Robust estimation of principal components from depth-based multivariate rank covariance matrix

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Summary

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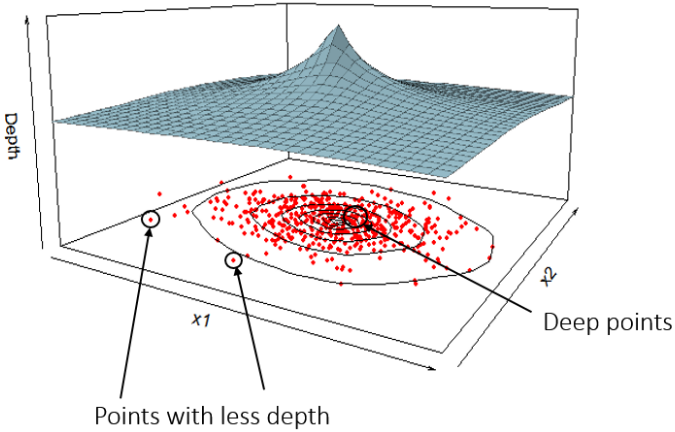
What is depth?

Example: 500 points from $\mathcal{N}_2((0,0)^T, \text{diag}(2,1))$



A scalar measure of how much inside a point is with respect to a data cloud

Formal definition

For any multivariate distribution $F = F_{\mathbf{X}}$, the depth of a point $\mathbf{x} \in \mathbb{R}^p$, say $D(\mathbf{x}, F_{\mathbf{X}})$ is any real-valued function that provides a 'center outward ordering' of $\mathbf{x}$ with respect to F (Zuo and Serfling, 2000).

Desirable properties (Liu, 1990)

(P1) *Affine invariance*: $D(A\mathbf{x} + \mathbf{b}, F_{A\mathbf{X}+\mathbf{b}}) = D(\mathbf{x}, F_{\mathbf{X}})$

(P2) *Maximality at center*: $D(\theta, F_{\mathbf{X}}) = \sup_{\mathbf{x}\in\mathbb{R}^p} D(\mathbf{x}, F_{\mathbf{X}})$ for $F_{\mathbf{X}}$ with center of symmetry θ, the *deepest point* of $F_{\mathbf{X}}$.

(P3) *Monotonicity w.r.t. deepest point*: $D(\mathbf{x}; F_{\mathbf{X}}) \leq D(\theta + a(\mathbf{x} - \theta), F_{\mathbf{X}})$

(P4) *Vanishing at infinity*: $D(\mathbf{x}; F_{\mathbf{X}}) \to \mathbf{0}$ as $\|\mathbf{x}\| \to \infty$.

- **Halfspace depth** (HD) (Tukey, 1975) is the minimum probability of all halfspaces containing a point.

$$HD(\mathbf{x}, F) = \inf_{\mathbf{u} \in \mathbb{R}^p; \mathbf{u} \neq \mathbf{0}} P(\mathbf{u}^T \mathbf{X} \geq \mathbf{u}^T \mathbf{x})$$

- **Projection depth** (PD) (Zuo, 2003) is based on an outlyingness function:

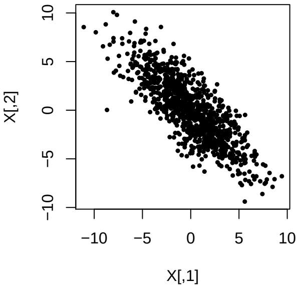
$$O(\mathbf{x}, F) = \sup_{\|\mathbf{u}\|=1} \frac{|\mathbf{u}^T \mathbf{x} - m(\mathbf{u}^T \mathbf{X})|}{s(\mathbf{u}^T \mathbf{X})}; \quad PD(\mathbf{x}, F) = \frac{1}{1 + O(\mathbf{x}, F)}$$

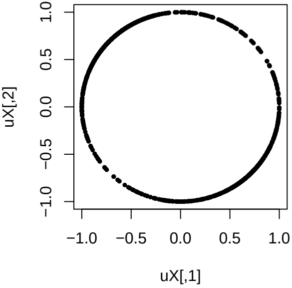
Robustness

- **Classification**
- Depth-weighted means and covariance matrices
- What we're going to do:
  Define multivariate rank vectors based on data depth, do PCA on them

$$\mathbf{S}(\mathbf{x}) = \begin{cases} \mathbf{x}\|\mathbf{x}\|^{-1} & \text{if } \mathbf{x} \neq \mathbf{0} \\ \mathbf{0} & \text{if } \mathbf{x} = \mathbf{0} \end{cases}$$

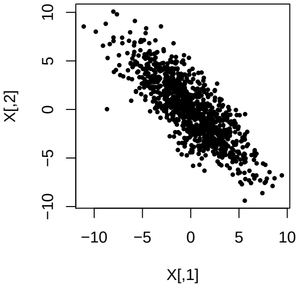
- Say $\mathbf{x}$ follows an elliptic distribution with mean μ, covariance matrix Σ.
- Sign covariance matrix (SCM): $\Sigma_S(\mathbf{X}) = E\mathbf{S}(\mathbf{X} - \mu)\mathbf{S}(\mathbf{X} - \mu)^T$
- SCM has same eigenvectors as Σ. PCA using SCM is robust, but not efficient.

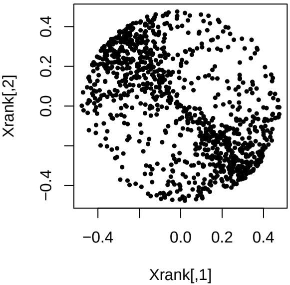




Spatial ranks

- Fix a depth function $D(\mathbf{x}, F) = D_\mathbf{X}(\mathbf{x})$. Define $\tilde{D}_\mathbf{X}(\mathbf{x}) = \sup_{\mathbf{x} \in \mathbb{R}^p} D_\mathbf{X}(\mathbf{x}) - D_\mathbf{X}(\mathbf{x})$
- Transform the original observation: $\tilde{\mathbf{x}} = \tilde{D}_\mathbf{X}(\mathbf{x}) \mathbf{S}(\mathbf{x} - \mu)$. This is the *Spatial Rank* of $\mathbf{x}$.
- Depth Covariance Matrix (DCM) = $Cov(\tilde{\mathbf{X}})$. Has more information than spatial signs, so more efficient.





Form of DCM

Theorem (1)

Let the random variable $\mathbf{X} \in \mathbb{R}^p$ *follow an elliptical distribution with center* $\boldsymbol{\mu}$ *and covariance matrix* $\Sigma = \Gamma\Lambda\Gamma^T$*, its spectral decomposition. Then, given a depth function* $D_{\mathbf{X}}(.)$ *the covariance matrix of the transformed random variable* $\tilde{\mathbf{X}}$ *is*

$$Cov(\tilde{\mathbf{X}}) = \Gamma\Lambda_{D,S}\Gamma^T, \quad with \quad \Lambda_{D,S} = E\left[(\tilde{D}_{\mathbf{Z}}(\mathbf{z}))^2 \frac{\Lambda^{1/2}\mathbf{z}\mathbf{z}^T\Lambda^{1/2}}{\mathbf{z}^T\Lambda\mathbf{z}}\right] \tag{1}$$

where $\mathbf{z} = (z_1, ..., z_p)^T \sim N(\mathbf{0}, I_p)$ *and* $\Lambda_{D,S}$ *a diagonal matrix with diagonal entries*

$$\lambda_{D,S,i} = E_{\mathbf{Z}}\left[\frac{(\tilde{D}_{\mathbf{Z}}(\mathbf{z}))^2\lambda_i z_i^2}{\sum_{j=1}^p \lambda_j z_j^2}\right]$$

TL; DR: Population eigenvectors are invariant under the spatial rank transformation.

Other results

- Asymptotic distribution of sample DCM, form of its asymptotic variance
- Asymptotic joint distribution of eigenvectors and eigenvalues of sample DCM
- Form and shape of influence function: a measure of robustness
- Asymptotic efficiency relative to sample covariance matrix

- 6 elliptical distributions: p-variate normal and t- distributions with df = 5, 6, 10, 15, 25.
- All distributions centered at $\mathbf{0}_p$, and have covariance matrix $\Sigma = \text{diag}(p, p-1, ...1)$.
- 3 choices of p: 2, 3 and 4.
- 10000 samples each for sample sizes $n = 20, 50, 100, 300, 500$
- For estimates $\hat{\gamma}_1$ of the first eigenvector $\hat{\gamma}_1$, prediction error is measured by the average smallest angle between the two lines, i.e. **Mean Squared Prediction Angle**:

$$MSPA(\hat{\gamma}_1) = \frac{1}{10000} \sum_{m=1}^{10000} \left(\cos^{-1} \left| \gamma_1^T \hat{\gamma}_1^{(m)} \right| \right)^2$$

Finite sample efficiency of some eigenvector estimate $\hat{\gamma}_1^E$ relative to that obtained from the sample covariance matrix, say $\hat{\gamma}_1^{Cov}$ is:

$$FSE(\hat{\gamma}_1^E, \hat{\gamma}_1^{Cov}) = \frac{MSPA(\hat{\gamma}_1^{Cov})}{MSPA(\hat{\gamma}_1^E)}$$

Table of FSE for $p = 2$

(HSD = Halfspace depth, MhD = Mahalanobis depth, PD = Projection depth)

F = Bivariate t_5	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.80	0.95	0.95	0.89
n=50	0.86	1.25	1.10	1.21
n=100	1.02	1.58	1.20	1.54
n=300	1.24	1.81	1.36	1.82
n=500	1.25	1.80	1.33	1.84
F = Bivariate t_6	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.77	0.92	0.92	0.86
n=50	0.76	1.11	1.00	1.08
n=100	0.78	1.27	1.06	1.33
n=300	0.88	1.29	1.09	1.35
n=500	0.93	1.37	1.13	1.40
F = Bivariate t_{10}	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.70	0.83	0.84	0.77
n=50	0.58	0.90	0.84	0.86
n=100	0.57	0.92	0.87	0.97
n=300	0.62	0.93	0.85	0.99
n=500	0.62	0.93	0.86	1.00

Table of FSE for $p = 2$

(HSD = Halfspace depth, MhD = Mahalanobis depth, PD = Projection depth)

F = Bivariate t_{15}	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.63	0.76	0.78	0.72
n=50	0.52	0.79	0.75	0.80
n=100	0.51	0.83	0.77	0.88
n=300	0.55	0.84	0.79	0.91
n=500	0.56	0.85	0.80	0.93
F = Bivariate t_{25}	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.63	0.77	0.79	0.74
n=50	0.49	0.73	0.71	0.76
n=100	0.45	0.73	0.69	0.81
n=300	0.51	0.78	0.75	0.87
n=500	0.53	0.79	0.75	0.87
F = BVN	SCM	HSD-CM	MhD-CM	PD-CM
n=20	0.56	0.69	0.71	0.67
n=50	0.42	0.66	0.66	0.70
n=100	0.42	0.69	0.66	0.77
n=300	0.47	0.71	0.69	0.82
n=500	0.48	0.73	0.71	0.83

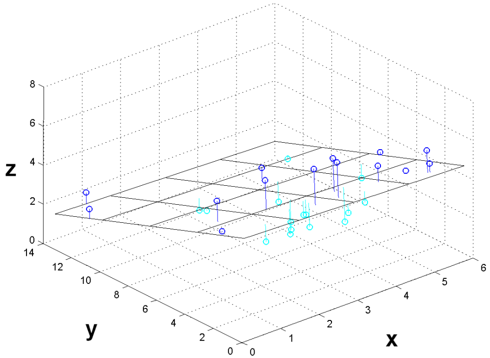
- Features extracted from images of 213 buses: 18 variables
- Methods compared:

  Classical PCA (CPCA)
  SCM PCA (SPCA)
  ROBPCA (Hubert et al., 2005)
  PCA based on MCD (MPCA)
  PCA based on projection-DCM (DPCA)

Score distance (SD) and orthogonal distance (OD)

$$SD_i = \sqrt{\sum_{j=1}^{k} \frac{s_{ij}^2}{\lambda_j}}; \quad OD_i = \|\mathbf{x}_i - P\mathbf{s}_i^T\|$$

where $S_{n \times k} = (\mathbf{s}_1, \ldots, \mathbf{s}_n)^T$ is the scoring matrix, $P_{p \times k}$ loading matrix, $\lambda_1, \ldots, \lambda_k$ are eigenvalues obtained from the PCA, and $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are the observation vectors.

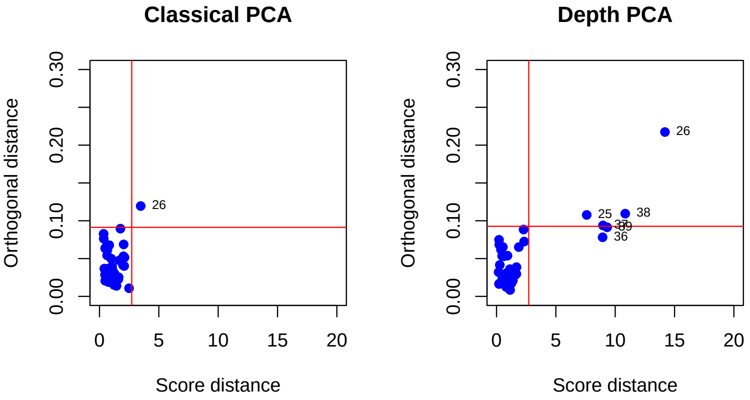


Quantile	Method of PCA				
	CPCA	SPCA	ROBPCA	MPCA	DPCA
10%	1.9	1.2	1.2	1.0	**1.2**
20%	2.3	1.6	1.6	1.3	**1.6**
30%	2.8	1.8	1.8	1.7	**1.9**
40%	3.2	2.2	2.1	2.1	**2.3**
50%	3.7	2.6	2.5	3.1	**2.6**
60%	4.4	3.1	3.0	5.9	**3.2**
70%	5.4	3.8	3.9	25.1	**3.9**
80%	6.5	5.2	4.8	86.1	**4.8**
90%	8.2	9.0	10.9	298.2	**6.9**
Max	24	1037	1055	1037	980

- Table lists quantiles of the squared orthogonal distance for a sample point from the hyperplane formed by top 3 PCs,
- For DPCA, more than 90% of points have a smaller orthogonal distance than CPCA

Data analysis: Octane data

- 226 variables and 39 observations. Each observation is a gasoline sample with a certain octane number, and have their NIR absorbance spectra measured in 2 nm intervals between 1100 - 1550 nm.
- 6 outliers: compounds 25, 26 and 36-39, which contain alcohol.



Extensions: Robust kernel PCA

- 20 points from each person. Noise added to one image from each person.
- Columns due to kernel CPCA, SPCA and DPCA, respectively. Rows due to top 2, 4, 6, 8 or 10 PCs considered.

Extensions: future work

- Explore properties of a depth-weighted M-estimator of scale matrix:

$$\Sigma_{Dw} = E\left[\frac{(\tilde{D}_{\mathbf{X}}(\mathbf{x}))^2(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^T}{(\mathbf{x}-\boldsymbol{\mu})^T\Sigma_{Dw}^{-1}(\mathbf{x}-\boldsymbol{\mu})}\right]$$

- Leverage the idea of depth based ranks: robust non-parametric testing
- Extending to high-dimensional and functional data

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THANK YOU!