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▶ To cite this version:

Paul-Gauthier Noé, Andreas Nautsch, Driss Matrouf, Pierre-Michel Bousquet, Jean-François Bonastre Overview. Compositional discriminant analysis through calibrated evidence functions. The 10th International Workshop on Compositional Data Analysis (CoDaWork2024), Jun 2024, Girona, Catalonia, Spain. hal-04625713

HAL Id: hal-04625713 https://hal.science/hal-04625713v1

Submitted on 26 Jun 2024

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Compositional discriminant analysis through calibrated evidence functions



Paul-Gauthier Noé, Andreas Nautsch, Driss Matrouf, Pierre-Michel Bousquet and Jean-François Bonastre

Overview

Compositional discriminant analysis is a non-linear discriminant function where the discriminant components form a calibrated isometric-log-ratio transformed likelihood function over the set of classes. The latter can be called evidence function and can be seen as a multiclass extension of the weight-of-evidence in Bayesian updating. The compositional nature of the approach is on the treatment of the likelihood function (not on the modelled data) allowing a novel analysis method.

Bayesian updating on the Aitchison simplex [1]

Considering a set of classes $C = \{c_i\}_{1 \le i \le N}$ and an individual who wants to infer the class of an observation x, its posterior probabilities are given by:

$$P(x) = w(x) \oplus \pi$$
, $\iff \operatorname{ilr} P(x) = \underbrace{\operatorname{ilr} w(x)}_{\text{Evidence function}} + \operatorname{ilr} \pi$,

where $\mathbf{P}(x) = [P(c_i \mid x)]_{1 \leq i \leq N}$, $\mathbf{w}(x) = [P(x \mid c_i)]_{1 \leq i \leq N}$ and $\mathbf{\pi} = [P(c_i)]_{1 \leq i \leq N}$ are respectively the posterior distribution, the likelihood function and the prior.

The idempotence and the distribution of evidence function

An evidence function $\boldsymbol{l}(x) = \operatorname{ilr} \boldsymbol{w}(x)$ is calibrated if it results in the same posterior probabilities whether $\boldsymbol{l}(x)$ or the data x is given [2]:

$$\forall i \in [1, N], P(c_i \mid x) = P(c_i \mid \boldsymbol{l}(x)) \iff \boldsymbol{l}(\boldsymbol{l}) = \boldsymbol{l}(x) \text{ (idempotence)},$$

leading to the following proposition extending a well-known result for LLRs [3],

Proposition 1 [2]: If
$$\boldsymbol{l} \mid c_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$
, then $\forall i \in [\![2,N]\!]$, $\boldsymbol{l} \mid c_i \sim \mathcal{N}(\boldsymbol{\mu}_i(\boldsymbol{\Sigma}), \boldsymbol{\Sigma})$, where $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_1(\boldsymbol{\Sigma}) = \boldsymbol{A}^{-1}\boldsymbol{B}\operatorname{vec}(\boldsymbol{\Sigma})$, and $\boldsymbol{\mu}_i(\boldsymbol{\Sigma}) = \boldsymbol{\mu}_1(\boldsymbol{\Sigma}) - \boldsymbol{\Sigma}\boldsymbol{a}_{i-1} - \sum_{j=1}^{i-2} \frac{1}{j+1}\boldsymbol{\Sigma}\boldsymbol{a}_j$,

 $m{A} \in \mathcal{M}_{N-1,N-1}(\mathbb{R})$ and $m{B} \in \mathcal{M}_{N-1,(N-1)^2}(\mathbb{R})$ are constant matrices, and $m{a}_i = \sqrt{rac{i+1}{i}}m{e}_i$ where e_i is the i^{th} vector of the standard canonical basis of \mathbb{R}^{N-1} .

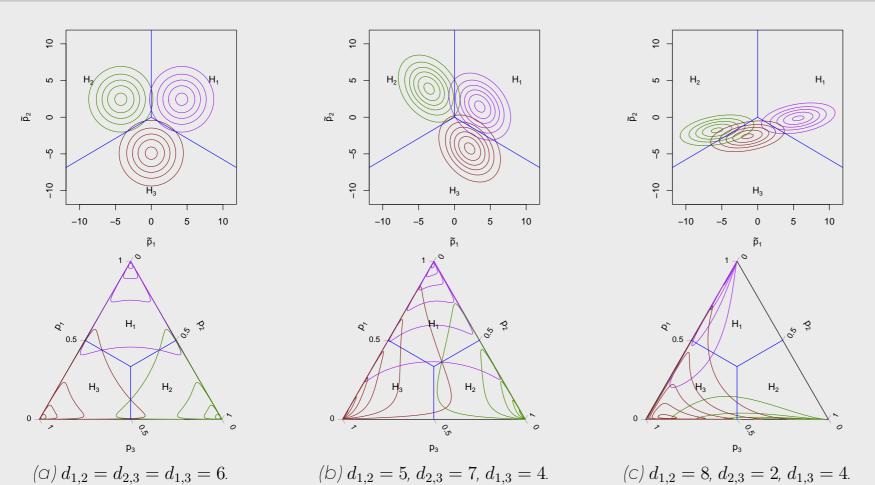


Figure: Gaussian conditional densities of the likelihood function in a 3 classes case. The covariance matrix can be expressed in terms of the three divergences between each density. The densities on the ILR space (top) are with respect to the Lebesgue measure while the densities on the simplex (bottom) are with respect to the Aitchison measure [4].

The method

Notations and objective

Let,

 $oldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^d$ be an observation, $\boldsymbol{l}(\boldsymbol{x}) \in \mathcal{L} \subset \mathbb{R}^{N-1}$ the evidence function,

 $\boldsymbol{r}(\boldsymbol{x}) \in \mathcal{R} \subset \mathbb{R}^{d-N+1}$ the residual,

 $\mathcal{Z} = \mathcal{L} \oplus \mathcal{R}$ the base space,

Find a diffeomorphism $g^{-1}: \mathcal{X} \mapsto \mathcal{Z}$, such that

 $\boldsymbol{z} = g^{-1}(\boldsymbol{x})$

 $\boldsymbol{z} = [l_1, \dots, l_{N-1}, r_1, \dots r_{d-N+1}] \in \mathcal{Z}$

evidence function

Class-conditional densities in the base space

We choose the densities in the base space according to Proposition 1:

$$\forall i \in [1, N], \boldsymbol{z} \mid c_i \sim \mathcal{N}\left(\boldsymbol{m_i}\left(\boldsymbol{\Sigma}\right), \boldsymbol{C}\left(\boldsymbol{\Sigma}\right)\right),$$

where the covariance matrix Σ is the **only parameter** and:

- $m_i(\Sigma)$ is the concatenation of $\mu_i(\Sigma)$ and the (d-N+1)-dimensional zero vector
- the covariance matrix $C(\Sigma)$ is the following block matrix:

$$oldsymbol{C}\left(oldsymbol{\Sigma}
ight) = egin{bmatrix} oldsymbol{\Sigma} & oldsymbol{0}_{N-1,d-N+1} \ oldsymbol{0}_{d-N+1,N-1} & oldsymbol{I}_{d-N+1} \end{bmatrix},$$

In this way,

- the first N-1 dimensions of z form the evidence function,
- the others form the **residual** normally distributed with a zero mean vector and an identity covariance matrix regardless of the class.

Learning the discriminant function with normalizing flow

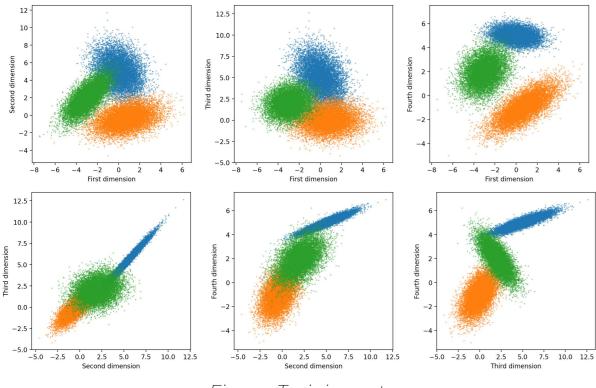
Normalizing flow—a cascade of invertible neural-networks [5]—is used to learn the mapping q through data likelihood maximization:

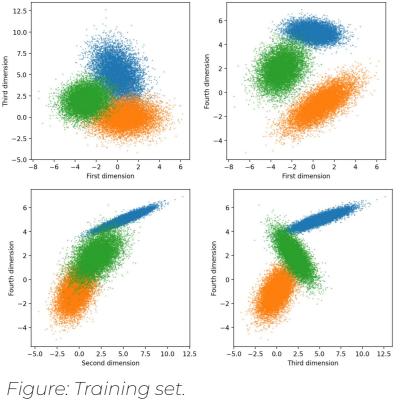
$$\log f\left(\mathcal{D} \mid \theta_g, \boldsymbol{\Sigma}\right) = \sum_{i=1}^{N} \left(\sum_{(x,c) \in \mathcal{D} \mid c = c_i} \log \left(f_{\mathcal{Z} \mid c_i, \boldsymbol{\Sigma}}\left(\boldsymbol{z}\right) \left| \det \left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{z}} \right) \right|^{-1} \right) \right),$$
Change of variable

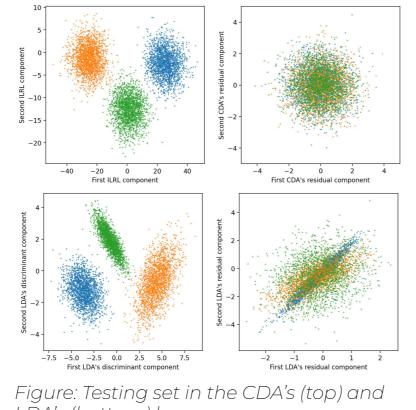
where the mapping's parameters $heta_g$ and the log-Cholesky parametrized $oldsymbol{\Sigma}$ are learned with automatic differentiation and gradient descent.

Toy experiments

With Gaussians







LDA's (bottom) base space.

Table: C_{llr} measures [6]. Samples from the non-concerned class are discarded.

compared classes	LDA		QDA		CDA	
	C_{IIr} [bit]	$C_{ m llr}^{ m min}$ [bit]	C_{IIr}	C_{IIr}^{min}	C_{IIr}	C_{IIr}^{min}
1 vs 2	$1.72_{10^{-3}}$	0.0	0.0	0.0	$4.85_{10^{-5}}$	0.0
1 vs 3	1.98	1.4310-1	$1.72_{10^{-9}}$	0.0	$9.46_{10^{-3}}$	$5.04_{10^{-3}}$
2 vs 3	$2.00_{10^{-1}}$	$1.76_{10^{-2}}$	6.3710-4	0.0	8.4610-3	$5.31_{10^{-3}}$

With MNIST

0123456789

The flattened images reduced to 40 principal components are used as inputs

Table: Cross-entropy and accuracy measures on the testing set for the MNIST's digit recognition task. empirical cross-entropy [nat] | accuracy [%]

	cripinear cross critiopy [nat] accuracy				Curacy [70]	
	LDA	$5.44_{10^{-1}}$			87.67	
	QDA	8.5610-1			96.24	
	CDA		2.23 ₁₀ ⁻¹		94.43	
10 -				8.0 - 7.5 -		
Second dimension				7.0 - 6.5 - 6.0 -		
0 -				5.5 -		
-4 -2 0	2 4 6 First dimension	8 10 12		3.5	4.0 4.5 5.0 5 First dim	.5 6.0 6.5 7.0 nension

Figure: UMAP visualization of the evidence function.

Figure: UMAP visualization of the residual.

Interpolation between digits in the space of evidence functions



Discussion

- The **discriminant components** form a calibrated isometric-log-ratio transformed likelihood function: an evidence function;
- No explicit assumption is made on the distribution of the data (except the existence of a diffeomorphism that would transform the data into the target Gaussians);
- Each discriminant component expresses a weight-of-evidence in favour of a group of classes against another group according to the used Aitchison basis;
- This can be used for uncertainty-aware decisions avoiding under or overconfident predictions;
- In addition, the discriminant space has the **intuitive** Euclidean vector space structure given by the Aitchison geometry, allowing interpretability, distance measures, interpolations, and straightforward computation of the posterior probability distribution by simply shifting the evidence function by the prior.

References

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