

Unsupervised linear discrimination using skewness

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Reference

This talk is based on the papers

- **Radojčić, U., Nordhausen, K. and Virta, J. (2025).**
Unsupervised linear discrimination using skewness. Accepted for publication in *Journal of Multivariate Analysis*.
- **Radojčić, U., Nordhausen, K. and Virta, J. (2021).**
Large-sample properties of unsupervised estimation of the linear discriminant using projection pursuit. *Electronic Journal of Statistics*, 15(2), 6677-6739.

These slides are available at the speaker's website
<https://users.utu.fi/jomivi/talks/>

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Normal mixture

Our model

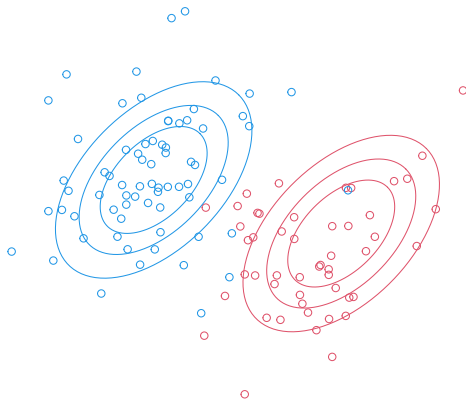
Let $X_1, \dots, X_n \in \mathbb{R}^p$ be a random sample from the normal location mixture,

$$X \sim \alpha_1 \mathcal{N}(\mu_1, \Sigma) + \alpha_2 \mathcal{N}(\mu_2, \Sigma),$$

where

- $\alpha_1, \alpha_2 \in (0, 1), \alpha_1 + \alpha_2 = 1,$
- $\mu_1 \neq \mu_2,$
- Σ is positive definite.

Illustration



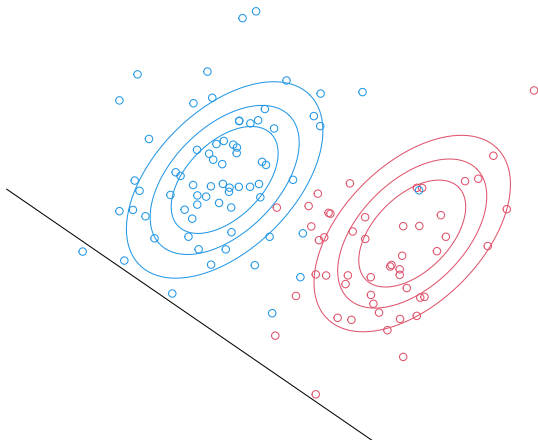
Separating projections

- We are interested in vectors $\theta \in \mathbb{R}^p$ such that the projection of the data

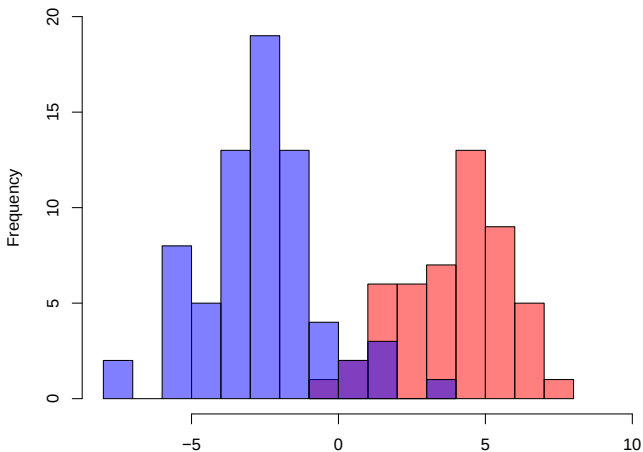
$$X \mapsto \theta' X$$

onto θ separates the two groups of the mixture

Illustration



The projection



Fisher's linear discriminant

- The projection direction on the previous slide is

$$\theta = \Sigma^{-1}(\mu_2 - \mu_1).$$

- This projection is used in **linear discriminant analysis** (LDA) and it leads to the Bayes optimal classifier under Gaussianity.

Sample estimator and asymptotic normality

- The sample LDA-estimator $\hat{\theta}$ is simple to compute given the sample $X_1, \dots, X_n$ and the labels $Y_1, \dots, Y_n$.
- $\hat{\theta}$ satisfies

$$\sqrt{n} \left(\frac{\hat{\theta}}{\|\hat{\theta}\|} - \frac{\theta}{\|\theta\|} \right) \rightsquigarrow \mathcal{N}_p(0, \Psi),$$

where

$$\Psi := \left(\frac{1 + \alpha_1 \alpha_2 \theta' \Sigma \theta}{\|\theta\|^2 \alpha_1 \alpha_2} \right) \left(I_p - \frac{\theta \theta'}{\|\theta\|^2} \right) \Sigma^{-1} \left(I_p - \frac{\theta \theta'}{\|\theta\|^2} \right).$$

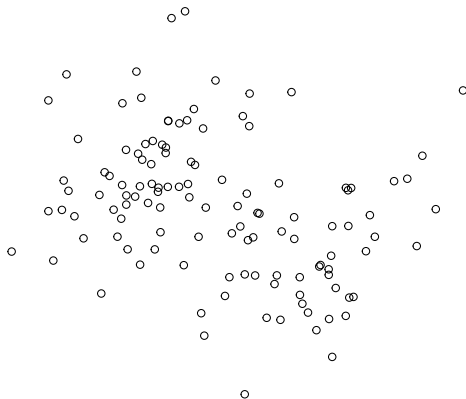
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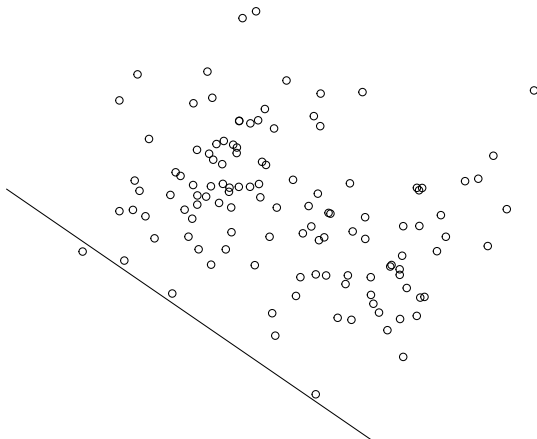
From classification to clustering

- The estimator $\hat{\theta}$ allows classification when (X_i, Y_i) are known.
- However, θ can be estimated also without the group labels $Y_i!$ [Peña and Prieto, 2001]
- This lets us use the projection $\theta'X_i$ for clustering.

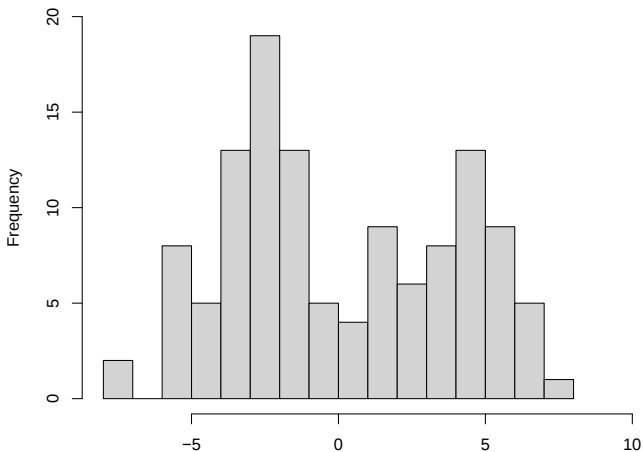
Unknown groups



Unknown groups



Histogram of the projection



Projection pursuit

- In projection pursuit [Huber, 1985], one chooses a projection index g which measures how “interesting” a random variable is and optimizes

$$\max_{\theta_0} g(\theta'_0 X).$$

- One particular choice is **squared Pearson's skewness**, g_{skew} , which searches for maximally skewed projections,

$$g_{\text{skew}}(\theta'_0 X) = \left\{ \frac{\mathbb{E}[\{\theta'_0 X - \mathbb{E}(\theta'_0 X)\}^3]}{(\mathbb{E}[\{\theta'_0 X - \mathbb{E}(\theta'_0 X)\}^2])^{3/2}} \right\}^2.$$

Skewness and θ

Proposition 1 in [Loperfido, 2013]

For our normal mixture, if $\alpha_1 \neq \alpha_2$, the maximizer θ_{skew} has

$$\frac{\theta_{\text{skew}}}{\|\theta_{\text{skew}}\|} = \frac{\theta}{\|\theta\|}.$$

Theorem 3 in [Radojičić et al., 2021]

Moreover,

$$\sqrt{n} \left(\frac{\hat{\theta}_{\text{skew}}}{\|\hat{\theta}_{\text{skew}}\|} - \frac{\theta}{\|\theta\|} \right) \rightsquigarrow \mathcal{N}_p(0, C\Psi),$$

for some constant $C \equiv C((\mu_2 - \mu_1)' \Sigma^{-1} (\mu_2 - \mu_1), \alpha_1 \alpha_2)$.

Relative efficiencies vs. LDA

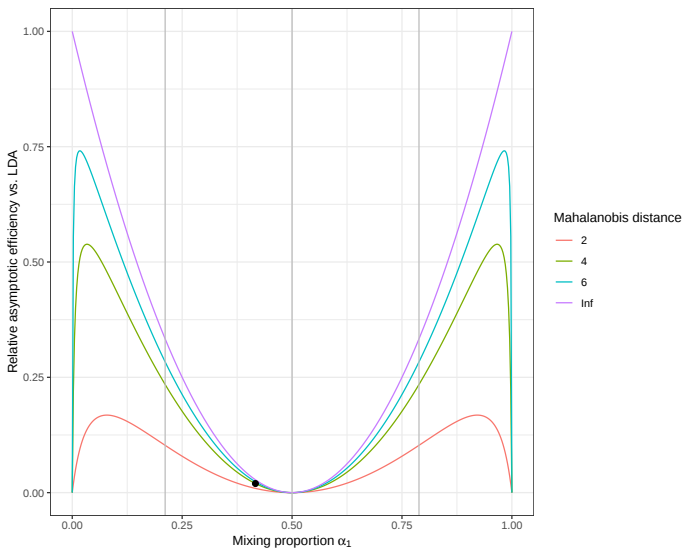


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Affine equivariance

- An estimator $u(X_i) \in \mathbb{R}^p$ is affine equivariant if

$$u(A'X_i + b) = A^{-1}u(X_i)$$

for all $b \in \mathbb{R}^p$ and all invertible $A \in \mathbb{R}^{p \times p}$.

- Projections onto affine equivariant directions are **unaffected by the choice of the coordinate system** of the data,

$$u(A'X_i + b)'(A'X_0 + b) = u(X_i)'X_0 + u(X_i)'(A^{-1})'b.$$

General result

Theorem 5 in [Radojičić et al., 2024]

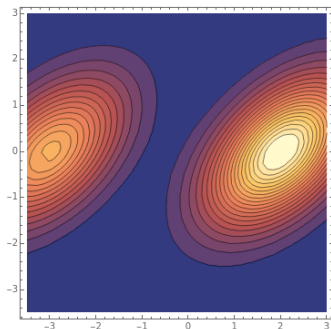
Any affine equivariant estimator of $\theta/\|\theta\|$ has asymptotic covariance matrix proportional to Ψ .

Standardization

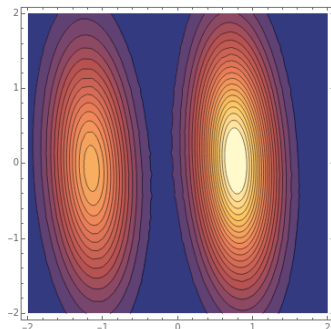
The standardized random vector X_{st} is obtained as

$$X_{\text{st}} = \text{Cov}(X)^{-1/2} \{X - E(X)\}.$$

Illustration



Original data, X



Standardized data, X_{st}

Estimator from Loperfido (2013)

- [Loperfido, 2013] defines the **affine equivariant** estimator $\theta_L = \text{Cov}(X)^{-1/2}u(X)$, where $u(X)$ is the leading unit-length eigenvector of the matrix

$$[E\{(X_{st} \otimes X_{st})X'_{st}\}]'[E\{(X_{st} \otimes X_{st})X'_{st}\}].$$

Proposition 3 in [Loperfido, 2013]

For our normal mixture, if $\alpha_1 \neq \alpha_2$, then

$$\frac{\theta_L}{\|\theta_L\|} = \frac{\theta}{\|\theta\|}.$$

A novel estimator

- [Radojičić et al., 2024] defines the **affine equivariant** estimator $\theta_J = \text{Cov}(X)^{-1/2} u(X)$, where $u(X)$ is the maximizer of

$$\max_{v \in \mathbb{R}^p, \|v\|=1} \sum_{k=1}^p \left\{ v^\top E(X_{\text{st}} X'_{\text{st}} e_k X'_{\text{st}}) v \right\}^2.$$

Lemma 7 in [Radojičić et al., 2024]

For our normal mixture, if $\alpha_1 \neq \alpha_2$, then

$$\frac{\theta_J}{\|\theta_J\|} = \frac{\theta}{\|\theta\|}.$$

Limiting covariance matrices

Theorems 6 and 7 in [Radojičić et al., 2024]

The asymptotic covariance matrices of $\hat{\theta}_J/\|\hat{\theta}_J\|$ and $\hat{\theta}_L/\|\hat{\theta}_L\|$ are exactly the same and equal to that of $\hat{\theta}_{\text{skew}}/\|\hat{\theta}_{\text{skew}}\|$.

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Simulation comparison

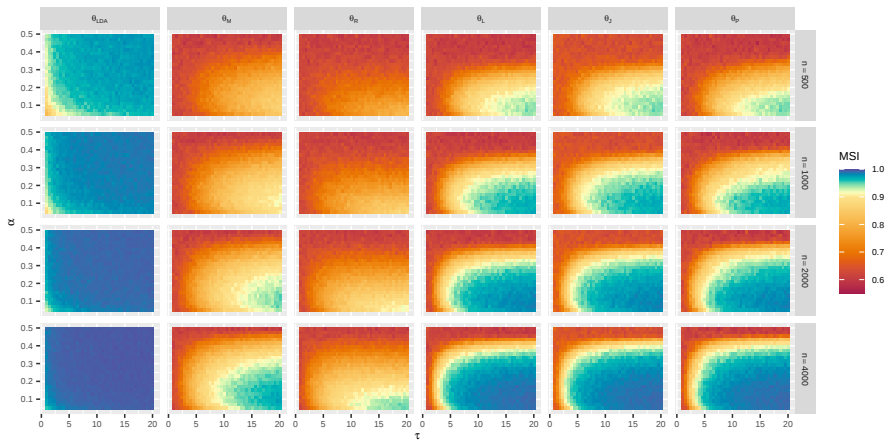


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History of the problem

Kurtosis-based approaches:

- [Peña and Prieto, 2001]
- [Peña et al., 2010]
- [Peña et al., 2017]
- [Radojičić et al., 2021]

Skewness-based approaches:

- [Loperfido, 2013]
- [Loperfido, 2015]
- [Radojičić et al., 2021]
- [Radojičić et al., 2024]

Future directions

- Analogous study for kurtosis would allow discarding the assumption that $\alpha_1 \neq \alpha_2$.
- Going beyond Gaussianity?
- Unequal covariance matrices?
- Multiple groups?
- High-dimensional variants?

Thank you for your attention!

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Projection pursuit.
Annals of Statistics, 13:435–475.



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Skewness and the linear discriminant function.
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Submitted.