Novel sample-efficient classification approaches for ERP data: **Time-decoupled LDA, Toeplitz-LDA, Unsupervised Mean-Difference Maximization**

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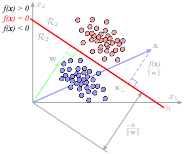
ERP classification with linear discriminant analysis (LDA): assumptions, parameters



LDA still state of the art for ERP data.

Assumptions made by LDA:

- Feature distributions are Gaussian
- Both classes share the same distribution

Trained LDA model is obtained by:

$$\mathbf{w} = \boldsymbol{\Sigma}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

and

$$b = -\frac{1}{2}\mathbf{w}^T(\mathbf{m}_1 + \mathbf{m}_2)$$

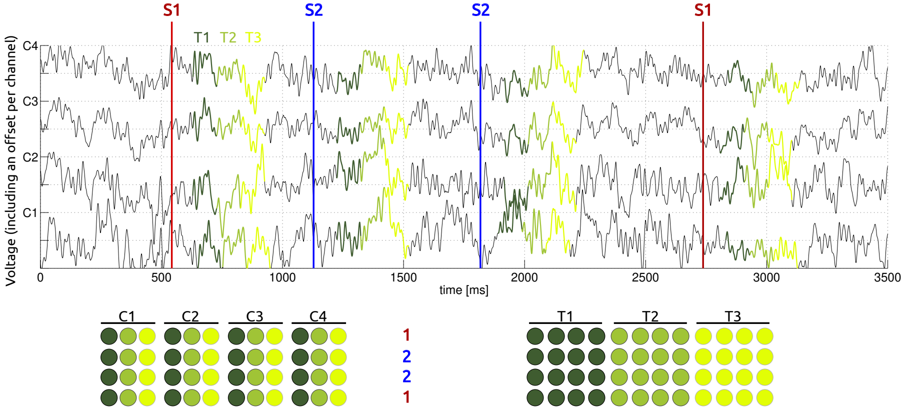
(*Note: this is the formulation for the case of equally probable classes, but it can easily be adapted.*)

From time series to ERP features

Toy example with target stimuli, non-target stimuli:

3 time features (T1, T2, T3) per channel, 4 channels (C1, C2, C3, C4).

$\rightarrow$ Data matrix $\mathbf{X}$ has 4 rows, each containing $3 * 4 = 12$ features.



Small data regimes: improve the estimation of covariance matrix by shrinking it towards a unit sphere

Seminal paper **on shrinkage regularization** forms the basis of the following approaches.

`https://doi.org/10.1016/j.neuroimage.2010.06.048`

ELSEVIER

NeuroImage
Volume 56, Issue 2, 15 May 2011, Pages 814-825

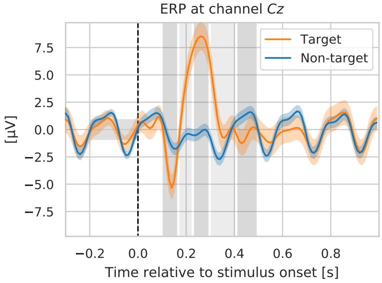
Single-trial analysis and classification of ERP components — A tutorial

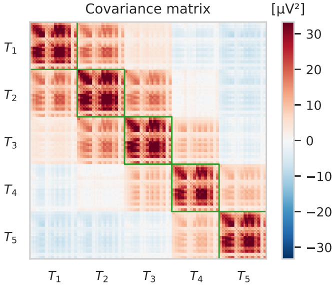
Benjamin Blankertz [a] [b], Steven Lemm [b], Matthias Treder [a], Stefan Haufe [a], Klaus-Robert Müller [a]

Three methods for small training datasets

1. Time-decoupled LDA (supervised)
2. Block-Toeplitz with tapering (supervised)
3. Unsupervised mean-difference maximization (UMM)

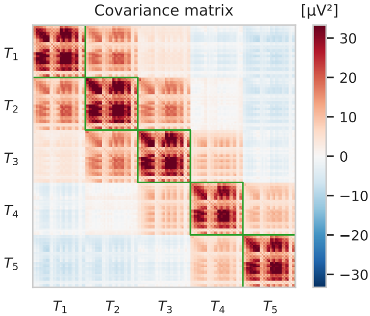
Very small auditory ERP datasets





- Training data: 78 epochs (13 target, 65 non-target), 155 features (31 channels and 5 time windows T_i) in *channel-prime* order.
- Upfront: Shrinkage regularization does a decent job.
- Can we do even better?

Estimating the empirical covariance matrix



- Observation: diagonal blocks of size 31×31 are similar
- Reminder: covariance matrix is calculated from **mean-free** data

$$\boldsymbol{\Sigma} = \frac{1}{N-1} \sum_N (\mathbf{x}_n - \mathbf{m})(\mathbf{x}_n - \mathbf{m})^T$$

(symmetric and positive semi-definite)

- $\rightarrow$ Covariance matrix describes background noise characteristic.

Two assumptions about background noise in ERP data

Given artifact-free data...

A1 : The noise on top of the ERP features is normally distributed.

Two assumptions about background noise in ERP data

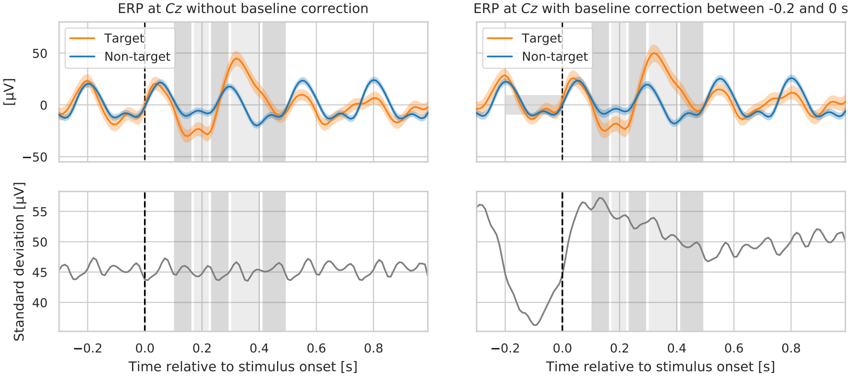
Given artifact-free data...

A1 : The noise on top of the ERP features is normally distributed.

A2 : Noise is unrelated to current user task, i.e.

- target or non-target epoch
- stimulation or no stimulation

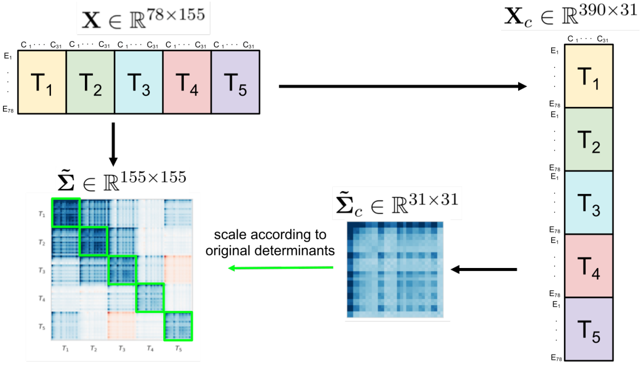
Checking assumption A2 by analyzing the noise



- A2 seems realistic if no baseline correction is performed.
- Not problematic: Can use *high-pass filter* instead (e.g., 0.5 Hz).
- High-pass filtering also helps to ensure A1!

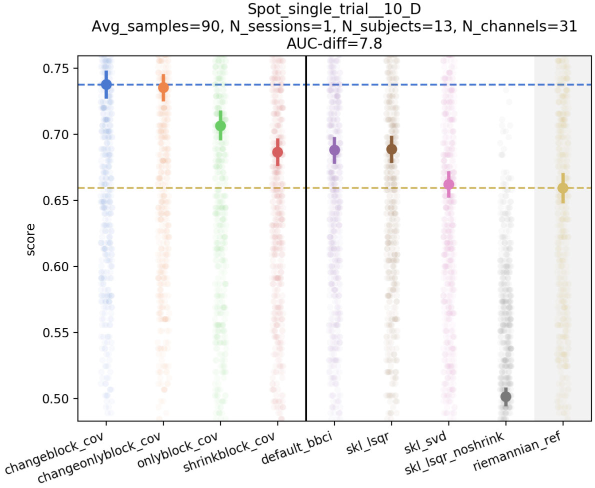
Assuming independence between time intervals (A2) → **Time-Decoupled LDA** (TD-LDA)

(1) Apply shrinkage regularization to empirical covariance matrix. **(2)** Improve estimate of diagonal blocks using *additional virtual* data points. **(3)** Exchange and re-scale the original diagonal blocks:



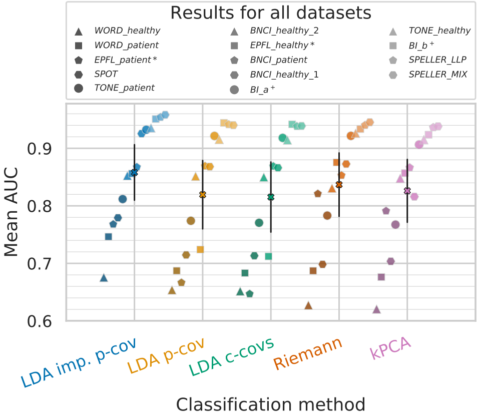
Using TD-LDA, the diagonal blocks are estimated from 5 times more data!

Improved $\tilde{\Sigma}$ together with the standard class means $\rightarrow$ **TD-LDA**.
Applied to small auditory ERP datasets:



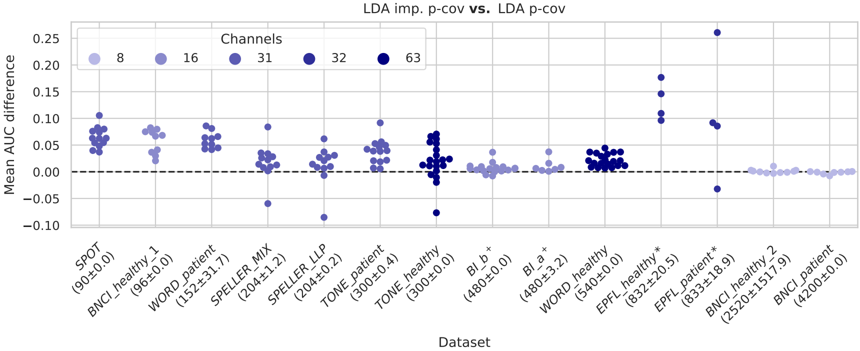
Results on various ERP datasets (auditory, visual)

TD-LDA ("LDA imp. p-cov") improves on many different ERP datasets compared to shrinkage regularized LDA ("LDA p-cov"):



[Sosulski et al.(2021), Neuroinformatics, 19(3):461-476.]

Improvements depend on size of training dataset



- TD-LDA is **specifically effective for small datasets** but does not hurt for large datasets.
- TD-LDA uses domain-specific regularization of covariance matrix.
- TD-LDA does **not** improve the quality of the class means.

Three methods for small training datasets

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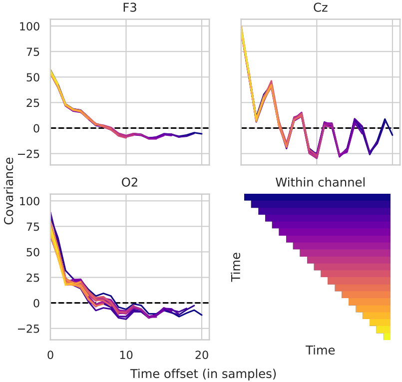
(Another) two assumptions about noise in ERP data

A3 : Only ERP signal is time-locked, EEG background is stationary. $\rightarrow$ covariance across time depends only on temporal distance δ between samples, i.e. $cov(x^{t_j}, x^{t_i}) = cov(x^{t_j+\delta}, x^{t_i+\delta}) \; \forall \delta \in \mathbb{R}$.

A4 For increasing temporal distances, i.e. $|t_i - t_j| \rightarrow \infty$, the covariance goes towards zero.

Checking assumption A4

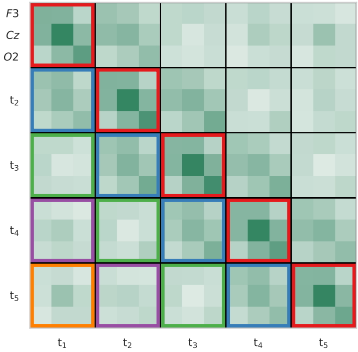


- Plots show covariances within three different channels across different temporal distances δ.
- Assumptions seems to hold for EEG channels F3 and Cz, but less so for channel O2 (Ideally: curves should overlap and approach zero).

Implementing assumption A3

With features in channel-prime order and after initial shrinkage:

If same temporal distances imply the same covariance within one channel, then we can average along the diagonal blocks AND along each of the off-diagonal blocks separately → **Toeplitz structure**.

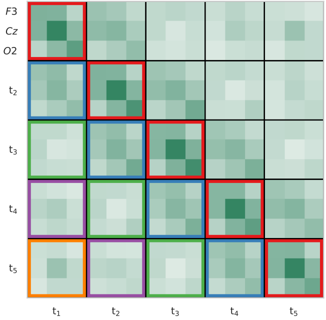


Memory requirements?

Implementing assumption A4

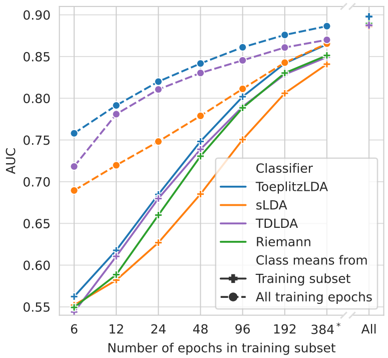
If covariance within one channel goes to zero with increased temporal distance, then we can taper down the blocks from the main diagonal to the corners. Practically:

- use a **linear tapering function**: strong weight on main diagonal, small weight on covariance blocks describing large temporal distance.
- simple implementation: add up the blocks across each diagonal



Results: Block-Toeplitz with tapering

Evaluated on 13 ERP dataset with over 200 subjects:



- solid lines: realistic performances
- dashed lines: performance with improved covariances, but maximally (unrealistic) informative class means

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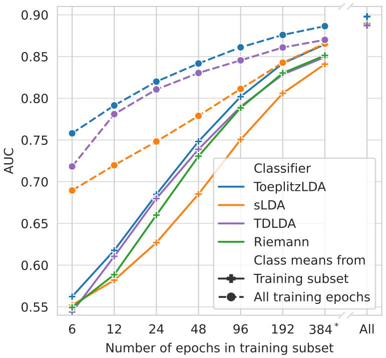


- solid lines: realistic performances
- dashed lines: performance with improved covariances, but maximally (unrealistic) informative class means
- Toeplitz-LDA slightly outperforms TD-LDA, strongly outperforms shrinkage-regularized LDA (sLDA).
- Improved class mean estimates *could* boost performance further.

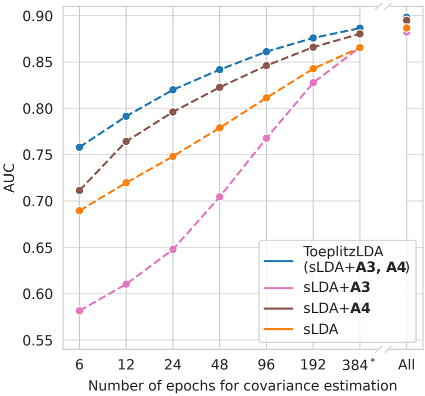
Block-Toeplitz with tapering: visual ERP speller

[Sosulski & Tangermann, Journal of Neural Eng., 2022, https://doi.org/10.1088/1741-2552/ac9c98]

Observation: Block-Toeplitz LDA drastically outperforms shrinkage-regularized LDA on this application metric (correctly spelled letters) for an *unsupervised approach*.

Influence of the assumptions

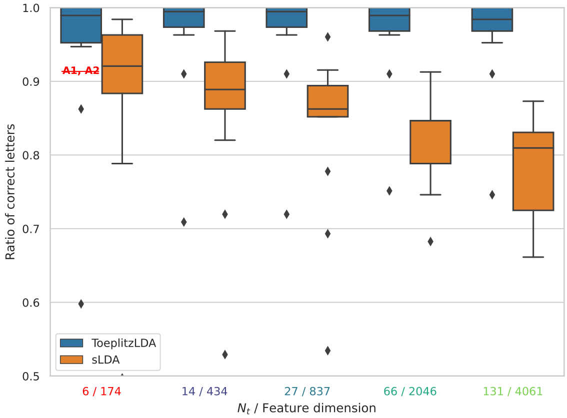
With (unrealistic) oracle for optimal class mean estimates:



- Major improvement by tapering alone (A4)
- Using A3 alone (block-wise averaging per diagonal without tapering) mimicks equally good estimates of covariances independent of temporal distance
  $\rightarrow$ performance drop!
- Combination of assumptions A3 and A4 works best.

Block-Toeplitz LDA scales well with many temporal features

Increasing the number of time intervals per channel:



- sLDA suffers from higher feature dimensionality (as covariance matrix is harder to estimate).
- Block-Toeplitz LDA can cope with original samples! Definition of feature intervals dispensable?

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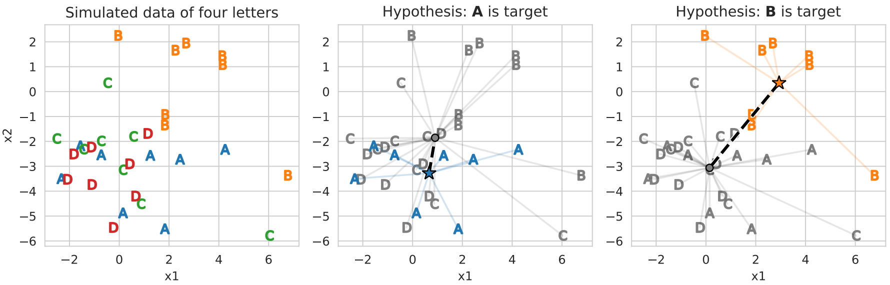
Unsupervised mean-difference maximization

Toy example: which of the four symbols is the attended target?



- Idea: The true target mean is expected to have largest distance to the mean of the other (non-target) symbols.

UMM acts instantaneously on single trial, and is unsupervised

Algorithm 1 Pseudocode for the basic UMM method. Variants of blue lines are described in Sections 2.2.2 and 2.2.3.

Require: available symbols S, epochs of i-th trial $E^{(i)}$

for every trial i **do**
    $\Sigma^{-1} \leftarrow \mathrm{cov}(E^{(i)})^{-1}$ ▷ no class labels needed
    $d^* \leftarrow -\infty$
    for s in S **do**
        $\Delta\boldsymbol{\mu}_s \leftarrow \mathrm{mean}(E^{(i)}_{A^{s+}}) - \mathrm{mean}(E^{(i)}_{A^{s-}})$
        $d \leftarrow \Delta\boldsymbol{\mu}_s \Sigma^{-1} \Delta\boldsymbol{\mu}_s^\intercal$
        if $d > d^*$ **then**
            $d^* \leftarrow d$
            $s^* \leftarrow s$
        end if
    end for ▷ s^* decoded symbol for trial i
end for

- Sequentially check all possible hypotheses for largest mean difference.
- Distances are computed using a covariance correction (cp. to Mahalanobis distances).
- Covariance matrices are estimated using shrinkage regularization with following block-Toeplitz regularization with tapering.

UMM is comes with a confidence and can learn across trials.

$$c = \frac{d^{\Sigma}(s^*) - d^{\Sigma}(s^r)}{\sigma_{S^-}}$$

- Confidence c is obtained by comparing the winner (*) distance to the runner-up (^{r}) distance.

$$\boldsymbol{\mu}_{s+}^{C} = \frac{\left[\sum_{l=1}^{N_t} (\hat{c}^{(l)} \cdot \boldsymbol{\mu}_{+}^{(l)}) + c^{(i)} \cdot \mathrm{mean}\left(E_{A^{s+}}^{(i)}\right)\right]}{\sum_{l=1}^{N_t} (\hat{c}^{(l)}) + c^{(i)}}$$

- Class means (and covariances) can be combined across trials either optimistically or based on the confidence obtained for each trial.

UMM results for binary classification

Target vs. non-target classification of multiple (MOABB) datasets:

UMM classification rates for all datasets and hyperparameters

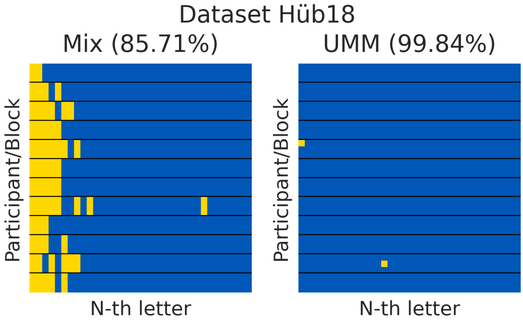
Dataset	Σ_s^1 μ^1	Σ_s^{all} μ^1	Σ_t^1 μ^1	Σ_t^{all} μ^1	Σ_s^1 μ^O	Σ_s^{all} μ^O	Σ_t^1 μ^O	Σ_t^{all} μ^O	Σ_s^1 μ^C	Σ_s^{all} μ^C	Σ_t^1 μ^C	Σ_t^{all} μ^C
Hüb17 (38)	76.02	72.18	92.19	91.44	80.58	95.95	99.37	**99.96**	81.83	98.66	99.37	**99.96**
Hüb18 (36)	80.16	74.84	96.11	94.44	72.70	98.97	99.21	**99.92**	73.65	99.05	99.52	99.84
Lee19 (107)	54.99	44.95	73.86	71.92	49.76	79.79	95.57	98.48	54.58	93.40	97.93	**99.47**
Ric13 (8)	50.00	42.14	62.50	59.29	42.86	47.14	58.93	59.64	41.43	**77.86**	60.71	59.64
Sch14 (21)	47.23	47.02	54.15	52.16	55.25	62.27	78.87	76.74	56.17	75.85	**82.52**	76.74

Used estimators

Classification rate: 0 – 25 – 50 – 75 – 100

- Block-Toeplitz rocks...
- Good instantaneous performances.
- Confidence-based history of means outperforms state-of-the-art for visual datasets Hüb17, Hüb18 and Lee19.
- Auditory datasets are harder (known).
- Patient dataset Ric13 can run into problems, if initial hypothesis is wrong. (For repair, see Poster 3-F-57)

UMM results for letter selection



- For visual ERP datasets, basically error-free letter selection (offline replay of MIX dataset obtained by Hübner et al.).

Wrap-up

- LDA with domain-specific regularizations can perform extremely well (**TD-LDA**, **Toeplitz-LDA**).
- With **UMM**, a novel *unsupervised* classification approach is available with potential to:
  - completely omit calibration
  - completely omit warm-up period (as in other unsupervised methods)
  - mitigate non-stationarity (UMM can be used instantaneously)
  - use confidence for, e.g., dynamic stopping, outlier detection, ...