Invariant coordinate selection - a guided tour of implementations

Aurore Archimbaud, Colombe Becquart,
Andreas Alfons & Klaus Nordhausen
joint w/ Anne M. Ruiz

ICS and Related Methods Conference
May 8, 2025

Outline of the presentation

Invariant coordinate selection
- Principle
- Interpretation of the components
- Summary

ICS - methodology

ICS - implementations

Conclusion

Tutorial

Invariant Component Selection (ICS)

ICS Tyler et al. (2009) - GPCA Caussinus and Ruiz-Gazen (1990)

Main characteristics

- Simultaneously diagonalizes two scatter matrices.
- Affine invariant.
- Dimension reduction method useful for multivariate data analysis.

Invariant Component Selection (ICS)

Main advantages

- Goes beyond PCA, which diagonalizes the covariance matrix.
- Can recover the Fisher's linear discriminant subspace under some elliptical mixture models, without knowing the class labels (Tyler et al., 2009; Becquart et al., 2024).

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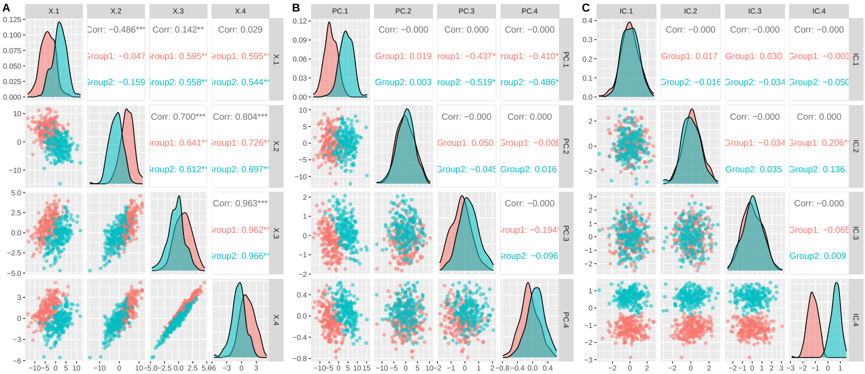
Main steps

1. Components calculation
2. Components selection

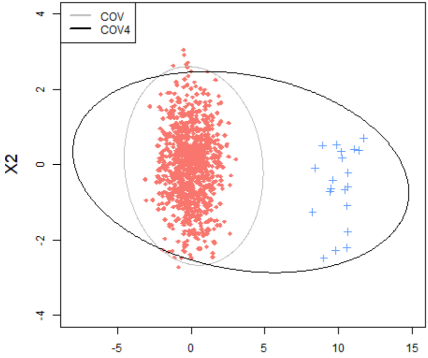


See the toy example from Nordhausen and Ruiz-Gazen (2021).

MEAN-SHIFT MODEL ($q = 1$)

$$980 \text{ obs } \sim \mathcal{N}_{p=2}(0, \mathbf{I}_p) \;\&\; 20 \text{ obs } \sim \mathcal{N}_{p=2}((10,0)', \mathbf{I}_p)$$

Suppose $\mathbf{V}_1 = \mathrm{COV}(\mathbf{X})$ and $\mathbf{V}_2 = \mathrm{COV}_4(\mathbf{X})$
with $\mathrm{COV}_4 = \frac{1}{p+2}\,\mathbb{E}\left[r^2(\mathbf{X})(\mathbf{X} - \mathbb{E}(\mathbf{X}))(\mathbf{X} - \mathbb{E}(\mathbf{X}))'\right]$.



Example: ICS with COV-COV4

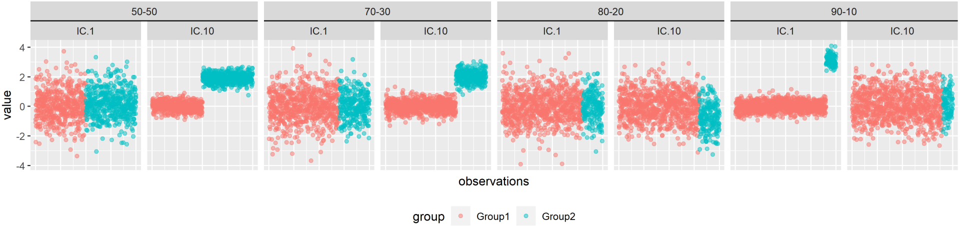


Figure: Mixture of 2 groups: first and last ICs

1. Components calculation

1. Two scatter matrices $\mathbf{V}_1$ and $\mathbf{V}_2$.
2. Eigendecomposition of $\mathbf{V}_1^{-1}\mathbf{V}_2$.
3. Decreasing eigenvalues: kurtosis.
4. Projection of the centered data on the eigenvectors $\rightarrow$ ICs.

1. Components calculation

1. $\mathbf{V}_1$: covariance matrix.
2. $\mathbf{V}_2$: fourth moment matrix.
3. Eigendecomposition of $\mathbf{V}_1^{-1}\mathbf{V}_2$
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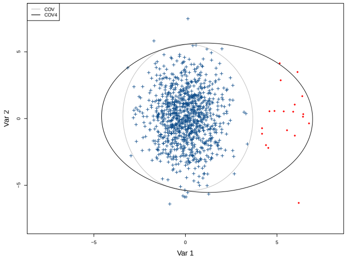

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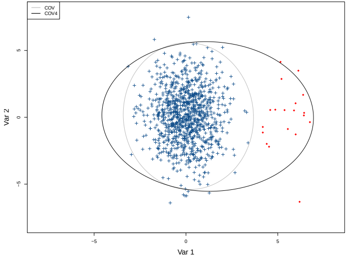
2. Components selection

1. Based on the eigenvalues.
2. Based on the components.
3. First and/or last $k \leq p$ components retained.



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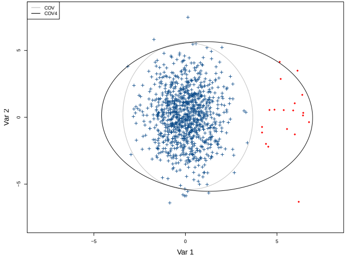

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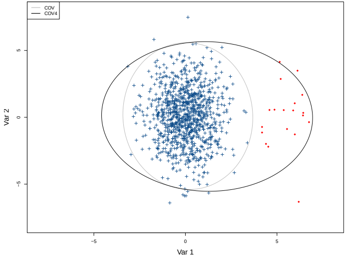

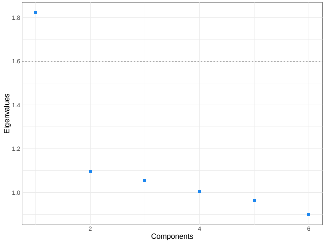

Applications

Outlier detection

1. Euclidian distance of the observations calculated using the k selected components.

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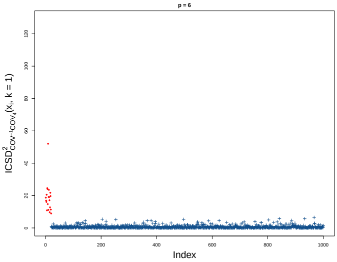

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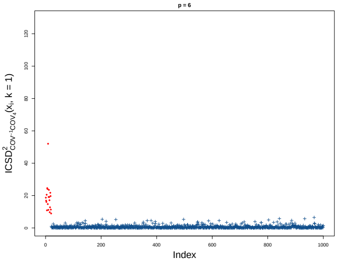

Tandem clustering with ICS

1. Clustering method.
2. Identification of clusters.

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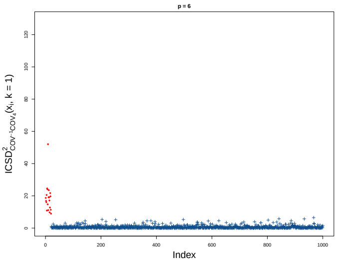

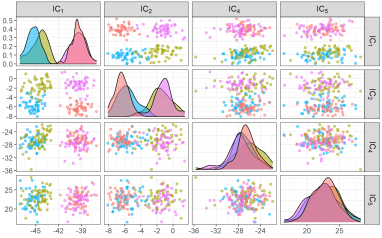

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Invariant coordinate selection

ICS - methodology

Choice of scatter matrices

Choice of components

ICS - implementations

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Choice of scatter matrices

Applications:

- For **outlier detection**: Archimbaud et al. (2018a) for a small proportion of outliers.

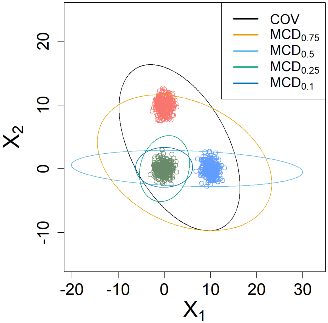
Choice of scatter matrices

Applications:

- For **outlier detection**: Archimbaud et al. (2018a) for a small proportion of outliers.
- For **clustering**: Becquart et al. (2024) and Alfons et al. (2024). One scatter matrix should reflect the within (local) cluster structure and one the between (global) cluster structure.

Choice of scatter matrices

- COV – COV_4 or FOBI Peña et al. (2010); Cardoso (1989); Nordhausen and Virta (2019); Fischer et al. (2017, 2020)
- MCD_α – COV, RMCD_α – COV with values of $\alpha \leq 0.5$ Rousseeuw (1985)
- TCOV – UCOV, TCOV – COV Caussinus and Ruiz-Gazen (1993a)
- LCOV – COV Hennig (2009)



Description	R - Scatter	R - ICS_scatter	Python `Scatter`
Covariance	`ICS::cov()`	`ICS::ICS_cov()`	`cov()`
Fourth-moment covariance	`ICS::cov4()`	`ICS::ICS_cov4()`	`cov4()`
One-step M-estimator	`ICS:: covW()`	`ICS::ICS_covW()`	`covW()`
One-step Tyler shape matrix	`ICS::covAxis()`	`ICS::ICS_covAxis()`	`covAxis()`
Multivariate t-distribution estimator	`ICS:: tM()`	`ICS:: ICS_tM()`	
Supervised scatter (quantiles)	`ICS::scovq()`	`ICS::ICS_scovq()`	
Minimum Covariance Determinant (MCD)	`rrcov::CovMcd()`	`ICSClust::ICS_mcd_raw()`, `ICS_mcd_rwt()`	`sklearn.covariance.MinCovDet()`
Cauchy location and scatter	`ICS::tM()`	`ICSClust::ICS_mlc()`	
Pairwise one-step M-estimate	`ICSClust::tcov()`	`ICSClust::ICS_tcov()`	
Simple robust estimates	`ICSClust::ucov()`	`ICSClust::ICS_ucov()`	
Local shape scatter	`ICSClust::lcov()`	`ICSClust::ICS_lcov()`	

CHOICE OF COMPONENTS WITH $q < p$

For outlier detection:

- First components

CHOICE OF COMPONENTS WITH $q < p$

For outlier detection:

- First components

For clustering:

- First and/or last components

CHOICE OF COMPONENTS WITH $q < p$

Archimbaud et al. (2018a), Alfons et al. (2024), Nordhausen et al. (2022), Radojicic and Nordhausen (2020)

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Based on the Invariant Components:

- Keep only non-gaussian components using marginal normality tests.

Choice of components with $q < p$

Archimbaud et al. (2018a), Alfons et al. (2024), Nordhausen et al. (2022), Radojicic and Nordhausen (2020)

Based on the Invariant Components:

- Keep only non-gaussian components using marginal normality tests.

In this context of particular sequential multiple testing, we apply the Bonferroni correction on the significance level: $\alpha_i = \alpha / i$ for $i = 1, \ldots, p$ with $\alpha = 5\%$ (see Dray (2008)).

Choice of components with $q < p$

Based on the eigenvalues and eigenvectors:

- Visually, using a scree plot.
- Using the number q of clusters a priori and the fact that some should be almost equal (med_criterion and var_criterion).
- Using asymptotic distribution of the eigenvalues or bootstrapping (ICSboot, FOBIasymp, FOBIboot).
- Using quasi inferential procedures (parallel analysis).
- Using ladle and data augmentation (FOBIladle).

Selection of components - summary

Criterion	Function	Notes
Marginal normality tests	`ICSClust::normal_crit()`	First and last few components are investigated
Median-based criterion	`ICSClust::med_crit()`	Requires a priori knowledge
Variance-based criterion	`ICSClust::var_crit()`	From `ICtest::ICSboot()`
Discriminatory power criterion	`ICSClust::discriminatory_crit()`	Supervised, requires a priori knowledge
Parallel analysis (simulation)	`ICSOutlier::comp_simu_test()`, `comp.simu.test()`	Only first components are investigated
Marginal normality tests	`ICSOutlier::comp_norm_test()`, `comp.norm.test()`	Only first components are investigated
Asymptotic and resampling based approaches	`ICtest:: ICSboot()`, `FOBIboot()`, `FOBIasymp()`, `FOBIladle()`	Focus on identifying Gaussian subspace

Outline of the presentation

Invariant coordinate selection

ICS - methodology

ICS - implementations
- R ecosystem
- Python ecosystem
- Julia ecosystem

Conclusion

Tutorial

Genesis: 2007/2008 - Klaus Nordhausen + Hannu Oja + David E. Tyler

ICS (v1.0-1.2)

ics (S4)

```
ics(X, S1 = cov, S2 = cov4, S1args = list(), S2args = list(),
    stdB = "Z", stdKurt = TRUE, na.action = na.fail)
```

```
@gKurt, @UnMix, @Scores
```

Scatter matrices:

```
cov4, cov4.wt,
covAxis, covOrigin, tM
```

2016-2018: + Aurore Archimbaud and Anne Ruiz-Gazen

+ Joris May

ICSShiny (v0.4-0.5)

ICSShiny (GUI)

1. *Choice of the scatter matrices*
2. *Selection of the ICs*
3. *Exploration of the output and identification of outliers*
4. *Download of graphs and components.*

ICSOutlier (v2.0-3.0)

ics.outlier (S4)

1. *Selection of ICs:* `comp.simu.test` `comp.norm.test`
2. *ICS distances:* `ics.distances`
3. *Identification of outliers:* `dist.simu.test`

ICtest (v2.0-3-1)

1. *Selection of ICs*

ICS (v1.3)

ics (S4)

```
ics(X, S1 = cov, S2 = cov4, S1args = list(), S2args = list(),
    stdB = "Z", stdKurt = TRUE, na.action = na.fail)
```

`@gKurt, @UnMix, @Scores`

ics2 (S4)

```
ics2(X, S1 = MeanCov, S2 = Mean3Cov4, S1args = list(), S2args = list(),
     na.action = na.fail)
```

two location functionals used to fix the signs of the components and to center them.

2023: + Andreas Alfons + Zlatko Drmač

ICSClust (v1.0)

ICSClust(S3)

ICS_scatter : `ICS_lcov, ICS_mcd, ICS_mlc, ICS_tcov, ICS_ucov`
1. Computation of ICS: `ICS`
2. Selection of ICs and visualization:
`"med_crit", "normal_crit", "var_crit", "discriminatory_crit"`
3. Clustering and visualization :
`"kmeans_clust", "tkmeans_clust", "pam_clust", "mclust_clust", "rmclust_clust", "rimle_clust"`

ICSOutlier (v4.0)

ICS_outlier(S3)

0. Computation of ICS: `ICS`
1. Selection of ICs: `comp_simu_test comp_norm_test`
2. ICS distances: `ics_distances`
3. Identification of outliers: `dist_simu_test`

ICS (v1.4-2)

```
ICS(
  X,
  S1 = ICS_cov,
  S2 = ICS_cov4,
  S1_args = list(),
  S2_args = list(),
  algorithm = c("whiten", "standard", "QR"),
  center = FALSE,
  fix_signs = c("scores", "W"),
  na.action = na.fail
)
```

```
@gKurt   → $gen_kurtosis
@UnMix   → $W
@Scores  → $scores
```

ICS (S3)

1. `ICS_scatter` *class*
2. *Different algorithms*
3. *Centering*
4. *Fixing signs*

ICS - ALGORITHMS

Let $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)'$ be a p-variate dataset.
Simultaneous diagonalization of two scatter matrices $\mathbf{S}_{1,n}$ and $\mathbf{S}_{2,n}$:

$$\mathbf{W}_n \mathbf{S}_{1,n} \mathbf{W}_n^\top = \mathbf{I}_p \quad \text{and} \quad \mathbf{W}_n \mathbf{S}_{2,n} \mathbf{W}_n^\top = \mathbf{D}_n$$

where the diagonal matrix $\mathbf{D}_n$ contains the eigenvalues $\rho_1, \ldots, \rho_p$ of $\mathbf{S}_{1,n}^{-1}\mathbf{S}_{2,n}$ in decreasing order and $\mathbf{W}_n = (\mathbf{w}_1, \ldots, \mathbf{w}_p)'$ contains the corresponding eigenvectors as its rows.

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where the diagonal matrix $\mathbf{D}_n$ contains the eigenvalues $\rho_1, \ldots, \rho_p$ of $\mathbf{S}_{1,n}^{-1}\mathbf{S}_{2,n}$ in decreasing order and $\mathbf{W}_n = (\mathbf{w}_1, \ldots, \mathbf{w}_p)'$ contains the corresponding eigenvectors as its rows.
The (affine) invariant coordinates or scores are:

$$\mathbf{Z}_n = \mathbf{X}_n^c \mathbf{W}_n^\top.$$

$\mathbf{X}_n^c$ can be the centered version of $\mathbf{X}_n$ with respect to the location estimator associated with $\mathbf{S}_{1,n}$.

ICS - ALGORITHMS

- **whiten**: whitens X_n with respect to $\mathbf{S}_1$ before computing $\mathbf{S}_2$ (should be a function).
- **standard**: performs the spectral decomposition of the symmetric matrix $M(X_n)$.

ICS - ALGORITHMS

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whiten:

- $Y_n = X_n S_1(X_n)^{-1/2}$
- $S_2(Y_n)$
- $S_2(Y_n) = UDU'$
- $W = U' S_1(X_n)^{-1/2}$
- $Z = X_n^c W^\top$

standard:

- $S_1(X_n), S_2(X_n)$
- $M(X_n) = S_1(X_n)^{-1/2} S_2(X_n) S_1(X_n)^{-1/2}$
- $M(X_n) = UDU'$
- $W = U' S_1(X_n)^{-1/2}$
- $Z = X_n^c W^\top$

ICS - ALGORITHMS

The signs of W can be fixed with `fix_signs`:

- **`"scores"`**: the generalized skewness values of all components are positive.
  Common for ICS framework.
- **`"W"`**: the maximum element in each row of W is positive and each row has norm 1.
  Common with ICA framework.

Z can be centered through the boolean `center` input parameter.

ICS - QR - based on pivoted QR decomposition

Archimbaud et al. (2023b), numerically stable algorithm for $\text{COV} - \text{COV}_w$ focusing on:

$$M(X_n) = \text{COV}^{-1/2}\text{COV}_w\text{COV}^{-1/2}.$$

ICS - QR - BASED ON PIVOTED QR DECOMPOSITION

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Algorithm:

- Pivoted QR factorization: $\Pi_2^\top \left(\frac{1}{\sqrt{n-1}} X_n^{c\top}\right) \Pi_1 = QR$
- $Q = \Pi_2 Q$, $R = R\Pi_1^\top$
- Leverage scores $q_i = \|Q(i,:)\|_2^2$, $i = 1, \ldots, n$
- SVD of Diag $\left(\sqrt{w((n-1)q_i)}\right)_{i=1}^{n} Q$ to obtain

$$\widetilde{M}(X_n) = \frac{n-1}{n} Q^\top \ \mathrm{Diag}(w((n-1)q_i))_{i=1}^{n} \ Q = \widetilde{U}_2\widetilde{D}_2\widetilde{U}_2^\top$$

- $W = (R^{-1}\widetilde{U}_2)^\top$
- $Z = \sqrt{n-1}Q\widetilde{U}_2$ *or equivalently* $Z = X_n^c \Pi_1 W^\top$.

ICS - SUMMARY

Main attributes

Description	R - `ics()`, `ics2()`	R - `ICS()`	Python `ICS`
Generalized eigenvalues	`@gKurt`	`$gen_kurtosis`, `gen_kurtosis()`	`.kurtosis_`
Unmixing matrix.	`@UnMix`	`$W`	`.W_`
Scores	`@Scores`	`$scores`, `components()`	`.scores_`

Methods

Description	R - `ics()`, `ics2()`, `ICS()`	Python `ICS`
Print basic information	`print()`	
Coefficient matrix of ICS	`coef()`	
Summary	`summary()`	`.describe()`
Component scatterplot matrix	`plot()`	`.plot()`
Plots the kurtosis measures	`screeplot()`	`.plot_kurtosis()`

Python - 2023: Colombe Becquart + Abdallah Abdelsameia

Package ICSpyLab

- Created to make ICS accessible to the Python community.
- Main features:
  - the ICS class;
  - several scatter matrices;
  - supported algorithms: standard, whiten, QR.

Python - 2023: Colombe Becquart + Abdallah Abdelsameia

- Main difference from R: computing the invariant coordinates is divided into `fit` and `transform` methods, in line with popular machine learning frameworks such as scikit-learn:
  - `fit` computes the matrix W containing the eigenvectors;
  - `transform` computes the (affine) invariant coordinates or scores with the fitted matrix W. This transformation can be applied to a different dataset than the one used to compute W;
  - use the method `fit_transform` to perform both steps in a single call (equivalent of the function `ICS-S3()` from the R package `ICS`).

Python - 2023: Colombe Becquart + Abdallah Abdelsameia

- Next steps:
  - additional scatter matrices (TCOV);
  - component selection.
- For more details about the implementation, its installation and usage, see the documentation.

Julia - 2023: + Christopher Claassen (EUR)

Master dissertation

- *Generalising Invariant Coordinate Selection to a non-linear dimensionality reduction method* $\Longrightarrow$ work in progress Claassen (2023).
- Julia - code: `https://github.com/CClaassen/SimultaneousDiagonalisation.jl/`.

Julia - 2023: + Christopher Claassen (EUR)

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Short description of all source files:

- *SimultaneousDiagonalisation*.*jl* contains the main module of the package.
- *factorisatons*.*jl* contains the main methods to compute PCA and ICS.
- *component_selection*.*jl* contains functions related to component selection.
- *normality_tests*.*jl* contains functions for univariate normality tests.
- *scatters*.*jl* contains functions for computing various scatter matrices.

JULIA - 2023: + CHRISTOPHER CLAASSEN (EUR)

- *smoothing_kernels.jl* contains functions for using smoothing kernels.
- *reproducing_kernels.jl* contains functions for using reproducing kernels.
- *kernel_manipulation.jl* contains functions for transforming kernels.
- *classification.jl* contains functions related to classification.
- *evaluation.jl* contains functions for evaluating classification results.
- *external_methods.jl* contains bindings to external methods.
- *figures.jl* contains functions for plotting different types of figures.
- *data_manipulation.jl* contains functions for transforming data.
- *utilities.jl* contains various useful auxiliary functions.
- *external_data.jl* contains functions for loading external data.
- *experiments.jl* contains functions for replicating all results from the paper.

factorisatons.jl	component_selection.jl	normality_tests.jl	scatters.jl	smoothing_kernels.jl	reproducing_kernels.jl	kernel_manipulation.jl
#Main Methods#	#Main Method#	#Main Method#	#Locations and Scatters#	#Main Methods#	#Main Method#	#Input Transformations#
ics()	**component_selection()**	**normal_test()**	**mean1()**	**kernel_smoother()**	kernel()	scale_input()
gpca()			**cov2()**	**adaptive_kernel_smoother()**		scale_output()
	#Index Methods#	#Moment Tests#	**mean3()**		#Polynomial Kernels#	ard_transform()
#Simultaneous Diagonalisations#	retain_all()	jarque_bera()	**cov4()**	#Limited Support Kernels#	**linear_kernel()**	linear_transform()
REG_EIG()	retain_first()	bonnett_seier()		uniform_kernel_w()	**polynomial_kernel()**	
SYM_EIG()	retain_last()	agostino_pearson()	#Robust Scatters#	triangular_kernel_w()		#Kernel Manipulations#
REG_SVD()		ansecombe_glynn()	**fastMCD()**	epanechnikov_kernel_w()	#Exponential Kernels#	kernel_centered()
SYM_SVD()	#Eigenvalue Methods#	omnibus_K2()	**FastMVE()**	quartic_kernel_w()	abelian_kernel()	kernel_normalized()
	retain_var()			triweight_kernel_w()	**laplacian_kernel()**	kernel2distance()
#Regular Diagonalisations#	kramer_rule()	#ECDF Tests#	#Local Scatters#	tricube_kernel_w()	**gaussian_kernel()**	
EIG()	cluster_priori()	anderson_darling()	**lcov()**	cosine_kernel_w()	gibbs_kernel()	#Nystrom Appoximations#
SVD()		kolmogorov_smirnov()	**rlcov()**		gamma_exponential_kernel()	nystrom_ind()
	#Component Methods#	lilliefors()	**alcov()**	#Infinite Support Kernels#	exponentiated_kernel()	nystrom_ratio()
#Alternative Diagonalisations#	normality()	cramer_mises()	**arlcov()**	gaussian_kernel_w()		
custom_eig()	pick_tsne()	watson()		logistic_kernel_w()	#Rational kernels#	#Kernel Combinations#
custom_svd()	marginal_div()		#Auxiliary Functions#	sigmoid_kernel_w()	**rational_kernel()**	kernel_sum()
reduced_svd()	joint_div()	#Misc Tests#	*opt_h()*	silverman_kernel_w()	rational_quadratic_kernel()	kernel_prod()
custom_gsvd()	batch_joint_div()	shapiro_wilk()	*breakdown()*		gamma_rational_kernel()	
		shapiro_francia()		#Aliases#		#Scale Parameter Settings#
#Rank Reducing Methods#	#t-SNE Loss Functions#	pearson_chi2()		parabolic_kernel_w()	#Periodic Kernels#	**median_trick()**
constrained_svd()	*tsne_loss()*			biweight_kernel_w()	**cosine_kernel()**	**quantile_trick()**
reduce_mat_svd()	*opt_beta()*	#Data Transformations#			**neural_network_kernel()**	
reduce_mat_qr()	*Hbeta()*	*z_score()*			periodic_kernel()	
		rob_score()				
	#Divergences#	*mad_n()*			#Misc Kernels#	
	kl_div()				fbm_kernel()	
	sym_kl_div()	#Auxiliary Functions#			gabor_kernel()	
	gen_kl_div()	*skewness_moments()*			matern_kernel()	
	renyi_div()	*kurtosis_moments()*			wiener_kernel()	
	js_div()	*round_retain_sum()*			**mahalanobis_kernel()**	
		count_sample_regions()				
		geary_kurt()				

classification.jl	evaluation.jl	external_methods.jl	figures.jl	data_manipulation.jl	utilities.jl	external_data.jl	experiments.jl
#Main Methods#	#Cross-validation#	#Visualisation Methods#	#Pairwise Scatters#	#Moment Calculations#	#Diagonal Matrix Shorthands#	#Data Retrieval#	#Thesis Reproduction#
ols2()	**k_fold()**	**tsne2()**	**scatter_plot()**	*raw_moment()*	*eye()*	iris_data()	all_experiments()
logit2()	**stratified_k_fold()**	**umap2()**	**scatter_plot_ind()**	*central_moment()*	*diag_eye()*	word2vec_data()	iris_experiments()
svm2()				*standard_moment()*	*diag_eye_nan()*	glove_data()	wine_experiments()
	#Auxiliary Functions#	#Robust Scatters from R#	#Pairwise Contour Scatters#			fasttext_data()	wbc_experiments()
#Used for Logit#	*split_data_ind()*	FastMCD2()	**contour_plot()**	#Weighted Locations#	#Matrix Shorthands#	ODDS_data()	word2vec_experiments()
loglike()	*stratified_split_data_ind()*	FastMVE2()	**contour_plot_ind()**	weighted_mean()	*self_inner()*	mnist_data()	glove_experiments()
	ind2labels()			geometric_median()	*self_outer()*		fasttext_experiments()
			#Misc Figures#	weighted_median()	*symmetrize()*	#MNIST Manipulation#	code_experiment()
	#Evaluation Metrics#		**contour_plot()**			*flatten2d()*	weighting_kernel_graph()
	diagnostics()		**heatmap_plot()**	#Distances#	#RNG Manipulation	*faltten1d()*	
	diagnostics2D()		**component_plot()**	data2dist()	*get_seed()*	*mnist_mean()*	
	get_all_eval()		**bshape_plot()**	*mahalanobis2()*	*next_seed()*		
	mcc()			*mahalanobis1()*		#Word Embeddings#	
			#Auxiliary Functions#		#Auxiliary Functions#	word2vec_data_scratch()	
	#Auxiliary Functions#		*method_title()*	#Categorical Encodings#	*text_subscript()*	glove_data_scratch()	
	confusion_matrix()		*fast_contour_plot()*	vec_cat_encode()	*ts()*	fasttext_data_scratch()	
	reduce_mat()		*get_default_colour()*	mat_cat_encode()	*duplicates()*	*get_embedding()*	
			get_different_colour()			*get_embeddings()*	
			bshape()	#Data Transformations#			
				transform_loc()			
				transform_01()			
				transform_z()			
				transform_rob()			
				#Used for gpca/ics#			
				fix_signs!()			

To do

- Check the code.
- Put it as a package.

All contributors are welcome.

Outline of the presentation

Invariant coordinate selection

ICS - methodology

ICS - implementations

Conclusion

Tutorial

Conclusion

ICS is an attractive unsupervised multivariate method:

- Designed to find structure in a low-dimensional subspace:
  - for outlier detection,
  - as pre-processing for clustering
- Affine invariant.

Conclusion

ICS is an attractive unsupervised multivariate method:

- Designed to find structure in a low-dimensional subspace:
  - for outlier detection,
  - as pre-processing for clustering
- Affine invariant.

Still presents some challenges:

- Choice of scatter matrices.
- Choice of components.

Some perspectives

Implementation:

- R ecosystem to maintain and improve:

  ICS, **ICSShiny**, ICtest, ICSOutlier, ICSClust.
  Add algorithms for functional, compositional, collinear or HDLSS data.
- Python (work in progress)
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- Python (work in progress)
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Github repository:

- https://github.com/AuroreAA/ICS-implementation

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Notations

- $\mathbf{X}$ is a p-dimensional random vector, $F_{\mathbf{X}}$ its cumulative distribution function and $\mathbf{m}(F_{\mathbf{X}})$ an affine equivariant location estimator.
- $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n)'$ a p-variate dataset. $\mathbf{x}_1, \ldots, \mathbf{x}_n$ follow the same distribution as $\mathbf{X}$.

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- $\mathcal{P}_p$ is the set of all symmetric positive definite matrices of order p.
- A scatter functional is defined as a matrix $\mathbf{S}(F_{\mathbf{X}}) \in \mathcal{P}_p$, uniquely defined at $F_{\mathbf{X}}$, which is affine equivariant in the sense that:

$$\mathbf{S}(F_{\mathbf{AX}+\boldsymbol{\gamma}}) = \mathbf{AS}(F_{\mathbf{X}})\mathbf{A}',$$

for all $p \times p$ non-singular matrices $\mathbf{A}$ and all $\boldsymbol{\gamma} \in \mathbb{R}^p$.

For sake of simplicity, the dependence on $F_{\mathbf{X}}$ is dropped.

Choice of scatter matrices I

- COV – COV_4 or FOBI Peña et al. (2010); Cardoso (1989); Nordhausen and Virta (2019); Fischer et al. (2017, 2020)

$$\text{COV}_4(\boldsymbol{X}_n) = \frac{1}{n}\sum_{i=1}^{n} r^2(\boldsymbol{x}_i)(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_n)(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_n)^\top,$$

where $r^2(\boldsymbol{x}_i) = (\boldsymbol{x}_i - \bar{\mathbf{x}}_n)^\top \text{COV}(\boldsymbol{x}_n)^{-1}(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_n)$ is the squared Mahalanobis distance.

Choice of scatter matrices II

- $\mathrm{MCD}_\alpha - \mathrm{COV}$ and $\mathrm{RMCD}_\alpha - \mathrm{COV}$: (Reweighted) Minimum Covariance Determinant Rousseeuw (1985).

$$\mathrm{MCD}_\alpha(\boldsymbol{X}_n) = c_\alpha \frac{1}{n_\alpha} \sum_{j=1}^{n_\alpha} (\boldsymbol{x}_{i_j} - \bar{\boldsymbol{x}}_{\alpha,n})(\boldsymbol{x}_{i_j} - \bar{\boldsymbol{x}}_{\alpha,n})^\top,$$

where $n_\alpha = \lceil \alpha n \rceil$ observations for which the sample covariance matrix has the smallest determinant and usually $\alpha \in [0.5, 1]$.
In our ecosystem it is also interesting to consider values of α that are smaller than 0.5.

CHOICE OF SCATTER MATRICES III

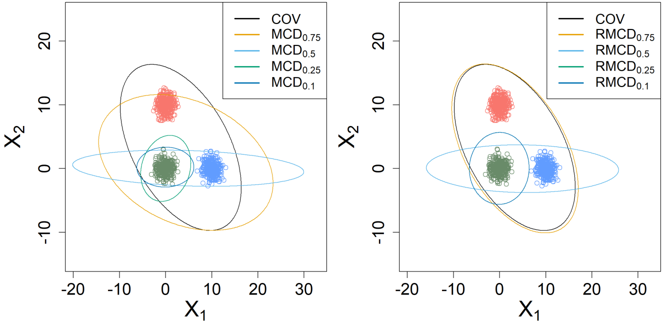

Figure: Shapes of different scatter matrices for a sample from a bivariate Gaussian mixture distribution with three balanced clusters.

Choice of scatter matrices IV

- SCOV – COV, TCOV – UCOV Caussinus and Ruiz-Gazen (1993a, 1995, 2007); Ruiz-Gazen (1996); Caussinus and Ruiz-Gazen (1990); Fekri and Ruiz-Gazen (2015)

Choice of scatter matrices IV

- SCOV − COV, TCOV − UCOV Caussinus and Ruiz-Gazen (1993a, 1995, 2007); Ruiz-Gazen (1996); Caussinus and Ruiz-Gazen (1990); Fekri and Ruiz-Gazen (2015) ⇒ TCOV − COV:

$$\mathrm{TCOV}_\beta(\boldsymbol{X}_n) = \frac{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w(\beta\, r^2(\boldsymbol{x}_i, \boldsymbol{x}_j))(\boldsymbol{x}_i - \boldsymbol{x}_j)(\boldsymbol{x}_i - \boldsymbol{x}_j)^\top}{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w(\beta, r^2(\boldsymbol{x}_i, \boldsymbol{x}_j))},$$

where $r^2(\boldsymbol{x}_i, \boldsymbol{x}_j) = (\boldsymbol{x}_i - \boldsymbol{x}_j)^\top \mathrm{COV}(\boldsymbol{x}_n)^{-1}(\boldsymbol{x}_i - \boldsymbol{x}_j)$,
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  where $r^2(\boldsymbol{x}_i,\boldsymbol{x}_j) = (\boldsymbol{x}_i-\boldsymbol{x}_j)^\top \mathrm{COV}(\boldsymbol{x}_n)^{-1}(\boldsymbol{x}_i-\boldsymbol{x}_j)$, $w(x) = \exp(-x/2)$, $\beta = 4$.

- LCOV – COV Hennig (2009), a local shape matrix based on the aggregation of covariance matrices computed based on 10% of the nearest neighbors (with regard to the Mahalanobis distance).

Parallel Analysis (PA)

As in Peres-Neto et al. (2005) for PCA or in Caussinus et al. (2003).

Computation of cut-offs:

- 10 000 simulations of $\mathcal{N}_n(0, I_p)$
- ICS with $\mathrm{COV}(\mathbf{X}_n)^{-1}\mathrm{COV}_4(\mathbf{X}_n)$
- Quantiles of the ICS eigenvalues at level $1 - \frac{\alpha}{i}$ for each component i, with $\alpha = 5\%$ and $i = 1, \ldots, p$.

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Test:

- Sequentially testing if the ICS eigenvalues are higher than corresponding quantiles.
- Stop as soon as one is lower than the cut-off.

Normality Tests

Finding the first i^{th} coordinate with no longer information about the structure of the data through normality tests.

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Finding the first i^{th} coordinate with no longer information about the structure of the data through normality tests.

Normality tests:

- The D'Agostino test of skewness (DA),
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- The Bonett-Seier (BS) test of Geary's kurtosis,
- The Jarque-Bera (JB) test for normality which is based on both skewness and kurtosis measures,
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Stopping rule

- Sequentially testing if the ICs are gaussian or not.
- Stop as soon as one is gaussian based on the corrected level of 5%.