Unsupervised linear discrimination using skewness

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Reference

This talk is based on the papers

- **Radojičić, U., Nordhausen, K. and Virta, J.** (2025). Unsupervised linear discrimination using skewness. Accepted for publication in *Journal of Multivariate Analysis*.
- **Radojičić, 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

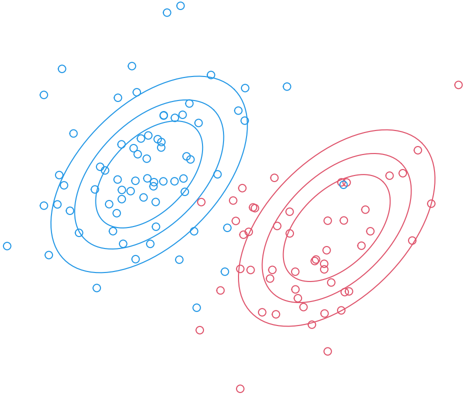
Let $X_1, \ldots, X_n \in \mathbb{R}^p$ be a random sample from the normal location mixture,

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

where

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

Illustration



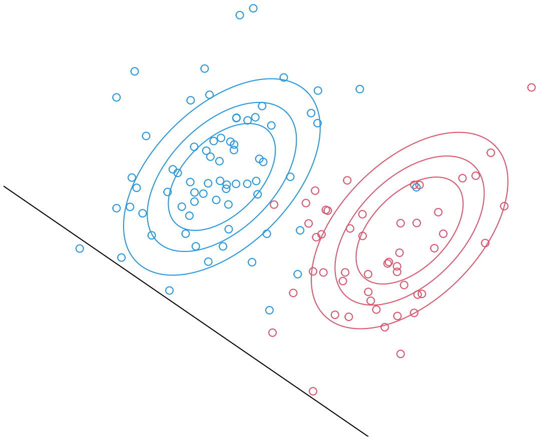
Separating projections

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

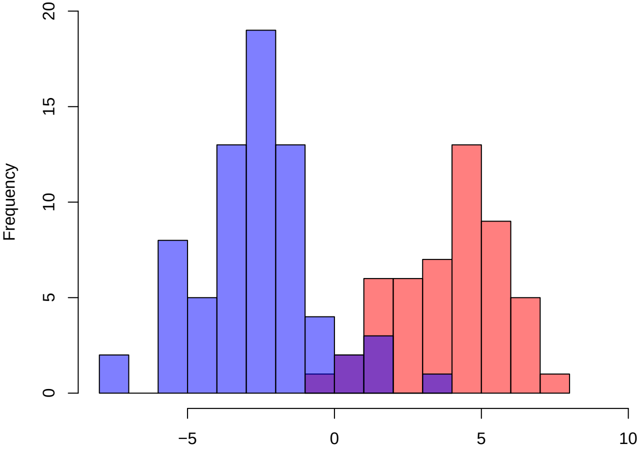
$$X \mapsto \theta' X$$

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 $X_1, \ldots, X_n$ and the labels $Y_1, \ldots, Y_n$.
- $\hat{\theta}$ 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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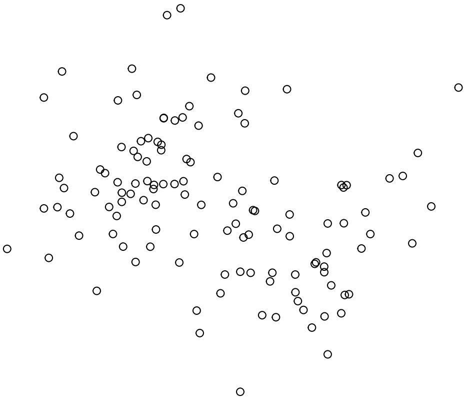
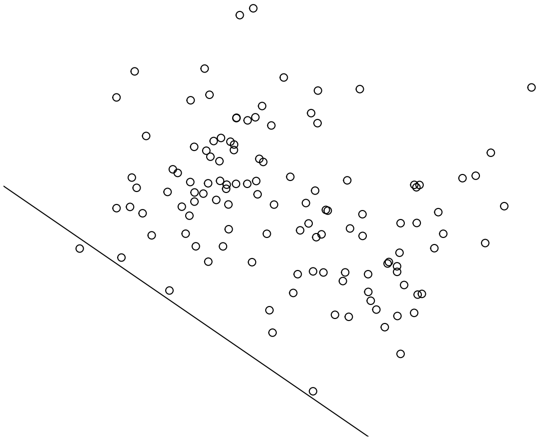
From classification to clustering

- 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.

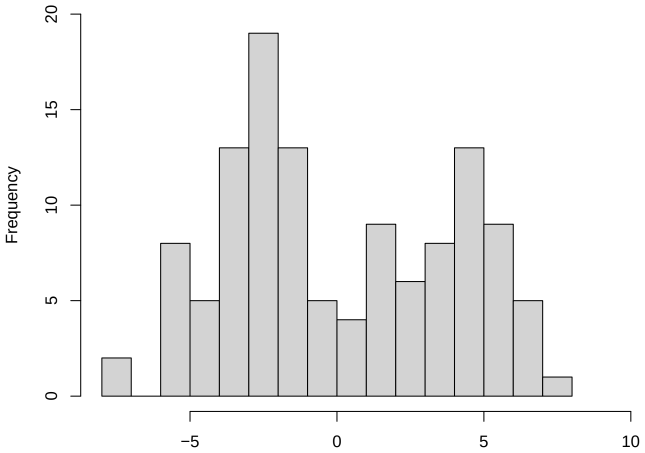
Unknown groups



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,

$$g_{\mathrm{skew}}(\theta_0' X) = \left\{ \frac{\mathrm{E}[\{\theta_0' X - \mathrm{E}(\theta_0' X)\}^3]}{(\mathrm{E}[\{\theta_0' X - \mathrm{E}(\theta_0' X)\}^2])^{3/2}} \right\}^2 .$$

Skewness and θ

Proposition 1 in [Loperfido, 2013]

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

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

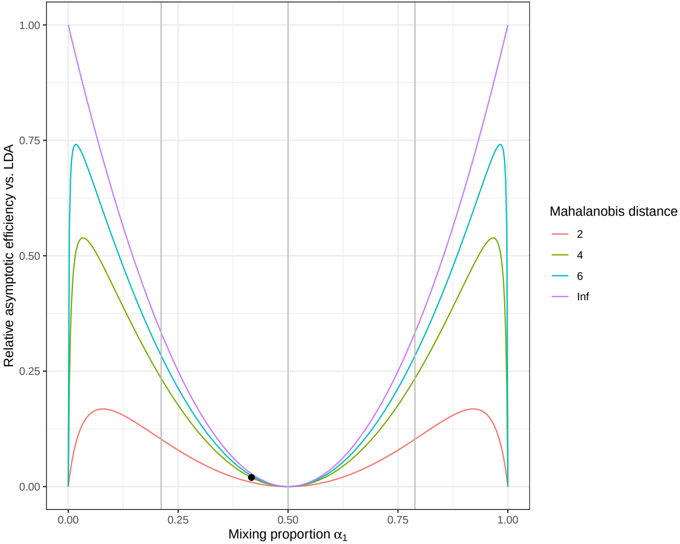
Theorem 3 in [Radojičić et al., 2021]

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., 2025]

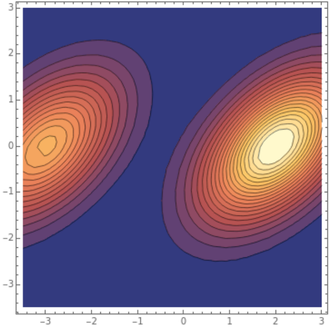
Any affine equivariant estimator of $\theta/\|\theta\|$ has asymptotic covariance matrix proportional to Ψ.

Standardization

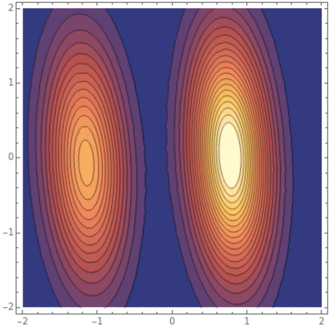
The standardized random vector X_{st} is obtained as

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

Illustration



Original data, X



Stndardized data, X_{st}

Estimator from Loperfido (2013)

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

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

Proposition 3 in [Loperfido, 2013]

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

$$\frac{\theta_{\mathrm{L}}}{\|\theta_{\mathrm{L}}\|} = \frac{\theta}{\|\theta\|}.$$

A novel estimator

- [Radojičić et al., 2025] defines the affine equivariant estimator $\theta_{\mathrm{J}} = \mathrm{Cov}(X)^{-1/2} u(X)$, where $u(X)$ is the maximizer of

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

Lemma 7 in [Radojičić et al., 2025]

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

$$\frac{\theta_{\mathrm{J}}}{\|\theta_{\mathrm{J}}\|} = \frac{\theta}{\|\theta\|}.$$

Limiting covariance matrices

Theorems 6 and 7 in [Radojičić et al., 2025]

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

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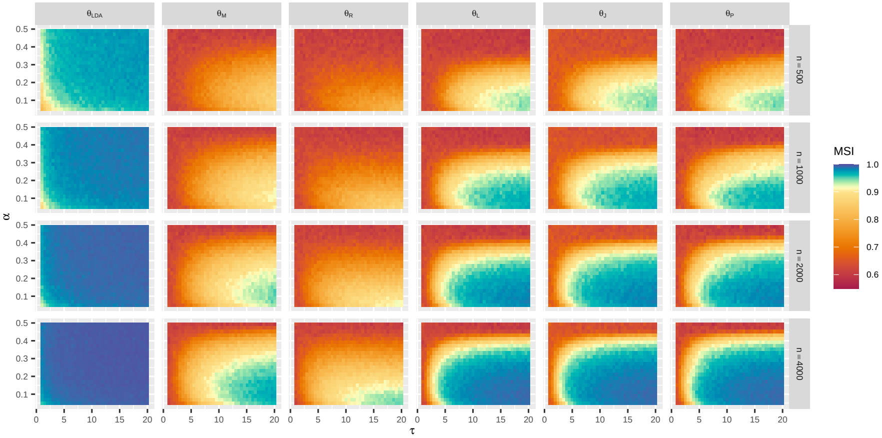
Simulation comparison



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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., 2025]

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!

References I

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