monotonic on $[0, \infty)$,

$$\lim_{r \rightarrow \infty} g_1(r) = 0, \quad g_{p+2}(r) = -\frac{1}{\pi} g'_p(r),$$

for $p \geq 1, r \geq 0$ and

$$g_2(r) = 2 \int_0^\infty g_3(r + y^2) dy \quad (r \geq 0).$$

$$\int_0^\infty r^{-1/2} g_1(r) dr = 1$$

$\implies \{g_p\}_{p \geq 1}$ is a consistent family of density generators.

Algorithm for the construction of consistent families of density generators

Consistent Families of Generators

$\{g_p\}_{p=1,2,\dots}$ consistent family of density generators

\implies

$$(g_p(-u))^{(1/2)} = \sqrt{\pi} g_{p+1}(-u) \quad (u \leq 0, p \geq 1),$$

Let $a \in [-\infty, \infty)$, $\nu > 0$, $\nu \notin \mathbb{N}$ and $n = [\nu] + 1$, where $[\alpha]$ is the integer part of α . the fractional derivative of order ν in the sense of Caputo of function $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ is defined by

$${}_c D_a^\nu \varphi(x) = \frac{1}{\Gamma(n-\nu)} \int_a^x \frac{\varphi^{(n)}(t)}{(x-t)^{\nu-n+1}} dt \quad \text{for } x > a.$$

Examples of Generator Families

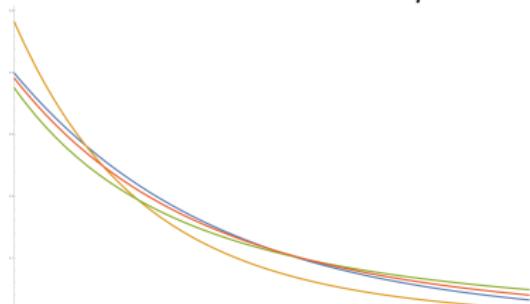
- **normal distribution**

$$g_p(r) = \frac{1}{(2\pi)^{p/2}} \exp\left(-\frac{r}{2}\right)$$

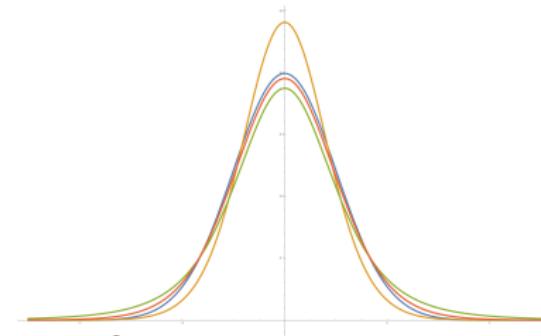
- **normal mixture generator**

$$g_p(r) = \frac{1}{(2\pi)^{p/2}} \left(qa^{p/2} \exp\left(-\frac{ar}{2}\right) + (1 - q) \exp\left(-\frac{r}{2}\right) \right)$$

generator fcn. g_p



one-dimensional density



- ***t*-distribution (Pearson VII), $m > 0$**

$$g_p(r) = \frac{\Gamma(p/2 + m)}{(2m)^{p/2} \pi^{p/2} \Gamma(m)} \left(1 + \frac{r}{2m}\right)^{-p/2-m}$$

Examples of Generator Families

- **logarithmic generator** $a > 1, b > 0, b \leq a - 1$

$$g_1(r) = \frac{\sqrt{b} \ln(r + a)}{2\pi \ln(\sqrt{a} + \sqrt{b}) (r + b)} \rightarrow g_3, g_2$$

- **fractional-exponential generator**

$$\begin{aligned} g_1(r) &= \frac{e^{-a-r}\sqrt{a}}{(r+a)\operatorname{erfc}(\sqrt{a})\pi} \rightarrow \\ g_p(r) &= \frac{\sqrt{a}\bar{\Gamma}(\frac{p+1}{2}, a+r)}{\operatorname{erfc}(\sqrt{a})\pi^{(p+1)/2}(a+r)^{(p+1)/2}}, \end{aligned}$$

- **mixtures**

- **Kotz-type family**

$$g_p(r) = \frac{t}{\Gamma(\frac{s+d}{t})} r^s e^{-r^t} \text{ for } r > 0.$$

problem: no explicit formulas for $g_q, q \neq p$



Moments and Identifiability

$$f_X(x) = \det(\Sigma)^{-1/2} g\left((x - \mu)^T \Sigma^{-1} (x - \mu)\right), \quad x \in \mathbb{R}^p,$$

$$\mathbb{E}(X) = \mu, \quad \text{cov}(X) = \frac{2\pi^{p/2}}{p\Gamma(p/2)} \int_0^\infty r^{p+1} g_p(r^2) dr \quad \Sigma$$

Theorem.

$X \sim EC_p(\mu; \Sigma; g_p)$, $X \sim EC_p(\bar{\mu}; \bar{\Sigma}; \bar{g}_p) \implies$

$$\bar{\mu} = \mu, \quad \bar{\Sigma} = c\Sigma, \quad \bar{g}_p(z) = c^{p/2} g_p(cz) \quad \forall z \geq 0$$

Choose c such that

$$\frac{2\pi^{p/2}}{p\Gamma(p/2)} \int_0^\infty r^{p+1} g_p(r^2) dr = 1 \iff \text{cov}(X) = \Sigma$$

Estimation problems

$$\mathbb{E}(X) = \mu, \text{cov}(X) = \Sigma$$

X_1, X_2, \dots, X_n sample, $X \sim EC_p(\mu; \Sigma; g_p)$

1) Nonparametric estimation of μ and Σ

$$\hat{\mu} = \bar{X}, \quad \hat{\Sigma} = \text{empirical covariance matrix}$$

alternatively: M-estimator  Maronna 1976

2) Parametric estimation of the density

Maximum-Likelihood estimator

3) Semiparametric estimation of the density: Kernel density estimator for

g_p

Maximum likelihood estimation

model for the density $g_p(\cdot | \tau)$ with parameter $\tau \in \Theta_1 \subset \mathbb{R}^{q_1}$

▷ Sample X_1, \dots, X_n , $X \sim EC_p(\mu; \Sigma; g_p)$

parameter $\theta = (\mu, \underbrace{\sigma_{11}, \sigma_{12}, \dots, \sigma_{pp}}_{\text{without repetition of identical entries}}, \tau)^T \in \Theta$

- Likelihood function

$$L(\theta) = \prod_{i=1}^n g_p \left((X_i - \mu)^T \Sigma^{-1} (X_i - \mu) \mid \tau \right)$$

Maximum-likelihood estimator

$$\hat{\theta} = \arg \max_{\theta \in \Theta} L(\theta)$$

The estimator $\hat{\theta}$ is asymptotically normally distributed.

Maximum likelihood estimation - Example

dataset 5 of Andrews and Herzberg (1985)

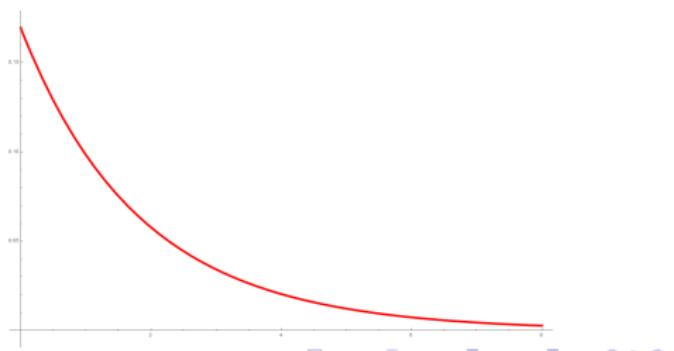
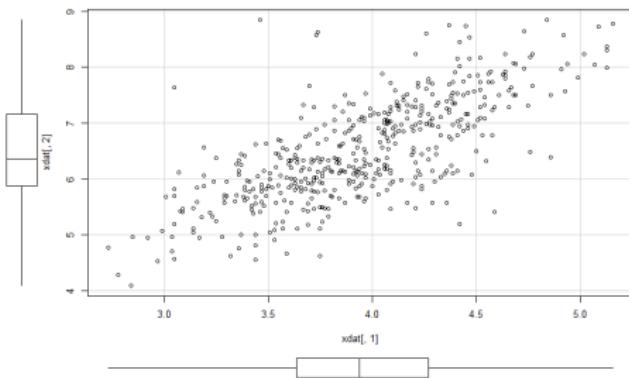
variables: yield of grain and straw

model function $g_p(r) = (qa^{p/2} \exp(-ra/2) + (1 - q) \exp(-r/2))/(2\pi)^{p/2}$

ml-method $\rightarrow \hat{q} = 0.09476697, \hat{a} = 1.68244509$

scatter plot of the data

plot of g_p ,

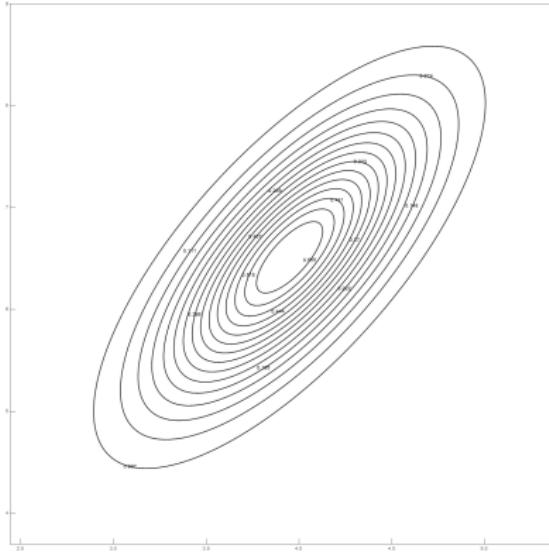


Maximum likelihood estimation - Example

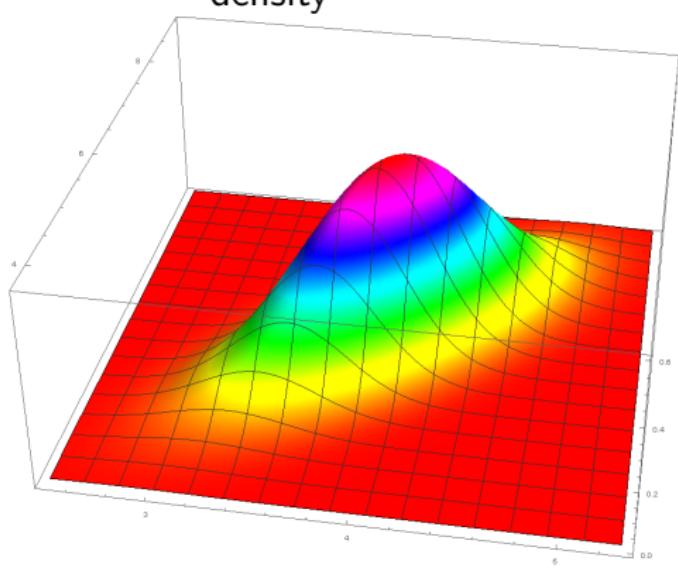
dataset 5 of Andrews and Herzberg (1985) - yield of grain and straw

ml-method $\rightarrow \hat{q} = 0.09476697, \hat{a} = 1.68244509$

contour plot of the density



density

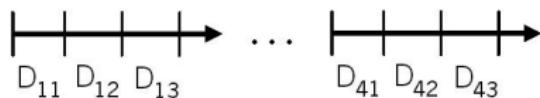


Curse of dimensionality

Data example: Liver-disorders (UCI Machine Learning Repository)

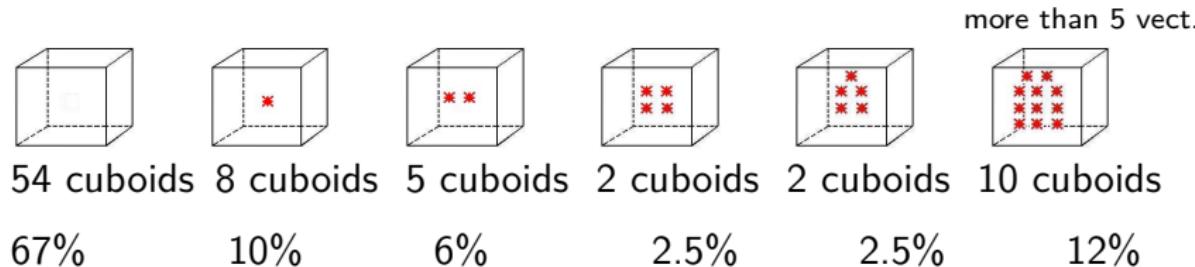
Variable $X^{(1)}, X^{(2)}, X^{(3)}, X^{(4)}$,

The range is divided into 3 subintervals:



81 cuboids are formed $D_{1i_1} \times D_{2i_2} \times D_{3i_3} \times D_{4i_4}$.

$n = 200$ data vectors are distributed as follows:



⇒ Dimension reduction techniques

Preliminaries - Volcano effect

We consider: $Y = (X - \mu)^T \Sigma^{-1} (X - \mu)$ with density

$$f_Y(y) = s_p \cdot y^{p/2-1} g(y) \quad (y \in \mathbb{R}^+), \quad s_p = \frac{\pi^{p/2}}{\Gamma(p/2)}$$

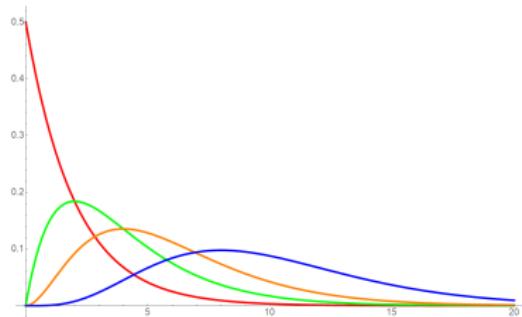
density of Y in the multinormal case

- **Idea 1:** \hat{f}_Y estimator for $f_Y \implies$

$$\hat{g}(y) = s_p^{-1} y^{-p/2+1} \hat{f}_Y(y)$$

estimator for g .

Problem: $\hat{g}(y) \rightarrow \infty$ for $y \rightarrow 0$.



the mass moves away from zero as $p \rightarrow \infty$

Construction of the estimator

$$f(x) = \det(\Sigma)^{-1/2} g\left((x - \mu)^T \Sigma^{-1} (x - \mu)\right) \quad (x \in \mathbb{R}^p)$$

transformation $\tilde{Y} = \psi(Y)$, $Y = (X - \mu)^T \Sigma^{-1} (X - \mu)$

Assume that $\psi : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ has a derivative ψ' with $\psi'(y) > 0$ for $y \geq 0$, and $\psi(0) = 0$. Ψ inverse function of ψ .

\tilde{Y} has density h :

$$h(t) = \Psi'(t) f_Y(\Psi(t)) = s_p \cdot \Psi'(t) \Psi(t)^{p/2-1} g(\Psi(t)),$$

\implies

$$g(y) = s_p^{-1} y^{-p/2+1} \psi'(y) h(\psi(y))$$

Transformation function ψ

Assumption $\mathcal{T}(p)$. $\Psi = \psi^{-1}$, $\Psi^{(p+1)}$ exists and is continuous on $(0, \infty)$, $\psi' > 0$, ψ' is supposed to be bounded on $(0, +\infty)$, and ψ'' is assumed to be bounded on $(0, +\infty)$. Function $x \mapsto x^{p/2-1}\psi'(x)^{-1}$ has a bounded derivative on $[0, M_1]$ with $M_1 > 0$,

$$\lim_{x \downarrow 0} x^{-p/2+1}\psi'(x) = C_1 > 0.$$

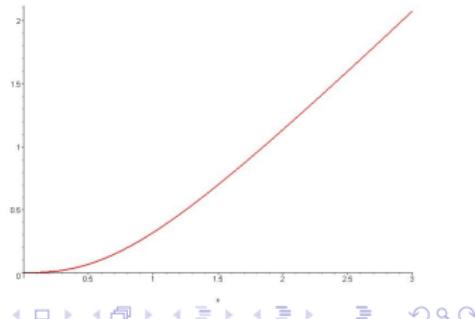
There exist constants $\alpha \in (0, 1]$, $C_2, M_2 > 0$, such that

$$|\Psi(t)| \leq C_2|t|^\alpha \quad \text{for } t \in [0, M_2].$$

Example:

$$\psi(x) = -a + (a^{p/2} + x^{p/2})^{2/p}$$

image for $p = 5$, $a = 1$:



Construction of the estimator

$$f(x) = \det(\Sigma)^{-1/2} g\left((x - \mu)^T \Sigma^{-1} (x - \mu)\right) \quad (x \in \mathbb{R}^p)$$

Transformation $\tilde{Y} = \psi(Y)$ mit Dichte h

$$g(y) = s_p^{-1} y^{-p/2+1} \psi'(y) h(\psi(y))$$

- **kernel estimators for g, f, h :**

$$\hat{g}_n(z) = s_p^{-1} z^{-p/2+1} \psi'(z) \hat{h}_n(\psi(z)) \quad (z \geq 0),$$

$$\hat{f}_n(x) = \det(\hat{\Sigma}_n)^{-1/2} \hat{g}_n\left((x - \hat{\mu}_n)^T \hat{\Sigma}_n^{-1} (x - \hat{\mu}_n)\right) \quad (x \geq 0).$$

Construction of the estimator

X_1, X_2, \dots, X_n sample, $X \sim EC_p(\mu; \Sigma; g_p)$

- transformed sample: Y_{n1}, \dots, Y_{nn} ,

$$Y_{ni} = \psi \left((X_i - \hat{\mu}_n)^T \hat{\Sigma}_n^{-1} (X_i - \hat{\mu}_n) \right), \quad i = 1, \dots, n.$$

- Assumption $\limsup_{n \rightarrow \infty} \sqrt{\frac{n}{\ln \ln(n)}} \|\hat{\theta}_n - \theta\| = C_0 \quad f.s.$

with a constant $C_0 > 0$.

- Kernel estimator for h :** mirror method

$$\hat{h}_n(y) = \frac{1}{nb} \sum_{i=1}^n \left(K((y - Y_{in})b^{-1}) + \underbrace{K((y + Y_{in})b^{-1})}_{\text{additional term}} \right) \quad (y \geq 0)$$

additional term

Construction of the estimator

- **Assumptions on the kernel function:** **Condition $\mathcal{K}(p)$**

$K : \mathbb{R} \rightarrow \mathbb{R}$ bounded, $K(-t) = K(t)$,

$$\int_{-1}^1 K(t) dt = 1, \quad K(t) = 0 \text{ for } |t| > 1,$$

$$\int_{-1}^1 u^j K(u) du = 1 \quad (j \leq p-1 \text{ even})$$

- **Assumptions on the bandwidth $b = b(n)$:**

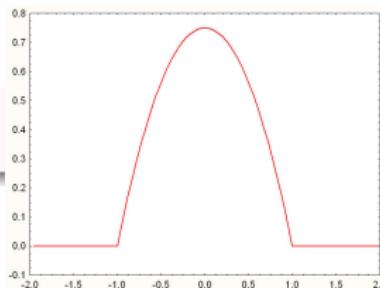
$$\lim_{n \rightarrow \infty} b(n) \ln \ln n = 0 \quad \text{and}$$

$$b(n) \geq C_5 \cdot n^{-1/5}.$$

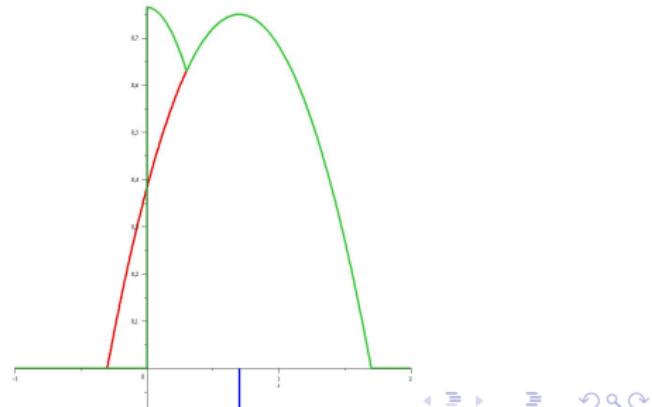
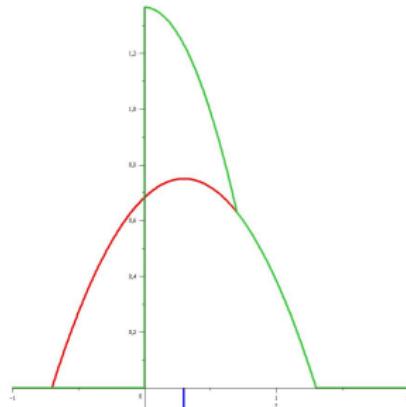
Construction of the estimator

- Epanechnikov kernel

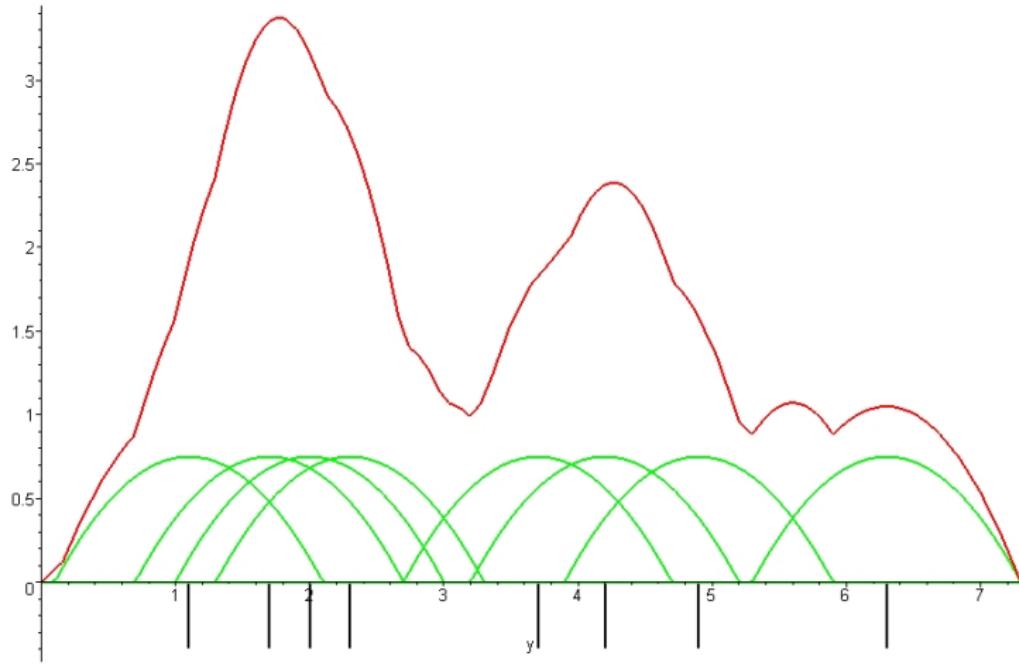
$$K(x) = 0.75(1 - x^2) \text{ for } -1 \leq x \leq 1$$



Kernel function at boundary for $b = 1$ and data items at 0.3 and 0.7



Kernel estimator



Covergence rate of the estimator

Theorem.

Assume that $g^{(q)}$ exists and is bounded on \mathbb{R}^+ for even $q \geq 2$,

Assumptions $\mathcal{K}(q)$, $\mathcal{T}(q)$ are satisfied. Then for a compact set D with $\mu \notin D$:

$$\sup_{x \in D} |\hat{f}_n(x) - f(x)| = O\left(\sqrt{\ln n}(nb(n))^{-1/2} + b^q(n)\right) \quad \text{a.s.}$$

For a compact set D with $\mu \in D$ we have

$$\sup_{x \in D} |\hat{f}_n(x) - f(x)| = O\left(\sqrt{\ln n}(nb(n))^{-1/2} + b^\gamma(n)\right) \quad \text{a.s.}$$

with $\gamma > 0$.

- optimized convergence rate: $O\left(\left(\frac{n}{\ln n}\right)^{-q/(2q+1)}\right)$

improves rates in  Cui and He (1995)

Asymptotic distribution of the estimator

Theorem.

$b(n) \sim C_1 n^{-1/(2p+1)}$ with a constant $C_1 > 0$,

$x \neq \mu$ such that $g^{(p)}$ is continuous in $u := (x - \mu)^T \Sigma^{-1} (x - \mu) \implies$

$$\sqrt{nb(n)} \left(\hat{f}_n(x) - f(x) \right) \xrightarrow{\mathcal{D}} \mathcal{N}(\bar{\mu}, \bar{\sigma}^2), \text{ where}$$

$$\bar{\sigma}^2 = \det(\Sigma)^{-1} s_d^{-1} u^{-d/2+1} \psi'(u) g(u) \int_{-1}^1 K^2(t) dt$$

$$\bar{\mu} = \det(\Sigma)^{-1/2} s_d^{-1} u^{-d/2+1} \psi'(u) C_1^{(2p+1)/2} \frac{1}{p!} h^{(p)}(\psi(u)) \int_{-1}^1 t^p K(t) dt.$$

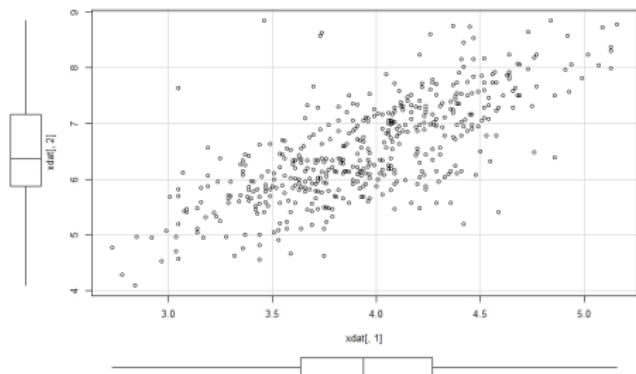
 Stute/Werner (1991): known μ and $\psi(x) \equiv x$

Semiparametric estimation - Example

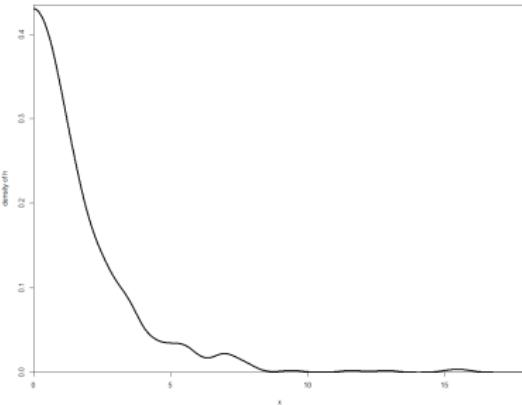
dataset 5 of Andrews and Herzberg (1985)

variables: yield of grain and straw

scatter plot of the data



plot of g_p ,



Semiparametric estimation - High-dimensional case

 Liebscher/Okhrin (2023)

dimension p may tend to ∞ , $p \leq n^{1/2}$

density h of R^2/p

$$g(r) = s_p^{-1} p^{-1} r^{-p/2+1} h(r/p)$$

h bounded

- **kernel estimators for g, f, h :** \hat{h}_n as before

$$\hat{g}_n(r) = s_p^{-1} r^{-p/2+1} \hat{h}_n(r) \quad (r \geq 0),$$

$$\hat{f}_n(x) = \det(\hat{\Sigma}_n)^{-1/2} \hat{g}_n \left((x - \hat{\mu}_n)^T \hat{\Sigma}_n^{-1} (x - \hat{\mu}_n) \right) \quad (x \geq 0).$$

Semiparametric estimation - High-dimensional case

$$p \rightarrow \infty$$

Assumption: $C_1 \leq \lambda_{min} \leq \|\Sigma\|_2 = \lambda_{max} \leq C_2$

$$\hat{f}_n(x) = \det(\hat{\Sigma}_n)^{-1/2} \hat{g}_n \left((x - \hat{\mu}_n)^T \hat{\Sigma}_n^{-1} (x - \hat{\mu}_n) \right) \quad (x \geq 0).$$

Theorem.

Assume that $g^{(q)}$ exists and is bounded on \mathbb{R}^+ for even $q \geq 2$, Assumption $\mathcal{K}(q)$ is satisfied, $b(n) \geq C_3 n^{-1/5}$. Then for $0 < m < M$:

$$\begin{aligned} \sup_{x: x^T \Sigma x \in [mp, Mp]} |\hat{f}_n(x) - f(x)| &= O \left(\sqrt{\ln n} (nb(n))^{-1/2} + b^q(n) \right) \\ &\quad + O(pn^{-1/2} \sqrt{\ln n} + p^2 n^{-1} \ln nb^{-2}) \quad a.s. \end{aligned}$$

- optimized convergence rate: $O((\frac{n}{\ln n})^{-q/(2q+1)})$

Contour function

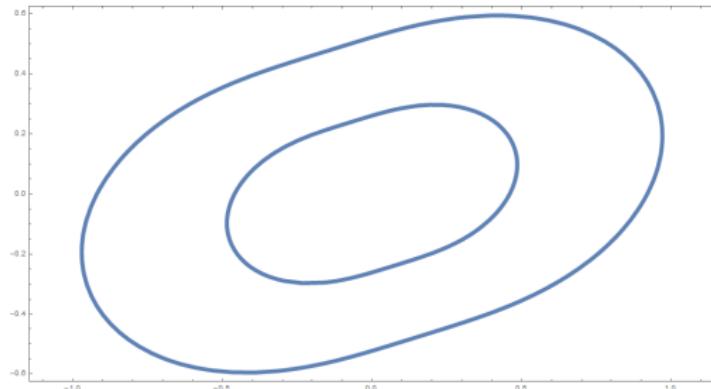
$h : \mathbb{R}^p \rightarrow [0, +\infty)$ positively homogeneous function:

$$h(\lambda x) = \lambda h(x) \quad \forall x \in \mathbb{R}^p, \lambda > 0$$

Let $x_0 \in \mathbb{R}^p$ belong to the star-shaped sphere $\{x : h(x) = 1\}$

$$\rightarrow h(\lambda x_0) = \lambda$$

star-shaped sphere and set $\{x : h(x) = 0.5\}$



Example for h

$$h(x) = \|x\|_q$$

Star-shaped density

- **Density of the random vector**

$X = (X^{(1)}, \dots, X^{(p)})^T \sim CSS(g, h, \mu, \Sigma)$:

$$f_X(x) = (C_0 \det(\Sigma))^{-1} g\left(h(\Sigma^{-1}(x - \mu))\right), \quad x \in \mathbb{R}^p,$$

generator fcn. $g : [0, +\infty) \rightarrow [0, +\infty)$, contour fcn. $h : \mathbb{R}^p \rightarrow [0, +\infty)$,
 location $\mu \in \mathbb{R}^d$, $\sigma = (\sigma_1, \dots, \sigma_p)$, scaling $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_p)$

- Representation:  Richter 2014

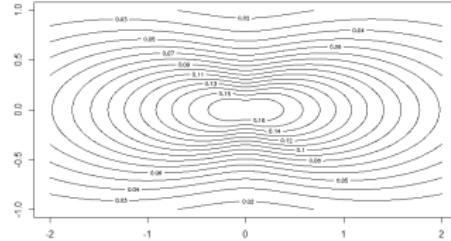
$$X \stackrel{d}{=} \mu + R \Sigma U$$

$R = h(\Sigma^{-1}(X - \mu)) \in [0, +\infty)$ and

$U = \frac{1}{R} (\Sigma^{-1}(X - \mu)) \in S_{p-1}$ independ.

$g(r) = r^{1-p} f_R(r)$, f_R density of R

density contour plot - example



volcano effect for bounded g

Models for h

- $h(x) = \|x\|_q \rightarrow l_q$ -elliptical distribution,  Gupta/Song 1997
- p -dimensional spherical coordinates \rightarrow transformation T

$$x_1 = \cos \alpha_1, \quad x_2 = \cos \alpha_2 \sin \alpha_1,$$

$$x_j = \cos \alpha_j \prod_{k=1}^{j-1} \sin \alpha_k, \quad x_p = \prod_{k=1}^{p-1} \sin \alpha_k$$

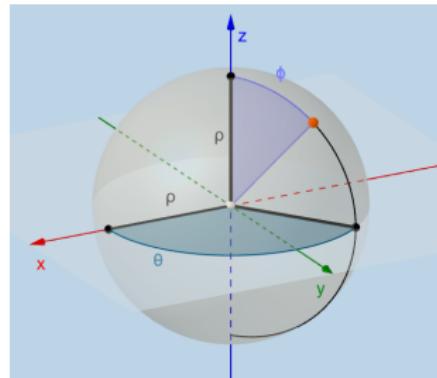
$$T : \{x \in \mathbb{R}^p : \|x\| = 1\} \rightarrow [0, \pi]^{p-2} \times [0, 2\pi),$$

$$x \mapsto (\alpha_1, \dots, \alpha_{p-1}),$$

- **Model function** $H_\eta : [0, \pi]^{p-2} \times [0, 2\pi) \rightarrow (0, \infty)$,

parameter $\eta \in \Theta_2 \subset \mathbb{R}^{q_2}$

$$h_\eta(x) = \|x\|_2 H_\eta(T(\|x\|_2^{-1} x))$$



source: geogebra

Models for h

- p -dimensional polar coordinate transformation

$T : \{x \in \mathbb{R}^d : \|x\| = 1\} \rightarrow [0, \pi)^{p-2} \times [0, 2\pi]$ with $x \rightsquigarrow (\alpha_1, \dots, \alpha_{p-1})$,

$$h_\eta(x) = \|x\|_2 H_\eta(T(\|x\|_2^{-1} x))$$

$$H_\eta(\alpha_1, \dots, \alpha_{p-1}) = h_\eta(T^{-1}(\alpha_1, \dots, \alpha_{p-1}))$$

Model function H_η , $\eta \in \Theta_2 \subset \mathbb{R}^{q_2}$

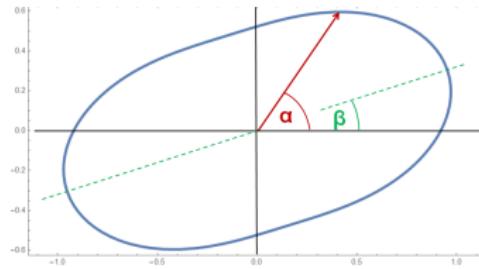
- Example for $d = 2$, $\alpha = \alpha_1$:

model with parameters $\eta = (a, \beta)^T$

$$H_\eta(\alpha) = 1 + a - a \cos(2\alpha - 2\beta)$$

length of the red arrow: $1/H(\alpha)$

contour of the density $h = 1$



Parametric Models for h - case $d = 2$

$$h_\eta(x) = \|x\|_2 H_\eta(\alpha)$$

α ... angle between point and x -axis, $H_\eta : [0, 2\pi) \rightarrow (0, \infty)$

- general properties: H_η is a bounded, continuously differentiable function,

$$\lim_{t \rightarrow 2\pi-0} H_\eta(t) = H_\eta(0), \quad H_\eta(\pi + \alpha) = H_\eta(\alpha), \quad \inf_{\alpha \in [0, 2\pi)} H_\eta(\alpha) > 0.$$

Model class 1:

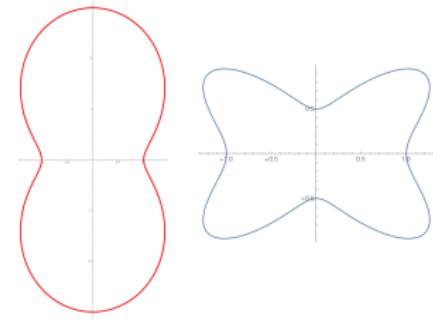
$$\eta = (a, b, c, \beta)^T, a, b, c > 0, \beta \in [0, \pi)$$

$$H(\alpha) = \left(\frac{1 + a \tan^2(\alpha - \beta)}{1 + b \tan^2(\alpha - \beta)} \right)^c \quad \text{for } \alpha \in [0, 2\pi)$$

Model class 2:

$$H(\alpha) = \left(1 + a \sin^2(\alpha - \beta) + b \sin^4(\alpha - \beta) \right)^c$$

$$\text{for } \alpha \in [0, 2\pi]$$



Models for higher-dimensional h

Assumption: $H : [0, \pi]^{d-2} \times [0, 2\pi) \rightarrow (0, \infty)$ is contin. differentiable,

$$\lim_{t \rightarrow 2\pi-0} H(\alpha_1, \dots, \alpha_{d-2}, t) = H(\alpha_1, \dots, \alpha_{d-2}, 0),$$

$$\lim_{\alpha_j \rightarrow 0+0} H(\alpha) = \lim_{\alpha_j \rightarrow \pi-0} H(\alpha) = \tilde{H}_j(\alpha_1, \dots, \alpha_{j-1}) \text{ for } j = 1, \dots, d-1$$

with a constant \tilde{H}_1 and appropriate functions $\tilde{H}_j : [0, \pi]^{j-1} \rightarrow (0, \infty), j \geq 2$

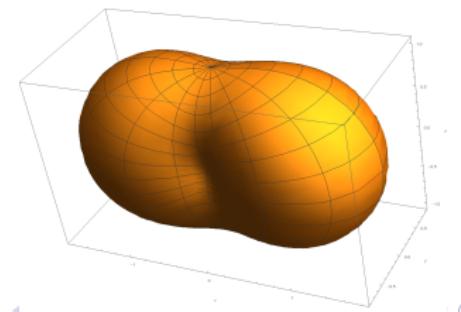
- Model function H_η with parameter $\eta \in \Theta_2 \subset \mathbb{R}^{q_2}$

Q_η orthogonal matrix describing the rotation

$$h_\eta(x) = \|x\|_2 H_\eta(T(\|Q_\eta x\|_2^{-1} Q_\eta x))$$

Example: contour plot of the density →

$$H(\alpha) = \left(1 + \sum_{j=1}^{d-1} a_j \prod_{k=1}^j \sin^2 \alpha_k \right)^{-1}$$



Estimation for star-shaped distributions

X_1, \dots, X_n sample of random vectors having density

$$f_Y(x) = (C_0 \det(\Sigma))^{-1} g\left(h(\Sigma^{-1}(x - \mu))\right), \forall x \in \mathbb{R}^p,$$

$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_p)$$

- for the sake of simplicity, assumption $h(-x) = h(x) \quad \forall x \in \mathbb{R}^p \rightarrow \mathbb{E}X = \mu$

• Estimation problems

- 1) Estimation of μ, σ
- 2) Parametric estimation of h
- 3) Maximum-likelihood estimation of f
- 4) Semiparametric estimation of f : kernel density estimator for g

Estimators for μ, σ

X_1, \dots, X_n sample, $X_i = (X_i^{(1)}, \dots, X_i^{(d)})^T$ has density f ,

$\mathbb{E} \|X\|_2 < +\infty$.

$\implies \mathbb{E} X = \mu$, w.l.o.g. we can assume $\mathbb{V}(X_i) = \sigma_i^2$ for $i = 1, \dots, n$.

- Estimator

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n X_i, \quad \hat{\sigma}_j = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (X_i^{(j)} - \hat{\mu}_j)^2}$$

where $\hat{\mu} = (\hat{\mu}_1, \dots, \hat{\mu}_d)^T$, $\hat{\Sigma} = \text{diag}(\hat{\sigma}_1, \dots, \hat{\sigma}_d)$

standardized sample items

$$\tilde{X}_i^{(j)} = \frac{1}{\hat{\sigma}_j} (X_i^{(j)} - \hat{\mu}_j), \quad \tilde{X}_i = (\tilde{X}_i^{(1)}, \dots, \tilde{X}_i^{(d)})^T.$$

Models for h - Parametric estimation

Model function $H = H_\eta$ with parameter $\eta \in \Theta_2 \subset \mathbb{R}^{q_2}$

- Density of spherical angle vect. $\Gamma = T \left(\|\Sigma^{-1}(X_i - \mu)\|_2^{-1} \Sigma^{-1}(X_i - \mu) \right)$:

$$f_\Gamma(\alpha) = C_0(\eta)^{-1} H_\eta(\alpha)^{-d} \prod_{k=1}^{d-2} \sin^{d-k-1} \alpha_k, \quad \alpha \in [0, \pi)^{d-1} \times [0, 2\pi]$$

standardized sample $\tilde{X}_1, \dots, \tilde{X}_n$,

spherical angle vectors $\Gamma_i = T \left(\|\tilde{X}_i\|_2^{-1} \tilde{X}_i \right)$

Maximizing the likelihood function by using the pseudo sample $\Gamma_1, \dots, \Gamma_n$

→ estimator $\hat{\eta}$

- Alternative: moment estimator for η

Maximum likelihood estimation

model functions g_τ, h_η with parameter $\tau \in \Theta_1 \subset \mathbb{R}^{q_1}, \eta \in \Theta_2 \subset \mathbb{R}^{q_2}$

▷ Sample $X_1, \dots, X_n, X_i \sim CSS(g, h, \mu, \Sigma)$,

parameter $\theta = (\mu^T, \sigma^T, \eta^T, \theta^T)^T \in \Theta = \mathbb{R}^p \times SPD(\mathbb{R}^p) \times \Theta_1 \times \Theta_2$

- Loglikelihood function

$$\ln L(\theta) = \sum_{i=1}^n \ln g_\tau(h_\eta(\Sigma^{-1}(X_i - \mu))) - n \sum_{j=1}^d \ln \sigma_j - n \ln(C_0(\eta)).$$

Maximum-likelihood estimator

$$\hat{\theta} = \arg \max_{\theta \in \Theta} \ln L(\theta)$$

Theorem.

Under regularity assumptions,

$$\sqrt{n} (\hat{\theta}_n - \theta) \xrightarrow{d} \mathcal{N}(0, I(\delta)^{-1}) \text{ for } n \rightarrow \infty, I \dots \text{information matrix}$$

Semiparametric estimator - transformation and sample

- **Transformation** $\psi : [0, \infty) \rightarrow [0, +\infty)$ as above

density χ of $Y = \psi(R)$, $R = h(\Sigma^{-1}(X - \mu))$, $\Psi = \psi^{-1}$:

$$\chi(y) = \Psi(y)^{d-1} g(\Psi(y)) \cdot \Psi'(y) \text{ for } y \geq 0.$$

$$\implies g(z) = z^{1-d} \psi'(z) \chi(\psi(z)) \text{ for } z \geq 0.$$

$$0 < \lim_{z \rightarrow 0+} z^{1-d} \psi'(z) < +\infty$$

- Sample X_1, \dots, X_n , $\hat{h} = h_{\hat{\eta}}$

transformed sample Y_{1n}, \dots, Y_{nn} ,

$$Y_{in} = \psi(\hat{h}(\hat{\Sigma}^{-1}(X_i - \hat{\mu})))$$

Density estimator

$$Y_{in} = \psi(\hat{h}(\hat{\Sigma}^{-1}(X_i - \hat{\mu})))$$

- kernel density estimator for density χ of $Y = \psi(R)$:

$$\hat{\chi}_n(y) = n^{-1} b^{-1} \sum_{i=1}^n \left(k\left((y - Y_{in})b^{-1}\right) + k\left((y + Y_{in})b^{-1}\right) \right) \quad \text{for } y \geq 0,$$

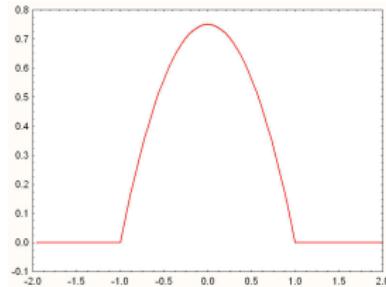
$b = b(n) \rightarrow 0$ bandwidth

Assumptions: $k : \mathbb{R} \rightarrow \mathbb{R}$ continuous kernel function, k' Lipschitz on $[-1, 1]$, $k(t) = 0$ for $t \in \mathbb{R} \setminus [-1, 1]$, $k(-t) = k(t)$ for $t \in [-1, 1]$,

$$\int_{-1}^1 k(t) dt = 1 \text{ and } \int_{-1}^1 t^j k(t) dt = 0$$

for $j : 0 < j < p \in \mathbb{Z}$, even $p \geq 2$

Epanechnikov kernel



Semiparametric density estimator

Assumptions:

$$\lim_{n \rightarrow \infty} b \ln \ln n = 0 \quad \text{and} \quad b_0 \geq b \geq C_1 \cdot n^{-1/5}$$

with constants $b_0, C_1 > 0$.

The partial derivatives G_1, \dots, G_d of h exist and are bounded. Moreover, $x \rightsquigarrow \psi'(h(x))G_j(x)$ is Hölder continuous of order $\alpha > 0.2$ for each j .

- **Estimator**

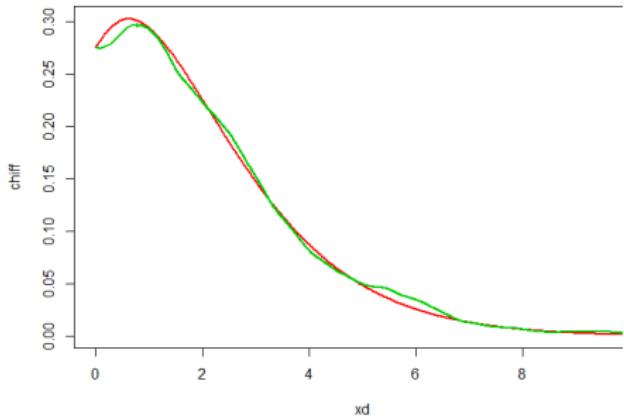
$$\hat{g}_n(z) = z^{1-d} \psi'(z) \hat{\chi}_n(\psi(z)),$$

$$\hat{f}_n(x) = (\hat{C}_0 \det(\hat{\Sigma}))^{-1} \hat{g}_n \left(\hat{h}(\hat{\Sigma}^{-1}(x - \hat{\mu})) \right)$$

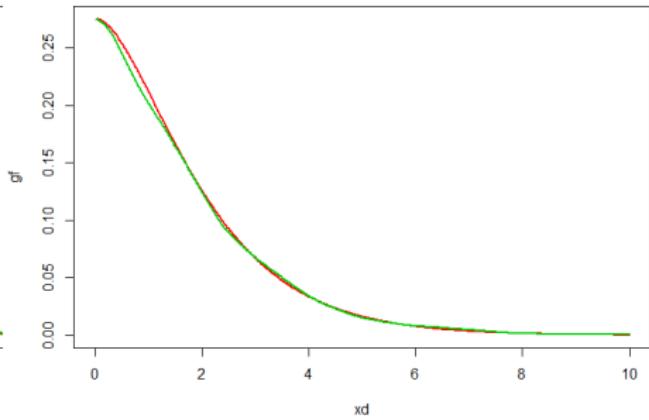
Density estimator - Simulated example

Simulation of the generalized q -norm-distribution, $q = 3, d = 2$,
 f_R modified exponential distribution, $n = 1000$ data points
green: estimator, red: true function

density χ of the transformed data



generator function g



Convergence of the density estimator

Suppose that $g^{(p)}$ exists, is bounded on $[0, \infty)$ for some even integer $p \geq 2$.

Theorem.

\implies for any compact set D with $\mu \notin D$ and $n \rightarrow \infty$,

$$\sup_{x \in D} |\hat{f}_n(x) - f(x)| = O\left(\sqrt{\ln n}(nb)^{-1/2} + b^p\right) \quad a.s.$$

case $\mu \in D$: b^p is replaced by $b^{1/d}$

- $\mu \notin D$: the same rate as for one-dimensional kernel density estimators, does not depend on d

Asymptotic normality of the density estimator

Assume that $g^{(p)}$ is continuous at $\tilde{x} := h(\Sigma^{-1}(x - \mu))$, $x \neq \mu$

Theorem.

$\lim_{n \rightarrow \infty} n^{1/(2p+1)} b = C_2$ with a constant $C_2 \geq 0$, \Rightarrow for $n \rightarrow \infty$

$$\sqrt{nb} (\hat{f}_n(x) - f(x)) \xrightarrow{d} \mathcal{N}(C_2^{(2p+1)/2} \Lambda(\tilde{x}), \bar{\sigma}^2(\tilde{x})).$$

where

$$\bar{\sigma}^2(\tilde{x}) = C_0^{-2} \tilde{x}^{1-d} \psi'(\tilde{x}) g(\tilde{x}) \int_{-1}^1 k^2(t) dt,$$

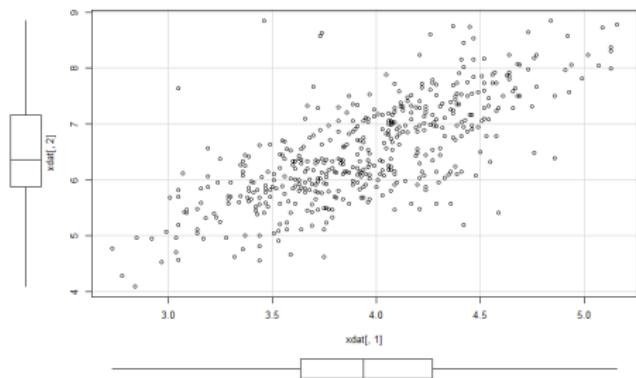
$$\Lambda(\tilde{x}) = C_0^{-1} \tilde{x}^{1-d} \psi'(\tilde{x}) \frac{1}{p!} \chi^{(p)}(\psi(\tilde{x})) \int_{-1}^1 t^p k(t) dt.$$

Data example

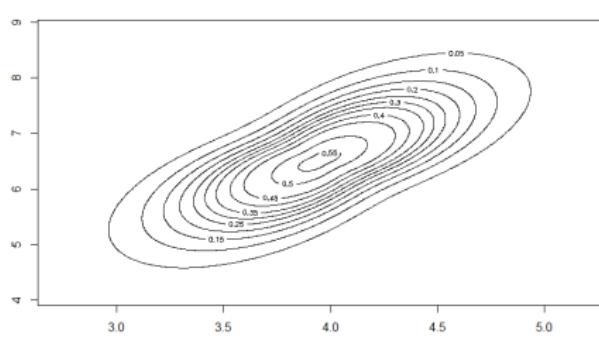
dataset 5 of Andrews and Herzberg (1985)

variables: yield of grain and straw

scatter plot of the data



contour plot of $\hat{\varphi}_n$, $b = 0.5$



moment estimator for a_1 : $\hat{a}_1 = 0.83641$

Data example

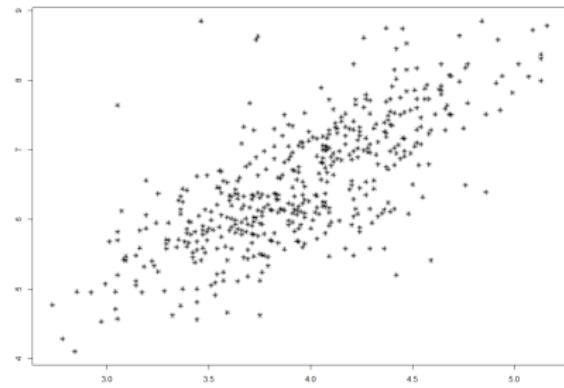
dataset 5 📈 Andrews/Herzberg 1985, variables: yield of grain and straw

model g : Pearson VII,

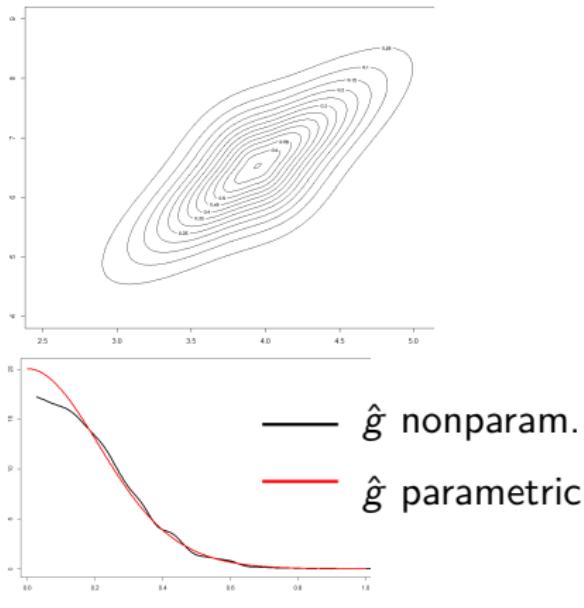
H class 1 with $c = 1$

goodness-of-fit $\rho = 0.9846$

scatter plot of the data



contour plot of $\varphi_{\hat{g}, \hat{h}, \hat{\mu}, \hat{\sigma}}$



Simulating the distribution

Theorem.

$R = h(\Sigma^{-1}(X - \mu))$ and $\Psi = T(\|\Sigma^{-1}(X - \mu)\|^{-1} \Sigma^{-1}(X - \mu))$ are independent with densities

$$f(r) = g(r)r^{d-1}, \quad \varphi_\Psi(\alpha) = \kappa^{-1} H(\alpha)^{-d} \prod_{k=1}^{d-2} \sin^{d-k-1} \alpha_k$$

- **algorithm** to simulate X :

- 1) Generate R with density f .
- 2) Generate Ψ (independent to R) with density φ_Ψ .

Formulas for marginal densities of every dimension are available.

- 3) Evaluate $U = H(\Psi)^{-1} T^{-1}(\Psi)$ and $X = \mu + \Sigma RU$

Summary

- very general class of star-shaped distributions including distributions with non-convex contours
 - parametric density estimators
 - flexible semiparametric density estimators on the basis of a one-dimensional kernel estimator
 - good performance, no dimensionality problems
-
- Tasks for future investigations:
 - model validation
 - skewed distributions

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