A Convex Hull Peeling Depth Approach to Nonparametric Massive Multivariate Data Analysis with Applications

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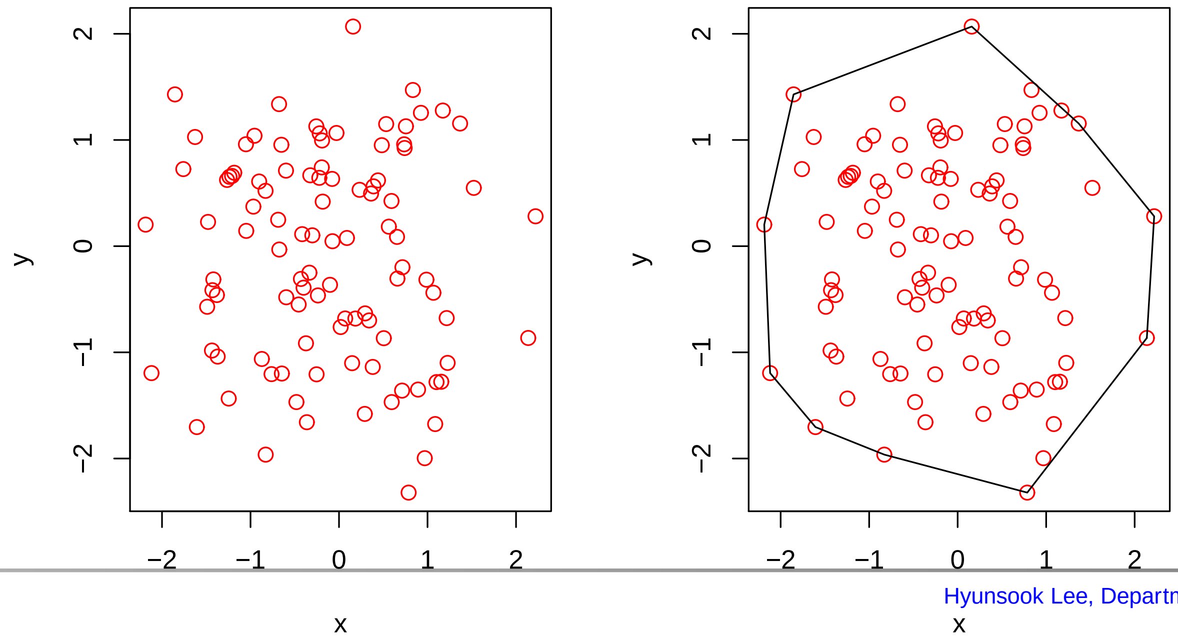
Outlines

- Convex Hull Peeling (CHP) and Multivariate Data Analysis
  - Definitions on CHP
  - Data Depth (Ordering Multivariate Data)
  - Quantiles and Density Estimation
- Color Magnitude (CM) Diagram and Sloan Digital Sky Survey
- Nonparametric Descriptive Statistics with CHP
  - Multivariate Median
  - Skewness and Kurtosis of a Multivariate Distribution
- Outlier Detection with CHP
  - Level α ; Shape Distortion; Balloon Plot
- Concluding Remarks

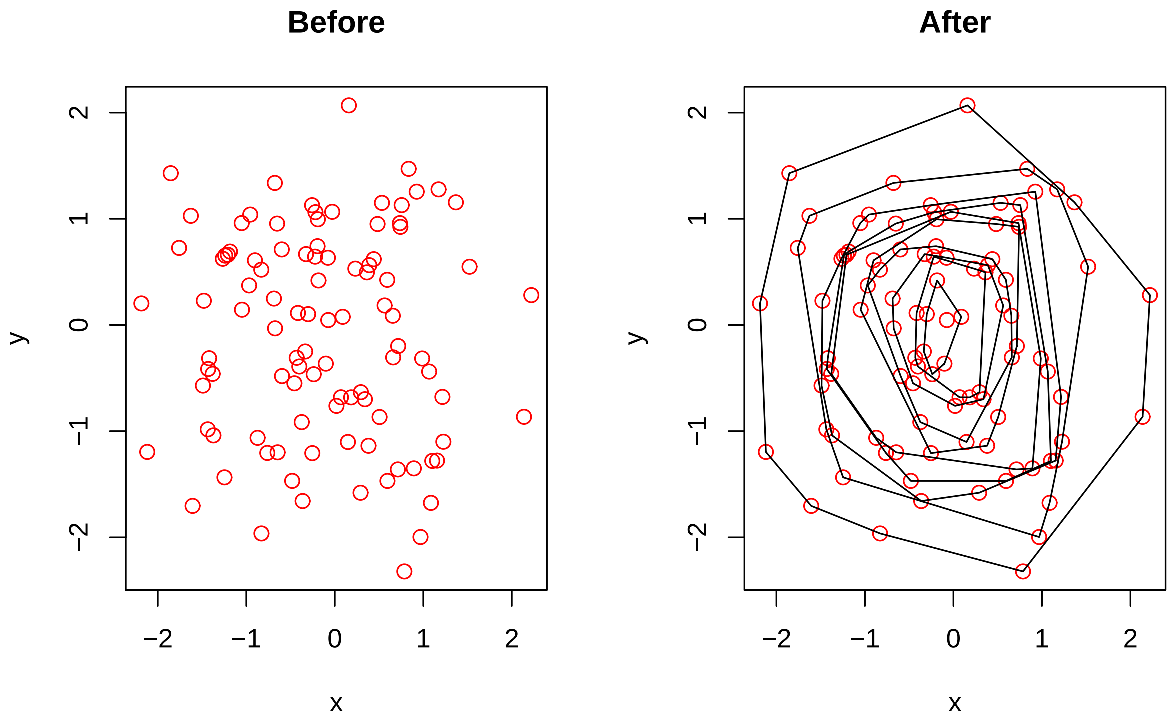
Definitions

Convex Set A set $C \subseteq R^d$ is convex if for every two points $x, y \in C$ the whole segment xy is also contained in C.

Convex Hull The convex hull of a set of points X in R^d is denoted by $CH(X)$, is the intersection of all convex sets in R^d containing X. In algorithms, a convex hull indicates points of a shape invariant minimal subset of $CH(X)$ (vertices, extreme points), connecting these points produces a wrap of $CH(X)$.



Convex Hull Peeling



Convex Hull Peeling Depth (CHPD)

[CHPD:] For a point $x \in R^d$ and the data set $X = \{X_1, ..., X_{N-1}\}$, let $C_1 = CH\{x, X\}$ and denote a set of its vertices V_1. We can get $C_j = C_{j-1} \backslash V_{j-1}$ through CHP until $x \in V_j$ $(j = 2, ...)$. Then, $\mathrm{CHPD}(x) = \frac{\sharp(\cup_{i=1}^{k} V_i)}{N}$ for k s.t. $k = \min_j\{j : x \in V_j\}$; otherwise CHPD is 0.

- Tukey (1974): Locating data center (median) by the Convex Hull Peeling Process.
- Barnett (1976): Ordering based on Depth
- $\hat{p}^{th}$ quantiles are $1 - \hat{p}^{th}$ CHPDs.
- Hyper-polygons of $1 - \hat{p}^{th}$ depth obtainable from any dimensional data.
- QHULL (Barber *et. al.*, 1996) works for general dimensions (http://qhull.org).
- Why CHPD...

Challenges in Nonparametric Multivariate Analysis

How to Order Multivariate Data?

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How to Order Multivariate Data?

Ordering Multivariate Data $\rightarrow$ Data Depth

- Mahalanobis Depth : Mahalanobis (1936)
- Convex Hull Peeling Depth: Barnett (1976)
- Half Space Depth: Tukey (1975)
- Simplical Depth : Liu (1990)
- Oja Depth : Oja (1983)
- Majority Depth : Singh (1991)
- Ordering is not uniformly defined

Statistical Data Depth
(Zuo and Serfling, 2000)

(P1) (Affine invariance) $D(Ax+b; F_{AX+b}) = D(x; F_X)$ for all X (A nonsingular matrix) holds for any random vector X in R^d, any $d \times d$ nonsingular matrix A, and any d-vector b;

(P2) (Maximality at center) $D(\theta; F) = \sup_{x \in R^d} D(x; F)$ holds for any $F \in \mathcal{F}$ having center θ;

(P3) (Monotonicity) for any $F \in \mathcal{F}$ having deepest point θ, $D(x; F) \leq D(\theta + \alpha(x-\theta); F)$ holds for $\alpha \in [0,1]$; and

(P4) $D(x; F) \to 0$ as $||x|| \to \infty$, for each $F \in \mathcal{F}$.

Convex Hull Peeling Depth

- affine invariance
- maximality at center
- monotonicity relative to deepest point
- vanishing at infinity

CHPD has these properties and points of smallest depth are possible outliers

Quantile Estimation

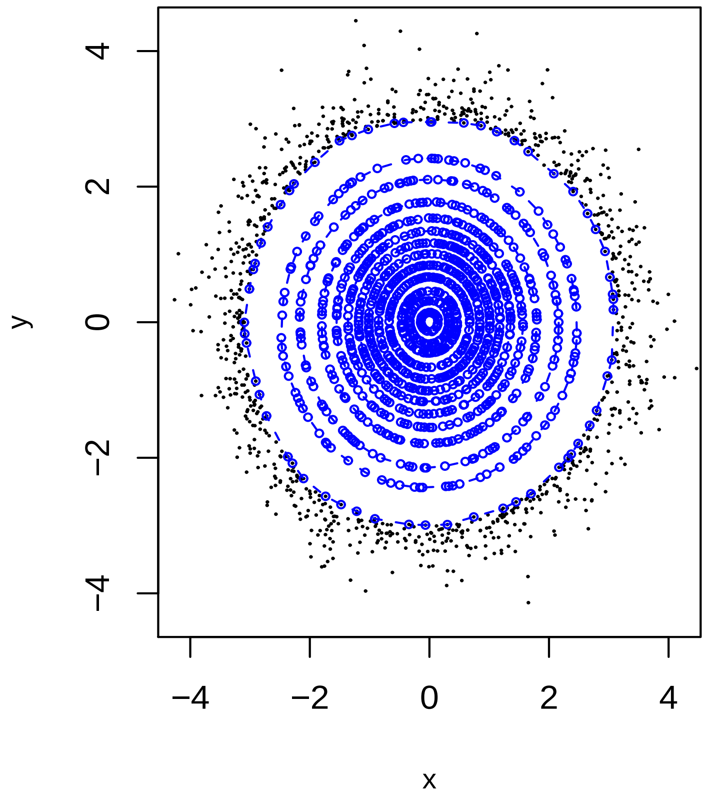
- Median: A point(s) left after peeling
  (will show robustness of this estimator later)
- p^{th} Quantile: Level set whose central region contains $\sim 100p\%$ data
  (will define the level set and the central region later)
- No Closed Form; Empirical Process

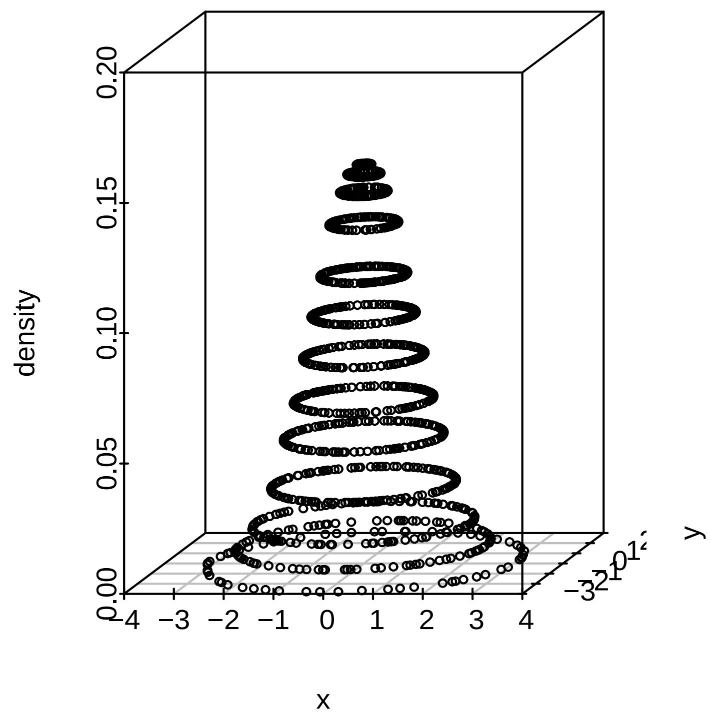
Empirical Density Estimation

Density Estimation with CHPD on Bivariate Normal Data (McDermott, 2003)

100000 Bivariate Normal Sample

Quantiles={0.99,0.95,0.90,0.80,...0.20,0.10,0.05,0.01}





Lessons and Further Studies

- Sample from a convex distribution (no doughnut shape)
- Works on Massive data
  $\longrightarrow$ Sequential Method
- Without previous knowledge, no model or prior is known to start an analysis. Exploratory data analysis for a large database
- Nonparametric and non-distance based approach
- Where CHP can be applied and how?
  $\longrightarrow$ Multi-color diagram from astronomy, where a plethora of free data archives is available.

Color Magnitude diagram

Two dimensional Color-Color diagram or
Celebrated Hertzsprung-Russell diagram (switch)

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What if we can see beyond 2 dimensions without bias (projection)
Then, 3 or higher dimensional color diagrams might have popularity.

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What if we can see beyond 2 dimensions without bias (projection)
Then, 3 or higher dimensional color diagrams might have popularity.

CHP may assist analyzing multi-color diagrams.
Need a suitable data set with colors.

Sloan Digital Sky Survey: SDSS

Commissioned 2000, now Data Release 5 is available.
5 bands; 4 variables (u-g, g-r, r-i, i-z)

- Studies on analyzing astronomical massive data received spotlights recently. http://www.sdss.org
- July, 2005: Data Release Four
  6670 square degrees, 180 million objects
  Available from http://www.sdss.org/dr4
  From SpecPhotoAll with SQL:
- Attributes of photometric data are color indices, *u,b,g,i,z* along with coordinates.

SQL for SDSS

```
select ra, dec, z, psfMag_u, psfMag_g, psfMag_r,
    psfMag_i, psfMag_z
from SpecPhotoAll
where specclass= 2
```

- Note — 2: galaxies, 3: QSO, 4: HighZ QSO
- Galaxies: 499043
- Quasars: 70204

Multivariate Descriptive Statistics

- CHP Median
- CHP Skewness
- CHP Kurtosis

with bivariate simulated data and SDSS DR4

Convex Hull Peeling Median (CHPM)

Multivariate Median: the inner most point among data

$\longrightarrow$ Survey of Multivariate Median (Small, 1990)

CHPM: recursive peeling leads to the inner most point(s). The average of these largest depth points is the median of a data set.

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Simulations: Sample from standard bivariate normal distribution

n	mean	median	CHPM
10^4	(0.001338, -0.02232)	(-0.005305, -0.01643)	(0.000918, -0.010589)
10^6	(0.000072, 0.000114)	(0.001185, -0.000717)	(0.002455, -0.000456)
		Sequential CHPM $\longrightarrow$	(0.004741, -0.004111)

Setting for the sequential method: m=10000 and d=0.05

Application: Median

Quasars	u-g	g-r	r-i	i-z
Mean	0.4619	0.2484	0.1649	0.1008
Median	0.2520	0.1750	0.1520	0.0770
CHPM	0.2530	0.1640	0.1913	0.0700
Galaxies	**u-g**	**g-r**	**r-i**	**i-z**
Mean	1.622	0.9211	0.4226	0.3439
Median	1.680	0.8930	0.4200	0.3540
CHPM	1.790	0.957	0.424	0.367
Seq. CHPM	1.772	0.950	0.4228	0.363

Robustness of Convex Hull Peeling Median

Breakdown point of a convex hull peeling median goes to zero as $n \to \infty$ (Donoho, 1982). Outliers are necessarily located at infinity.

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Empirical mean square error (EMSE) and Relative Efficiency (RE):

Model: $(1-\epsilon)N((0,0),\mathbf{I}) + \epsilon N(\cdot, 4\mathbf{I})$

$n = 5000$, $m = 500$, T_j=(CHPM, Mean)

$$EMSE = \frac{1}{m}\sum_{i=1}^{m} ||T_j - \mu||^2$$

	$N((5,5)^t, 4\mathbf{I})$			$N((10,10)^t, 4\mathbf{I})$		
ϵ	CHPM	Mean	RE	CHPM	Mean	RE
0	0.002178	0.000417	0.191689	0.002178	0.000417	0.191689
0.005	0.0028521	0.001682	0.589961	0.002891	0.005444	1.88291
0.05	0.016842	0.125522	7.45262	0.017824	0.500610	28.08597
0.2	0.139215	2.00109	14.37612	0.1435910	8.0017	55.7264

Generalized Quantile Process

EinMahl and Mason (1992)

$$U_n(t) = inf\{\lambda(A) : P_n(A) \geq t, A \in \mathbb{A}\}, 0 < t < 1.$$

- Central Region:

$$R_{CH}(t) = \{x \in \mathbb{R}^d : CHPD(x) \geq t\}$$

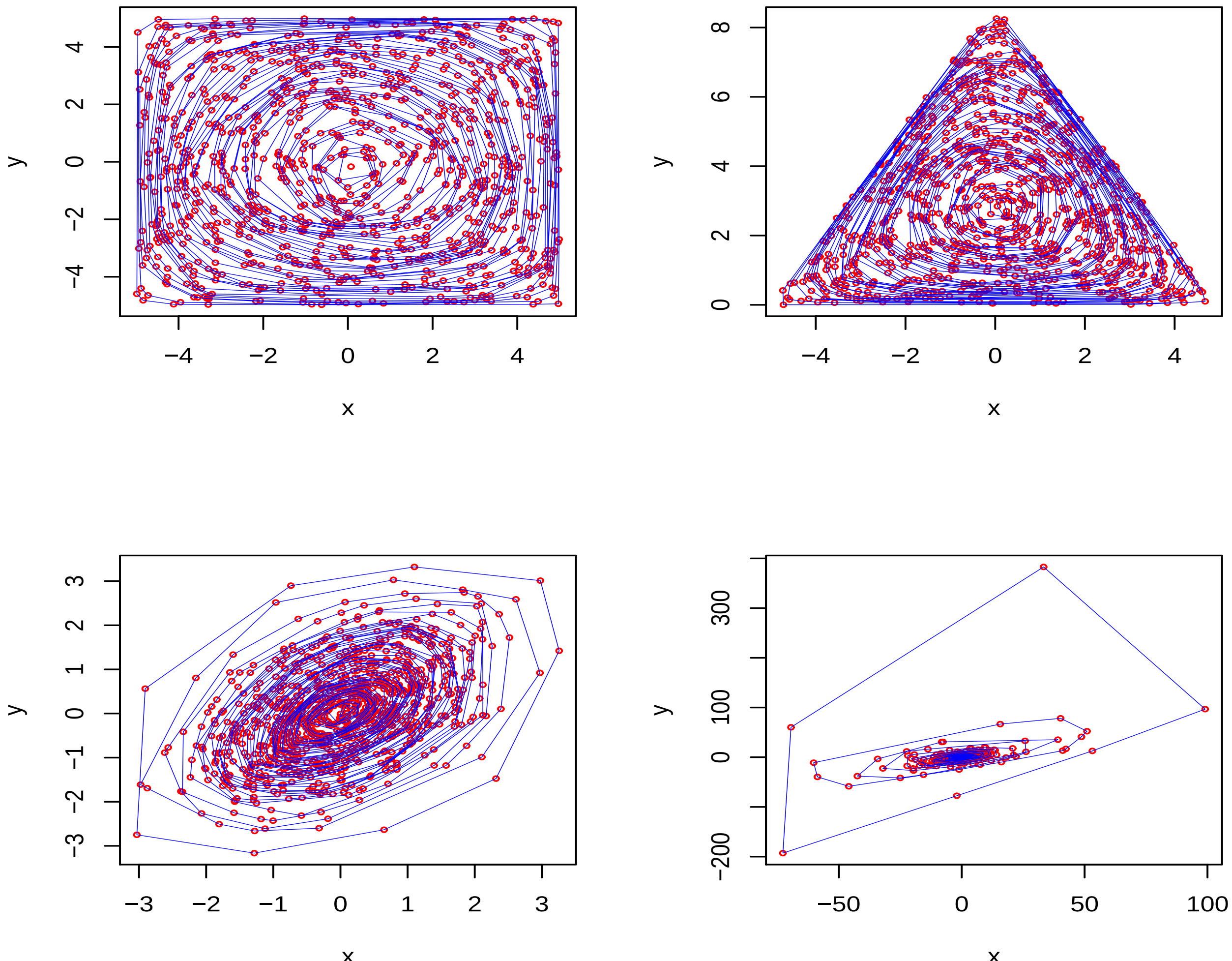
- Level Set:

$$\begin{aligned} B_{CH}(t) &= \partial R_{CH}(t) \\ &= \{x \in \mathbb{R}^d : CHPD(x) = t\} \end{aligned}$$

- Volume Functional:

$$V_{CH}(t) = Volume(R_{CH}(t))$$

$\longrightarrow$ One dimensional mapping.



→ not equi-probability contours, assume smooth convex distributions

Skewness Measure

Let $x_{j,i}$ be the i^{th} vertex in a level set $B_{CH,j}$ comprised by the j^{th} peeling process. A measure of skewness:

$$R_j = \frac{\max_i ||x_{j,i} - CHPM|| - \min_i ||x_{j,i} - CHPM||}{\min_i ||x_{j,i} - CHPM||}$$

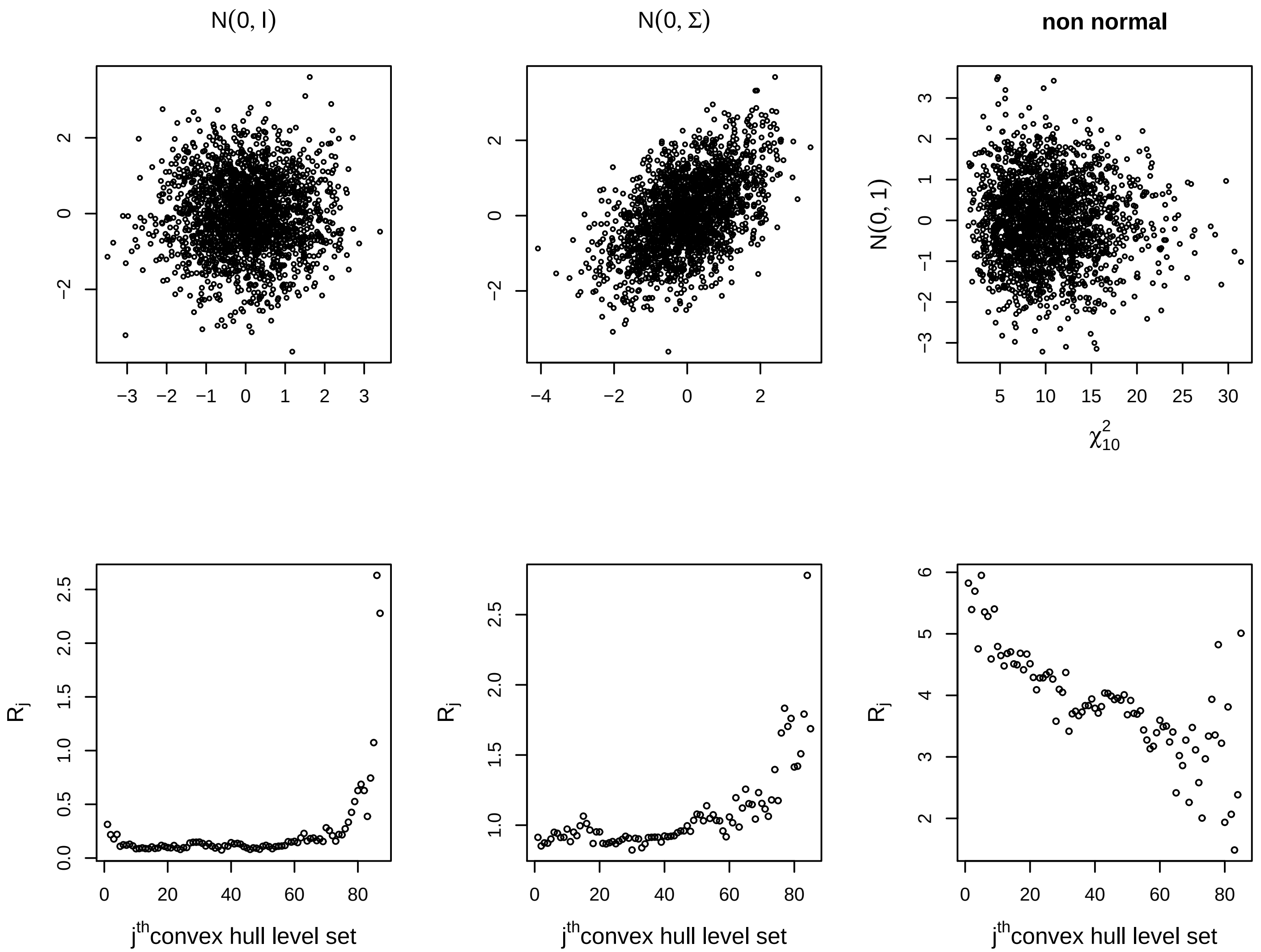
Not only a sequence of R_j visualizes but also quantizes the skewness along depths.

Denominator for the regularization $\rightarrow$ affine invariant R_j

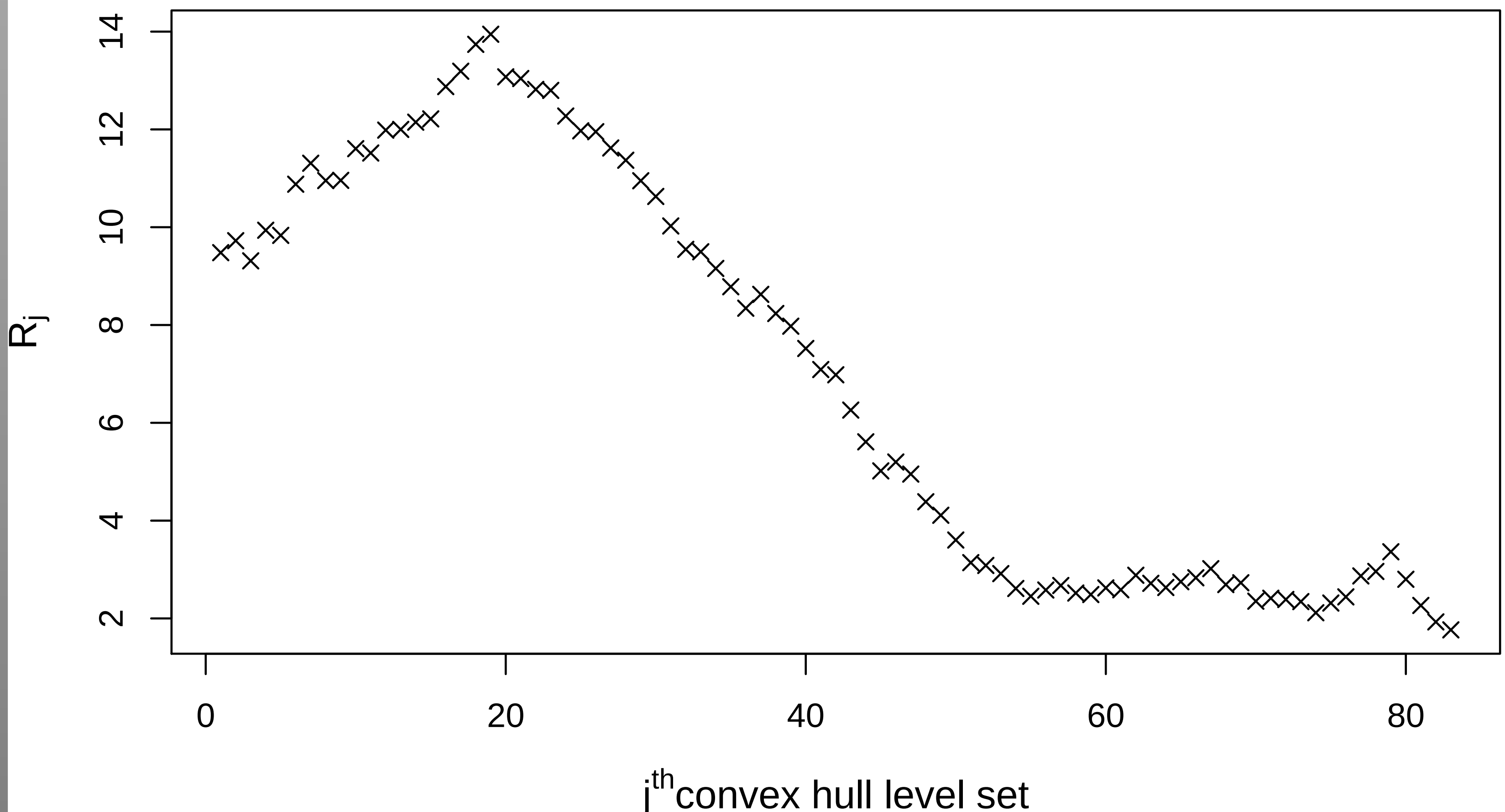
symmetric: flat R_j along convex hull peels

skewed: fluctuating R_j

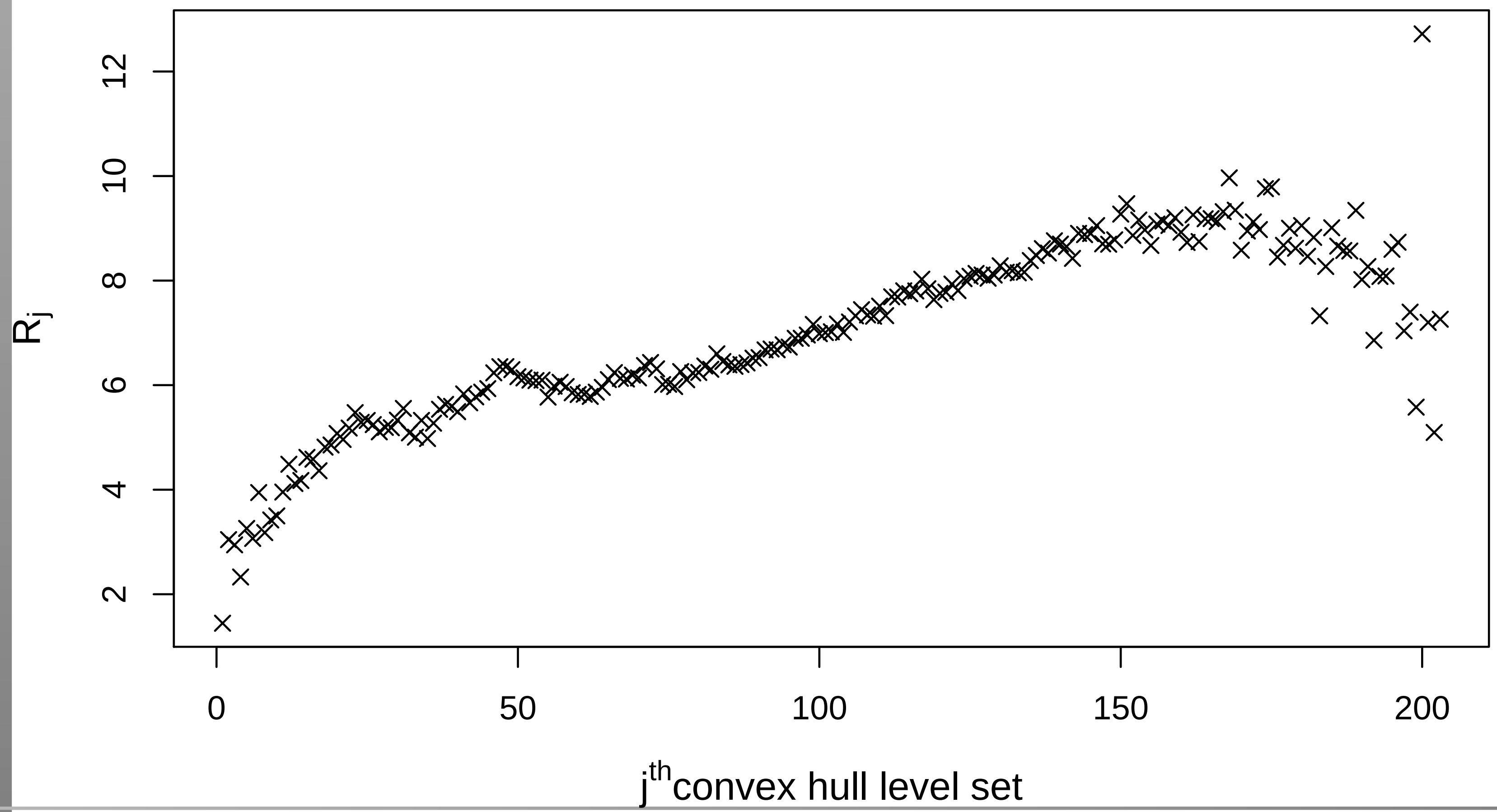
Simulation: Skewness Measure



Application: *Skewness Measure (Quasars)*



Application: *Skewness Measure (Galaxies)*



Kurtosis Measure

Quantile (Depth) based Kurtosis:

$$K_{CH}(r) = \frac{V_{CH}(\frac{1}{2} - \frac{r}{2}) + V_{CH}(\frac{1}{2} + \frac{r}{2}) - 2V_{CH}(\frac{1}{2})}{V_{CH}(\frac{1}{2} - \frac{r}{2}) - V_{CH}(\frac{1}{2} + \frac{r}{2})}$$

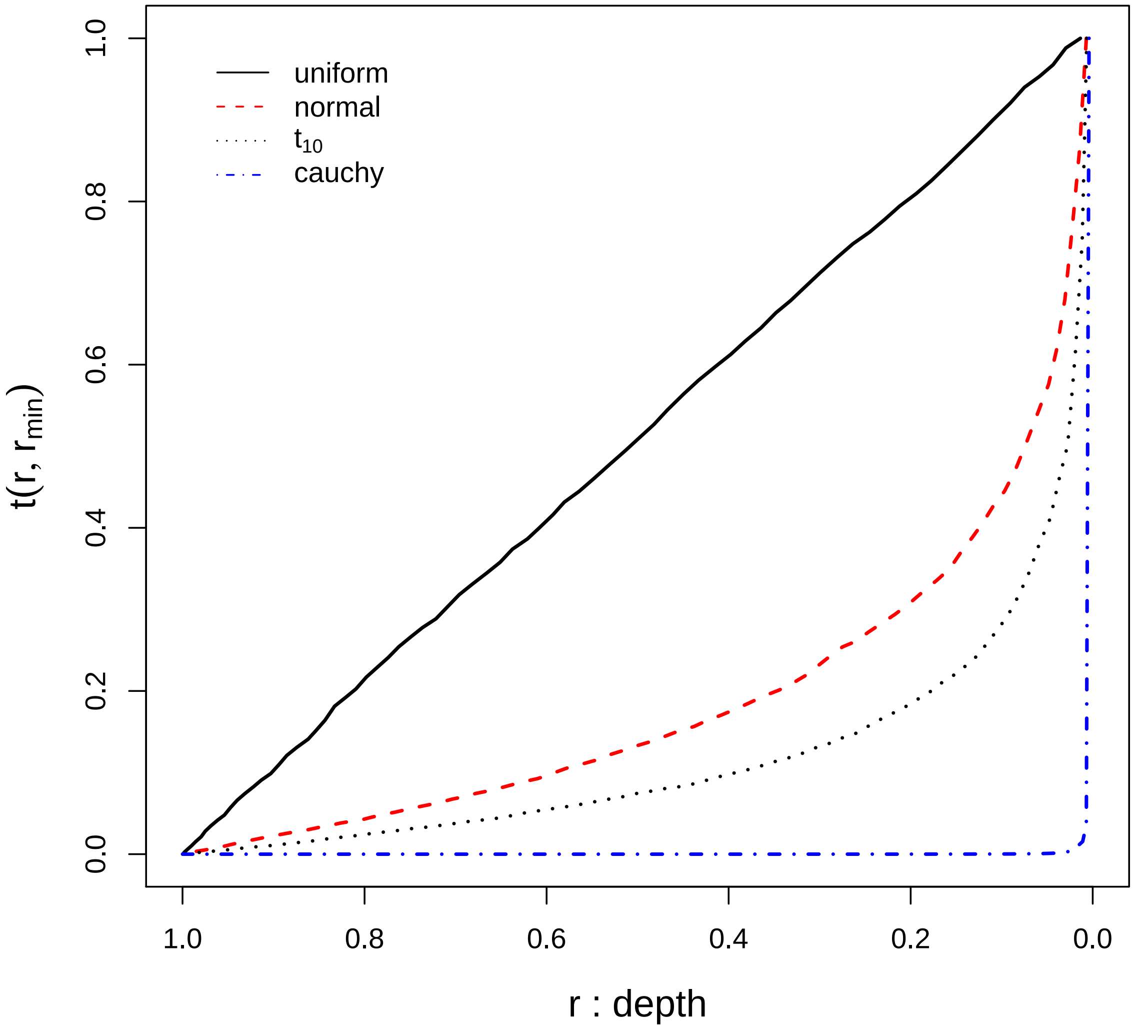
Tailweight:

$$t(r, s) = \frac{V_{CH}(r)}{V_{CH}(s)}$$

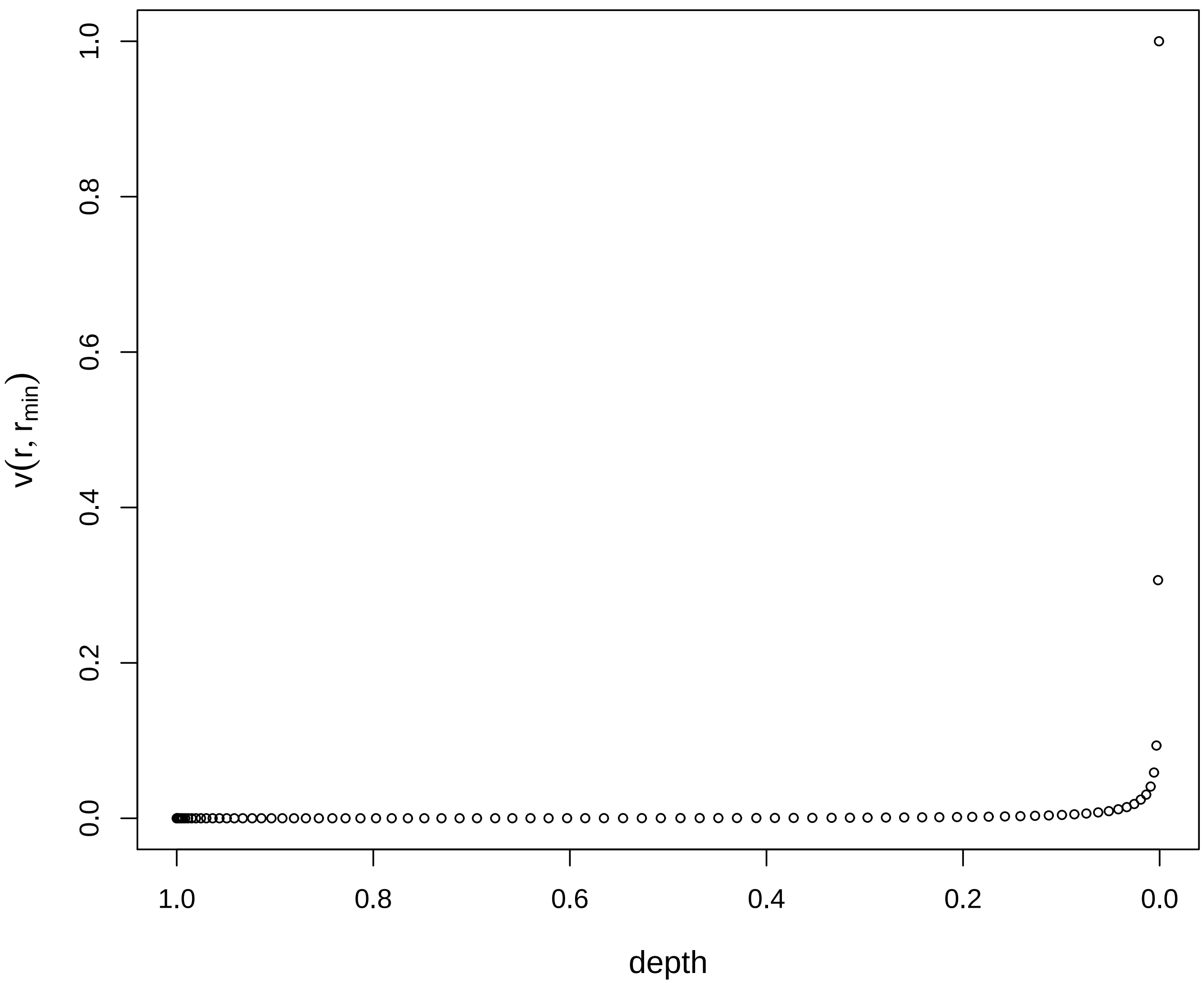
for $0 < s < r \leq 1$. Here,

$V_{CH}(r)$ indicates the volume functional at depth r.

Simulation: *Kurtosis Measure (Tailweight)*



Application: Kurtosis Measure (Quasars)



Multivariate Outlier Detection

- What are Outliers?
- Detecting Algorithms
    - Level α
    - Shape Distortion
    - Balloon Plot

What are Outliers?

Outliers are...

- Cumbersome Observations
- Lead to New Scientific Discoveries
- Improve Models (Robust Statistics)
- ...
- No Clear Objectives but Come Along Often

CHP: Experience and relative Robustness support the Idea of Outlier Detection.
$\Rightarrow$ We need a clear definition on outliers; especially, outliers of the 21st century. And outlier detecting methods.

Outliers are observations....

- Huber (1972): unlikely to belong to the main population.
- Barnett and Leroy (1994): appear inconsistent with the remainder.
- Hawkins (1980): deviated so much to arouse suspicion.
- Beckman and Cook (1983): surprising and discrepant to the investigator.
  Discordant Observations or Contaminants
- Rohlf (1975): somewhat isolated from the main cloud of points.

Yet, somewhat VAGUE!

Some Outlier Detection Methods

Univariate: Box-and-Whisker plot, Order statistics, ...

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Multivariate: Mostly bivariate applications

- Generalized Gap Test (Rolhf, 1975)
- Bivariate Box Plot (Zani et. al, 1999)
- Sunburst Plot (Liu et. al., 1999)
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and Mahalanobis distance $D(x) = (x - \hat{\mu})\hat{\Sigma}^{-1}(x - \hat{\mu})$.

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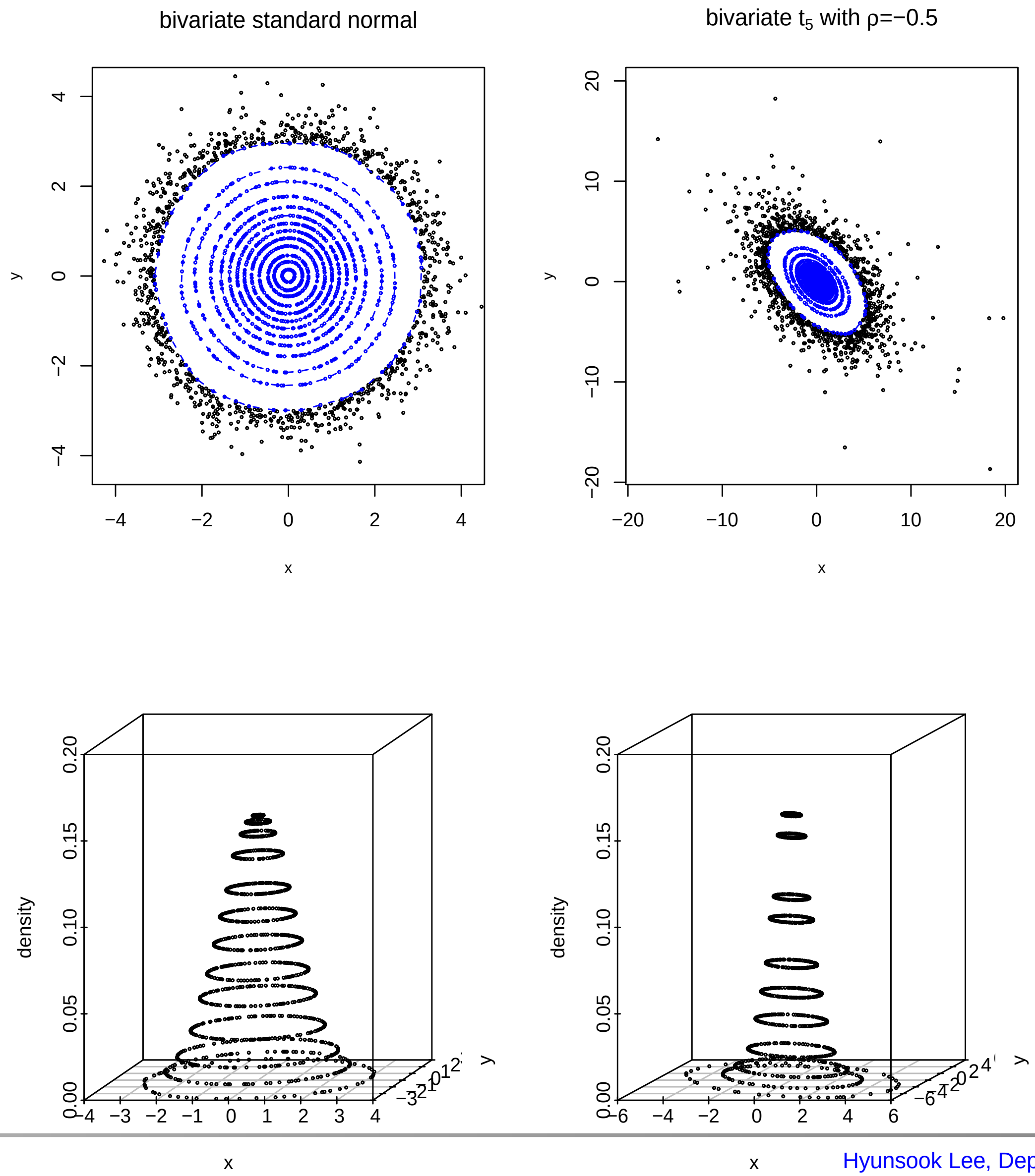
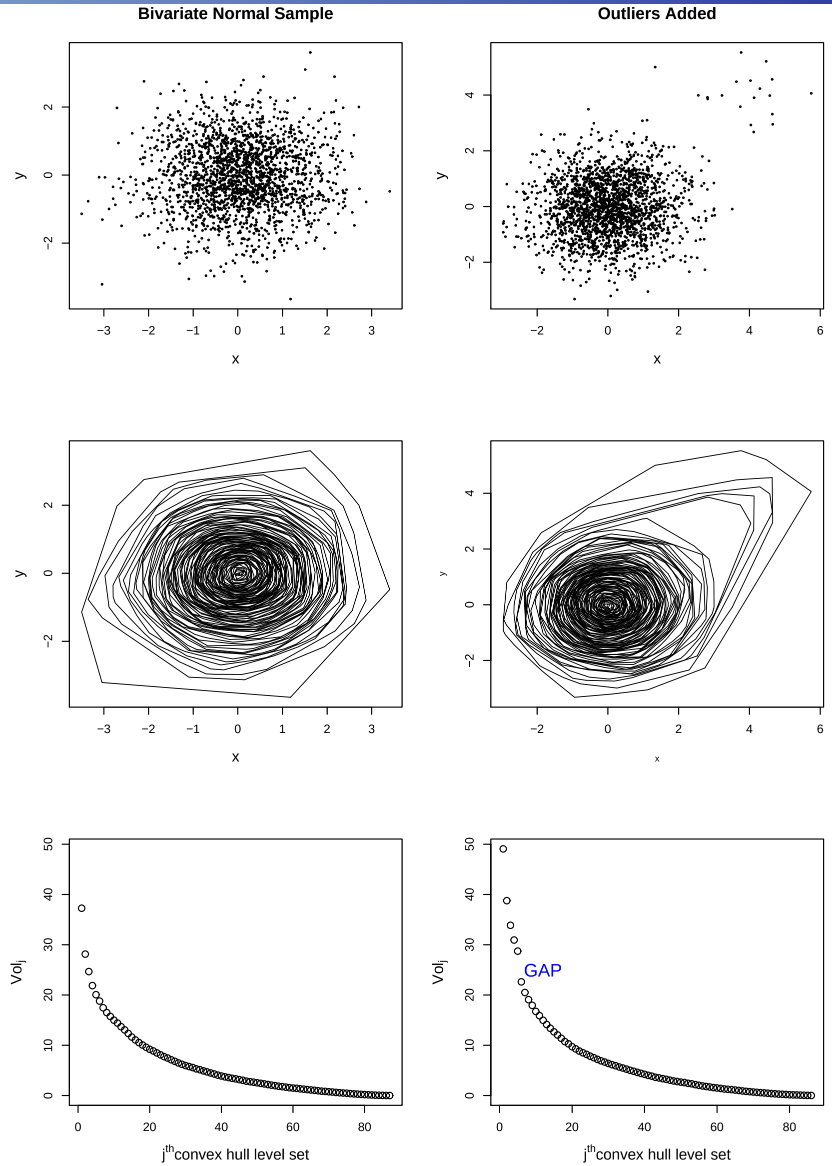
Difficulties of multivariate analysis arise from the complexity of ordering multivariate data.

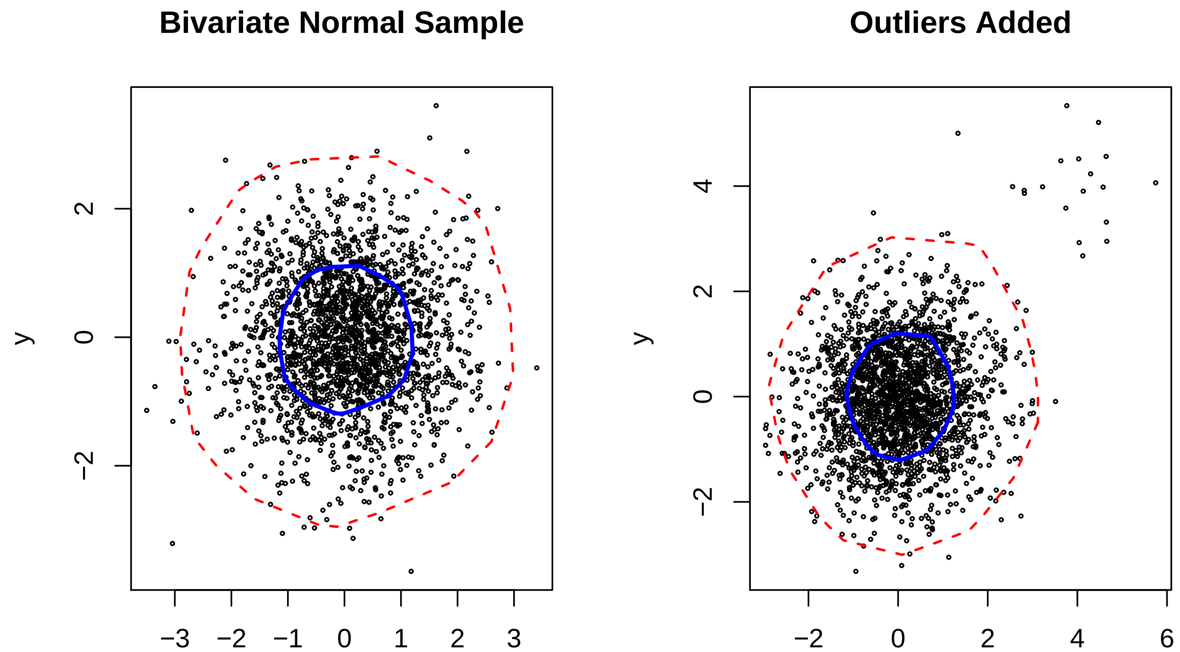
Quantile Based Outlier Detection



Contour Shape Changes



Balloon Plot

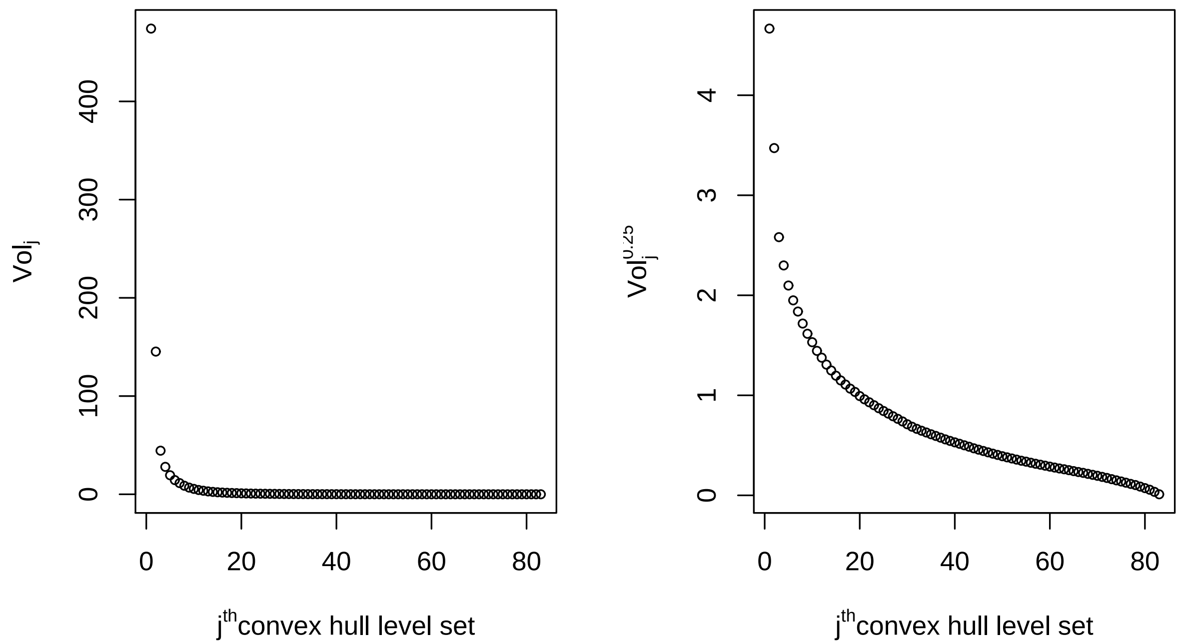


A Balloon Plot is obtained by blowing $.5^{th}$ CHPD polyhedron by 1.5 times (lengthwise). Let $V_{.5}$ be a set of vertices of $.5^{th}$ CHPD hull. The balloon for outlier detection is

$$B_{1.5} = \{y_i : y_i = x_i + 1.5(x_i - CHPM), x_i \in V_{.5}\}.$$

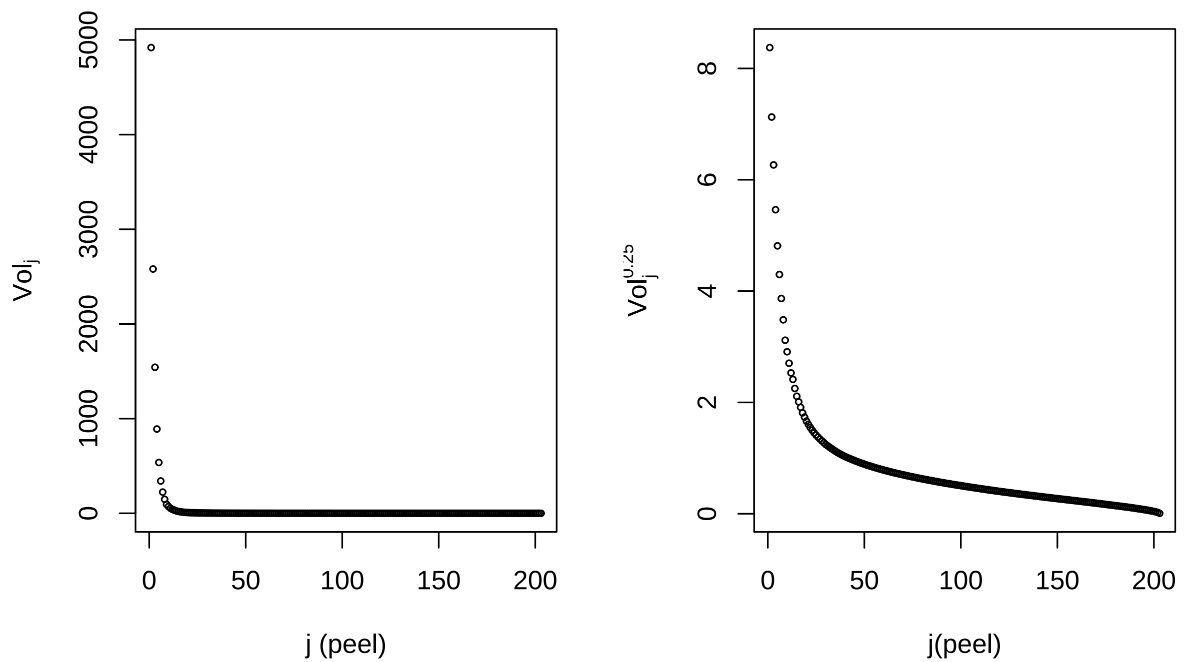
In other words, blow the balloon of IQR 1.5 times larger.

Outliers in Quasar Population



Volumes of 1st CH, .01 Depth CH, .05 Depth CH: (474.134, 14.442, 4.353)

Outliers in Galaxy Population



Volumes of 1st CH, .01 Depth CH, .05 Depth CH: (4919.492, 4.310, 1.075)

Discussion on CHP

Convex Hull Peeling is..

- a robust location estimator.
- a tool for descriptive statistics.
  Skewness and *Kurtosis* measure.
- a reasonable approach for detecting multivariate outliers.
- a starter for clustering.

$\Rightarrow$Our methods help to characterize multivariate distributions and identify outlier candidates from multivariate massive data; therefore, the results initiate scientists to study further with less bias.
CHP as Exploratory Data Analysis and Data Mining Tools.

Concluding Remarks

Drawbacks of CHPD

- Limited to moderate dimension data.
- CHPD estimates depths inward not outward.
- Convexity of a data set.
- No population/theoretical counterpart.

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No assumption on data distribution, Non-distance based, Affine invariant, Applicable to streaming data, Detecting Outliers, Providing Multivariate Descriptive Statistics, Exploratory data analysis