Statistical Depth Function

Zoltán Szabó

Machine Learning Journal Club, Gatsby Unit

June 27, 2016

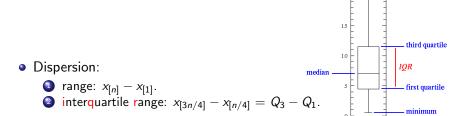
Outline

- L-statistics, order statistics, ranking.
- Instead of moments: median, dispersion, scale, skewness, ...
- New visualization tools: depth contours, sunburst plot.
- Testing: symmetry.
- Depth function properties.

L-statistics, ranking

- Given: $x_1, \ldots, x_n \in \mathbb{R}$ samples.
- Order statistics: $x_{[1]} \leq \ldots \leq x_{[n]}$.
- Linear combination of order statistics.
- Rank: position of x_i .

L-statistics: examples

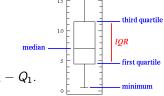


maximum

L-statistics: examples



- **1** range: $x_{[n]} x_{[1]}$.
- ② interquartile range: $x_{[3n/4]} x_{[n/4]} = Q_3 Q_1$.



maximum

- Location:
 - median: $x_{[n/2]}$.
 - α -trimmed mean = middle of the $(1-2\alpha)$ -th fraction of observations,

$$\frac{1}{(1-2\alpha)n}\sum_{i=\alpha n+1}^{(1-\alpha)n}x_{[i]}.$$

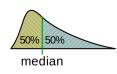
- Typical application: robust estimation.
- Question: Similar notions in \mathbb{R}^d ?

- Typical application: robust estimation.
- Question: Similar notions in \mathbb{R}^d ?
- Critical: $x_{[1]} \leq \ldots \leq x_{[n]}$.

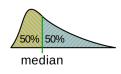
- Typical application: robust estimation.
- Question: Similar notions in \mathbb{R}^d ?
- Critical: $x_{[1]} \leq \ldots \leq x_{[n]}$.
- Idea: center-outward ordering.

Median

- F: continuous c.d.f. on \mathbb{R} .
- median:
 - point splitting the probability mass to $\frac{1}{2} \frac{1}{2}$.
 - solution of $F(m) = \frac{1}{2}$.



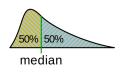
- F: continuous c.d.f. on \mathbb{R} .
- median:
 - point splitting the probability mass to $\frac{1}{2} \frac{1}{2}$.
 - solution of $F(m) = \frac{1}{2}$.



alternative view:

$$m := \underset{x \in \mathbb{R}}{\operatorname{arg max}} D(x) := 2F(x)[1 - F(x)]$$

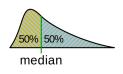
- F: continuous c.d.f. on \mathbb{R} .
- median:
 - point splitting the probability mass to $\frac{1}{2} \frac{1}{2}$.
 - solution of $F(m) = \frac{1}{2}$.



alternative view:

$$m:=rg\max_{x\in\mathbb{R}}D(x):=2F(x)[1-F(x)] \ =\mathbb{P}_{X_1,X_2\sim F}(x\in[X_1,X_2]).$$

- F: continuous c.d.f. on \mathbb{R} .
- median:
 - point splitting the probability mass to $\frac{1}{2} \frac{1}{2}$.
 - solution of $F(m) = \frac{1}{2}$.



alternative view:

$$m := \underset{x \in \mathbb{R}}{\arg \max} D(x) := 2F(x)[1 - F(x)]$$

= $\mathbb{P}_{X_1, X_2 \sim F}(x \in [X_1, X_2]).$

Moving away from m, D(x) decreases monotonically to 0.

Let us extend the median to \mathbb{R}^d !

• Simplitical depth [Liu, 1990]:

$$SD(\mathbf{x}; F) := \mathbb{P}_F (\mathbf{x} \in \Delta(X_1, \dots, X_{d+1})).$$

Let us extend the median to \mathbb{R}^d !

• Simplitical depth [Liu, 1990]:

$$SD(\mathbf{x}; F) := \mathbb{P}_F (\mathbf{x} \in \Delta(X_1, \dots, X_{d+1})).$$

• Half-space depth [Tukey, 1975]:

$$HD(\mathbf{x}; F) := \inf_{\mathbf{x} \in H \subset \mathbb{R}^d} \mathbb{P}_F(X \in H)$$

minimum probability of any closed halfspace containing x.

Let us extend the median to \mathbb{R}^d !

• Simplitical depth [Liu, 1990]:

$$SD(\mathbf{x}; F) := \mathbb{P}_F (\mathbf{x} \in \Delta(X_1, \dots, X_{d+1})).$$

• Half-space depth [Tukey, 1975]:

$$\underline{HD}(\mathbf{x}; F) := \inf_{\mathbf{x} \in H \subset \mathbb{R}^d} \mathbb{P}_F(X \in H)$$

minimum probability of any closed halfspace containing x.

median:
$$m = \arg \max_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}; F)$$
.

Side-note: these quantities are also computable

- depth R-package: simplicial, half-space, Oja's depth.
- Ref. (half-space depth): [Dyckerhoff and Mozharovskyi, 2016].

Side-note: these quantities are also computable

- depth R-package: simplicial, half-space, Oja's depth.
- Ref. (half-space depth): [Dyckerhoff and Mozharovskyi, 2016].
- Simplicial depth:

$$\mathbf{x} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i,$$

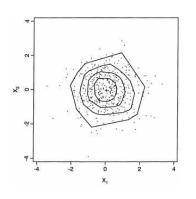
$$\sum_{i=1}^{n} \alpha_i = 1$$

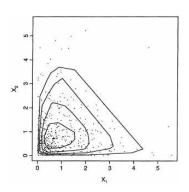
linear equation. If $\alpha_i \geq 0 \ (\forall i) \Rightarrow \text{Yes}$.

Example: SD – depth-induced contours

normal

exponential





- center-outward ordering.
- high-depth: 'center', low-depth: 'outlyingness'.
- expansion of contours: scale (dispersion), skewness, kurtosis.

• Median/center: deepest point.

- Median/center: deepest point.
- Other robust location statistics:
 - idea: assign smaller weights to more outlier data.
 - ullet given: $oldsymbol{w}:[0,1]
 ightarrow \mathbb{R}^{\geq 0}$ nonincreasing weight function

$$L_{w} = \frac{\sum_{i=1}^{n} \mathbf{x}_{[i]} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

- Median/center: deepest point.
- Other robust location statistics:
 - idea: assign smaller weights to more outlier data.
 - ullet given: ${\it w}:[0,1]
 ightarrow \mathbb{R}^{\geq 0}$ nonincreasing weight function

$$L_{w} = \frac{\sum_{i=1}^{n} \mathbf{x}_{[i]} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

- Specifically:
 - $w(t) = \mathbb{I}(t \le 1/n)$: sample median.
 - $w(t) = \mathbb{I}(t \le 1 \alpha)$: 100 α %-trimmed mean.

- Median/center: deepest point.
- Other robust location statistics:
 - idea: assign smaller weights to more outlier data.
 - ullet given: $oldsymbol{w}:[0,1]
 ightarrow \mathbb{R}^{\geq 0}$ nonincreasing weight function

$$L_{w} = \frac{\sum_{i=1}^{n} \mathbf{x}_{[i]} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

- Specifically:
 - $w(t) = \mathbb{I}(t \le 1/n)$: sample median.
 - $w(t) = \mathbb{I}(t \le 1 \alpha)$: 100 α %-trimmed mean.

No expectation requirement!

Dispersion, scale

Idea-1: similar to location, the dispersion

$$S = \frac{\sum_{i=1}^{n} (x_{[i]} - x_{[1]}) (x_{[i]} - x_{[1]})^{T} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

Dispersion, scale

Idea-1: similar to location, the dispersion

$$S = \frac{\sum_{i=1}^{n} (x_{[i]} - x_{[1]}) (x_{[i]} - x_{[1]})^{T} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

- Scale: det(S).
- Equivariance under affine tranformations:

$$\mathbf{y}_i = \mathbf{A}\mathbf{x}_i + \mathbf{b} \Rightarrow \mathbf{S}_{\mathbf{y}} = \mathbf{A}\mathbf{S}_{\mathbf{x}}\mathbf{A}^T.$$

Dispersion, scale

Idea-1: similar to location, the dispersion

$$S = \frac{\sum_{i=1}^{n} (x_{[i]} - x_{[1]}) (x_{[i]} - x_{[1]})^{T} w(i/n)}{\sum_{j=1}^{n} w(j/n)}.$$

- Scale: det(S).
- Equivariance under affine tranformations:

$$\mathbf{y}_i = \mathbf{A}\mathbf{x}_i + \mathbf{b} \Rightarrow \mathbf{S}_{\mathbf{y}} = \mathbf{A}\mathbf{S}_{\mathbf{x}}\mathbf{A}^T.$$

No moment constraints!

Dispersion: idea-2

Idea

Dispersion := speed how the data depth decreases.

• p-th (empirical) central region:

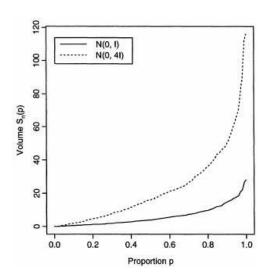
$$C_{n,p} := conv \left\{ \mathbf{x}_{[1]}, \ldots, \mathbf{x}_{[np]} \right\}.$$

scale curve:

$$S_n(p) := vol(C_{n,p}).$$

faster growing of $p \mapsto S_n(p) = \text{larger scale of the distribution}$.

Scale curve example



Skewness: departure from spherical symmetry

• Spherical symmetry around **c**:

$$X - \mathbf{c} = \mathbf{U}(X - \mathbf{c}), \forall \mathbf{U}$$
: orthogonal.

Skewness: departure from spherical symmetry

Spherical symmetry around c:

$$X - \mathbf{c} = \mathbf{U}(X - \mathbf{c}), \forall \mathbf{U}$$
: orthogonal.

- Strategy:
 - take the smallest sphere containing $C_{n,p}$,
 - determine the fraction of the data within this sphere,
 - plot it as function of $p \ (\geq p)$.

Skewness: departure from spherical symmetry

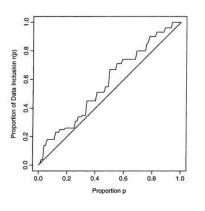
Spherical symmetry around c:

$$X - \mathbf{c} = \mathbf{U}(X - \mathbf{c}), \forall \mathbf{U}$$
: orthogonal.

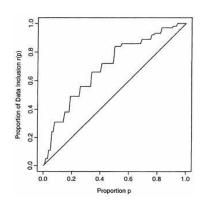
- Strategy:
 - take the smallest sphere containing $C_{n,p}$,
 - determine the fraction of the data within this sphere,
 - plot it as function of $p \ (\geq p)$.
- Sperical symmetry \Leftrightarrow $(0,0) \to (1,1)$ linear curve, i.e. area of the gap =0.

Spherical symmetric/skewed: demo

Spherical (area
$$= 0.08$$
)



Asymmetric (area = 0.2)



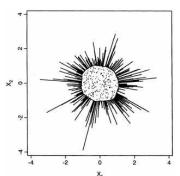
Sunburst plot

Sunburst plot = '2D boxplot'

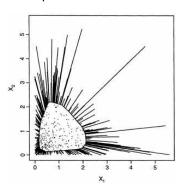
For a given depth function:

- identify the center,
- central 50% points (↔ IQR),
- ray from non-central points to center (\leftrightarrow whiskers).

normal



exponential



Testing

$$X \in \mathbb{R}^d$$
 is

• centrally symmetric around \mathbf{c} : $X - \mathbf{c} \stackrel{\textit{distr}}{=} \mathbf{c} - X$.

$$X \in \mathbb{R}^d$$
 is

- centrally symmetric around \mathbf{c} : $X \mathbf{c} \stackrel{distr}{=} \mathbf{c} X$.
- angularly symmetric around **c**: $\frac{X-c}{\|X-c\|_2}$ is C-sym. around **0**.

$$X \in \mathbb{R}^d$$
 is

- centrally symmetric around **c**: $X \mathbf{c} \stackrel{distr}{=} \mathbf{c} X$.
- angularly symmetric around **c**: $\frac{X-c}{\|X-c\|_2}$ is C-sym. around **0**.
- half-space symmetric around \mathbf{c} : $P(X \in H) \ge \frac{1}{2}$, for $\forall H \ni \mathbf{c}$, closed half-space.

$X \in \mathbb{R}^d$ is

- centrally symmetric around **c**: $X \mathbf{c} \stackrel{distr}{=} \mathbf{c} X$.
- angularly symmetric around **c**: $\frac{X-c}{\|X-c\|_2}$ is C-sym. around **0**.
- half-space symmetric around \mathbf{c} : $P(X \in H) \ge \frac{1}{2}$, for $\forall H \ni \mathbf{c}$, closed half-space.

Note:

- C-symmetry \Rightarrow A-symmetry \Rightarrow H-symmetry.
- d = 1: all = standard symmetry.

Testing: A-symmetry – idea

- SD is maximized at the center of symmetry, $=\frac{1}{2^d}$.
- F: absolutely continuous, $SD(\mathbf{c}^*; F) \leq \frac{1}{2^d}$, '=' $\Leftrightarrow F$: A-sym. around \mathbf{c}^* .

Testing: A-symmetry – idea

- SD is maximized at the center of symmetry, $=\frac{1}{2^d}$.
- F: absolutely continuous, $SD(\mathbf{c}^*; F) \leq \frac{1}{2^d}$, '=' $\Leftrightarrow F$: A-sym. around \mathbf{c}^* .
- c: hypothesized center.
- Decision: if $\frac{1}{2^d} SD(\mathbf{c}; F_n)$ is large \Rightarrow reject H_0 .

Testing: A-symmetry – idea

- SD is maximized at the center of symmetry, $=\frac{1}{2^d}$.
- F: absolutely continuous, $SD(\mathbf{c}^*; F) \leq \frac{1}{2^d}$, '=' $\Leftrightarrow F$: A-sym. around \mathbf{c}^* .
- c: hypothesized center.
- Decision: if $\frac{1}{2^d} SD(\mathbf{c}; F_n)$ is large \Rightarrow reject H_0 .
- Under the hood:
 - $\frac{1}{2^d} SD(\mathbf{c}; F_n)$: degenerate U-statistic,
 - $n\left[\frac{1}{2^d} SD(\mathbf{c}; F_n)\right] \to \infty$ -sum of χ^2 -s.

Depth function properties

 \mathcal{F} :=Borel probability measures on \mathbb{R}^d . $D(\cdot;\cdot): \mathbb{R}^d \times \mathcal{F} \to \mathbb{R}^{\geq 0}$ bounded, \bullet affine invariance:

$$D(\mathbf{A}\mathbf{x} + \mathbf{b}; F_{\mathbf{A}X + \mathbf{b}}) = D(\mathbf{x}; F_X) \ \forall \mathbf{A} : \text{invertible}, \mathbf{b}, X.$$

 $\mathfrak{F}:=$ Borel probability measures on \mathbb{R}^d . $D(\cdot;\cdot):\mathbb{R}^d\times\mathfrak{F}\to\mathbb{R}^{\geq 0}$ bounded,

affine invariance:

$$D(\mathbf{A}\mathbf{x} + \mathbf{b}; F_{\mathbf{A}X + \mathbf{b}}) = D(\mathbf{x}; F_X) \ \forall \mathbf{A} : \text{invertible}, \mathbf{b}, X.$$

maximality at center: For F with center c,

$$D(\mathbf{c}; F) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}; F).$$

 $\mathfrak{F}:=$ Borel probability measures on \mathbb{R}^d . $D(\cdot;\cdot):\mathbb{R}^d\times\mathfrak{F}\to\mathbb{R}^{\geq 0}$ bounded,

affine invariance:

$$D(\mathbf{A}\mathbf{x} + \mathbf{b}; F_{\mathbf{A}X + \mathbf{b}}) = D(\mathbf{x}; F_X) \ \forall \mathbf{A} : \text{invertible}, \mathbf{b}, X.$$

② maximality at center: For F with center c,

$$D(\mathbf{c}; F) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}; F).$$

9 monotonicity relative to the deepest point: For $\forall F$ with deepest point \mathbf{c} ,

$$D(\mathbf{x}; F) \leq D(\alpha \mathbf{x} + (1 - \alpha)\mathbf{c}; F), \forall \alpha \in [0, 1].$$

 $\mathfrak{F}:=$ Borel probability measures on \mathbb{R}^d . $D(\cdot;\cdot):\mathbb{R}^d\times\mathfrak{F}\to\mathbb{R}^{\geq 0}$ bounded,

affine invariance:

$$D(\mathbf{A}\mathbf{x} + \mathbf{b}; F_{\mathbf{A}X + \mathbf{b}}) = D(\mathbf{x}; F_X) \ \forall \mathbf{A} : \text{invertible}, \mathbf{b}, X.$$

② maximality at center: For F with center c,

$$D(\mathbf{c}; F) = \sup_{\mathbf{x} \in \mathbb{R}^d} D(\mathbf{x}; F).$$

9 monotonicity relative to the deepest point: For $\forall F$ with deepest point \mathbf{c} ,

$$D(\mathbf{x}; F) \leq D(\alpha \mathbf{x} + (1 - \alpha)\mathbf{c}; F), \forall \alpha \in [0, 1].$$

vanishing at infinity:

$$D(\mathbf{x}; F) \xrightarrow{\|\mathbf{x}\| \to \infty} 0, \forall F.$$



Categorization of depth functions [Zuo and Serfling, 2000]

Vanishing at infinity: useful for establishing

$$\sup_{\mathbf{x}} |D(\mathbf{x}; F_n) - D(\mathbf{x}; F)| \xrightarrow{n \to \infty} 0 \text{ (F-a.s.)}.$$

Categorization of depth functions [Zuo and Serfling, 2000]

- Properties of HD and SD:
 - half-space (HD): 1-4 √ (H-sym.)
 - simplicial (SD):
 - continuous distributions: 1-4 √ (A-sym.)
 - discrete: 2/3 might fail.

Types

$$D_{A}(\mathbf{x}; F) = \mathbb{E}_{F} \left[h_{A}(\mathbf{x}; X_{1}; \dots; X_{r}) \right] \xrightarrow{\text{example}} SD,$$

$$D_{B}(\mathbf{x}; F) = \frac{1}{1 + \mathbb{E}_{F} \left[h_{B}(\mathbf{x}; X_{1}; \dots; X_{r}) \right]},$$

$$D_{C}(\mathbf{x}; F) = \frac{1}{1 + O(\mathbf{x}; F)},$$

$$D_{D}(\mathbf{x}; F) = \inf_{\mathbf{x} \in C \in \mathcal{C}} \mathbb{P}_{F}(X \in C) \xrightarrow{\text{example}} HD.$$

- $h_A(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_r)$: bounded, closeness of \mathbf{x} to \mathbf{x}_i -s.
- $h_B(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_r)$: unbounded, distance of \mathbf{x} from \mathbf{x}_i -s.
- O(x; F): unbounded outlyingness function.
- C: closedness properties.

Types

$$D_{A}(\mathbf{x}; F) = \mathbb{E}_{F} [h_{A}(\mathbf{x}; X_{1}; \dots; X_{r})] \xrightarrow{\text{example}} SD,$$

$$D_{B}(\mathbf{x}; F) = \frac{1}{1 + \mathbb{E}_{F} [h_{B}(\mathbf{x}; X_{1}; \dots; X_{r})]},$$

$$D_{C}(\mathbf{x}; F) = \frac{1}{1 + O(\mathbf{x}; F)},$$

$$D_{D}(\mathbf{x}; F) = \inf_{\mathbf{x} \in C \in \mathcal{C}} \mathbb{P}_{F}(X \in C) \xrightarrow{\text{example}} HD.$$

- $h_A(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_r)$: bounded, closeness of \mathbf{x} to \mathbf{x}_i -s.
- $h_B(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_r)$: unbounded, distance of \mathbf{x} from \mathbf{x}_i -s.
- O(x; F): unbounded outlyingness function.
- C: closedness properties.

Note: $D_A(\mathbf{x}; F_n)$: U/V-statistic.

Type B examples

Let $\Sigma = cov(F)$. In simplicial volume depth $(D_{SVD^{\alpha}})$, $D_{\tilde{L^2}}$:

$$h(\mathbf{x}; \mathbf{x}_1, \dots, \mathbf{x}_d) = \left(\frac{vol[\Delta(\mathbf{x}, \mathbf{x}_1, \dots, \mathbf{x}_d)]}{\sqrt{\det(\Sigma)}}\right)^{\alpha}, \alpha > 0,$$
$$h(\mathbf{x}; \mathbf{x}_1) = \|\mathbf{x} - \mathbf{x}_1\|_{\Sigma^{-1}}, \ \|\mathbf{z}\|_{\mathbf{M}} = \sqrt{\mathbf{z}^T \mathbf{M} \mathbf{z}}.$$

Properties:

- D_{SVD}α: 1-4 √ (C-sym.),
- $D_{\tilde{L}^2}$: 1-4 \checkmark (A-sym.).

Type C example

Projection depth: worst case outlyingness w.r.t. 1d-median, for any 1d projection.

$$O(\mathbf{x}; F) = \sup_{\|\mathbf{u}\|_{2}=1} \frac{\left|\mathbf{u}^{T}\mathbf{x} - med(\mathbf{u}^{T}X)\right|}{MAD(\mathbf{u}^{T}X)}, X \sim F,$$

$$MAD(Y) = med(|Y - med(Y)|).$$

Properties: 1-4 ✓ (H-sym.)

Summary

- Depth functions: simplicial, half-space, ...
- They define: center-outward ordering, ranks, ⇒
- L-statistics, symmetry test.
- location (median,...), dispersion, scale, skewness, kurtosis (no moments),
- sunburst plot.

Thank you for the attention!



Dyckerhoff, R. and Mozharovskyi, P. (2016). Exact computation of the halfspace depth. Technical report, University of Cologne. http://arxiv.org/abs/1411.6927.

Liu, R. (1990).
On a notion of data depth based on random simplices.

The Annals of Statistics. 18:405–414.

Tukey, J. (1975).

Mathematics and picturing data.

In *International Congress on Mathematics*, pages 523–531.

Zuo, B. Y. and Serfling, R. (2000). General notions of statistical depth function. The Annals of Statistics, 28:461–482.