Archetypal Analysis

Mining the Extreme

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Benchmark Experiments – A Tool for Analyzing Statistical Learning Algorithms

Archetypal analysis

The Merriam-Webster Online Dictionary (2008) defines an archetype as

> *"the original pattern or model of which all things of the same type are representations or copies."*

The aim of archetypal analysis is to find these "pure types"—the archetypes.

Archetypes in psychology: "Ancient or archaic images that derive from the collective unconscious".

Realizations, for examples, in fairy tales:

Hero: the bravest and the cleverest of all

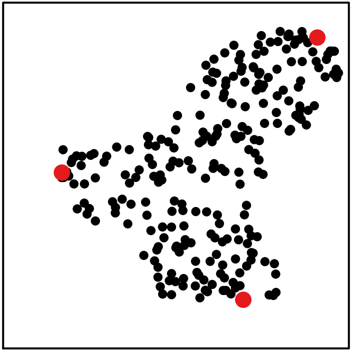
Monster: the scariest and most evil of all

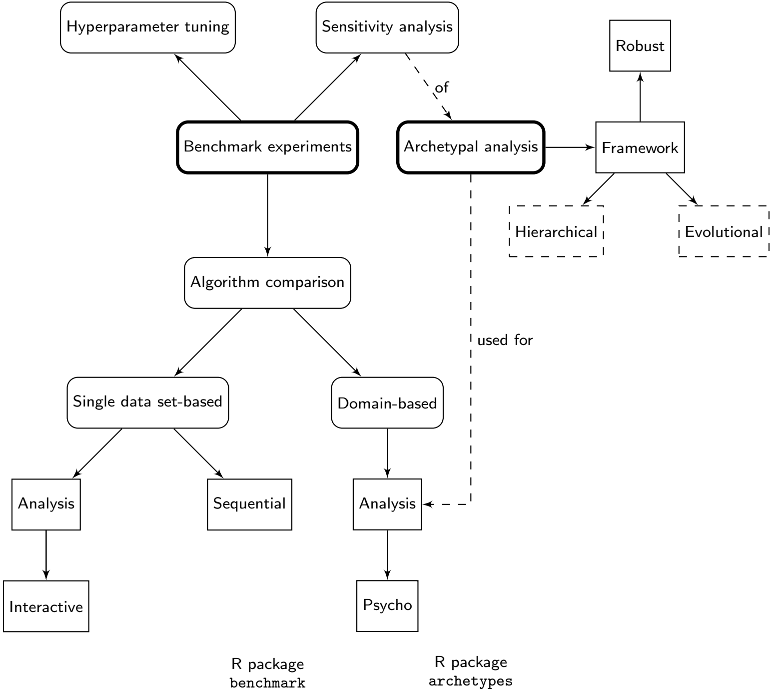
etc.: princess, stepmother, ...

Archetypes in everyday language: Archetypal symbolism often arises in our common usage.

- "There is only one *Lionel Messi*."
- "A little bit of *Chuck Norris* is in everyone."

Archetypes in data analysis: Extremal observations in a (multivariate) data set.

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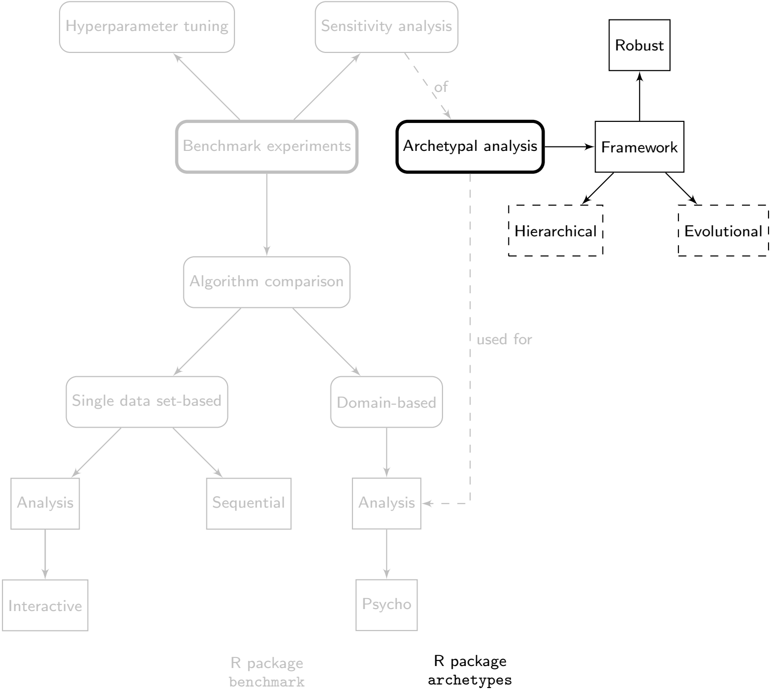
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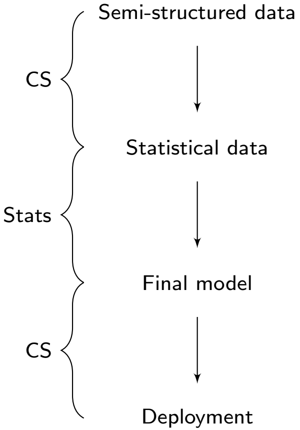
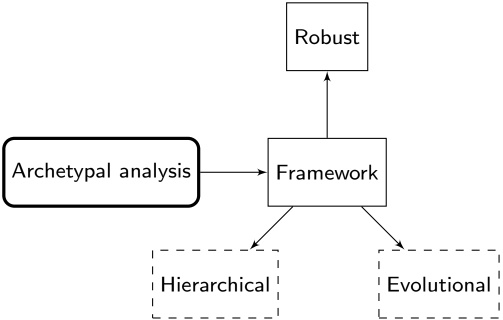




R package
`archetypes`

Archetypal analysis for data analysis

Archetypal analysis (Cutler and Breiman, 1994) has the aim to find a few, not necessarily observed, extremal observations (the archetypes) in a multivariate data set such that

1. all the observations are approximated by convex combinations of the archetypes, and
2. all the archetypes are convex combinations of the observations.

Optimization problem:

Consider an $n \times m$ matrix X. For a given k, the archetypal problem is to find the matrix Z of k m-dimensional archetypes. More precisely, to find the two $n \times k$ coefficient matrices α and β which minimize the residual sum of squares

$$\mathrm{RSS} = \|X - \alpha Z^\top\|_2 \text{ with } Z = X^\top \beta$$

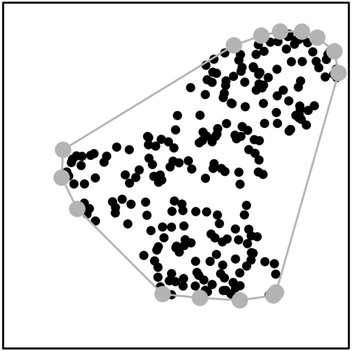
subject to the constraints

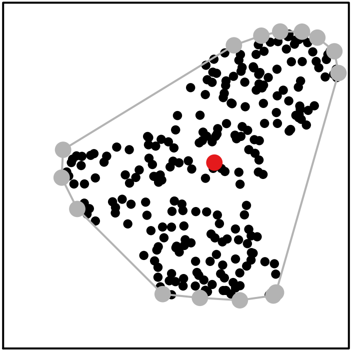
$$\sum_{j=1}^{k} \alpha_{ij} = 1 \text{ with } \alpha_{ij} \geq 0 \text{ and } i = 1, \dots, n,$$
$$\sum_{i=1}^{n} \beta_{ji} = 1 \text{ with } \beta_{ji} \geq 0 \text{ and } j = 1, \dots, k.$$

Approximation of the convex hull:

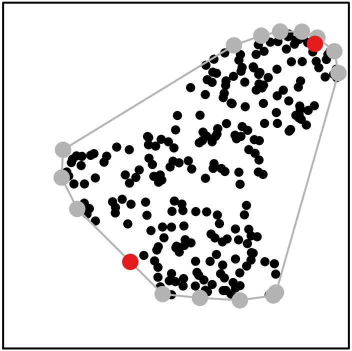
The archetypes lie on the boundary of the convex hull of the data; let N be the number of data points which define the boundary of the convex hull, then if ...

- $1 < k < N$, there are k archetypes on the boundary which minimize RSS;
- $k = N$, exactly the data points which define the convex hull are the archetypes with $\text{RSS} = 0$;
- $k = 1$, the sample mean minimizes the RSS.

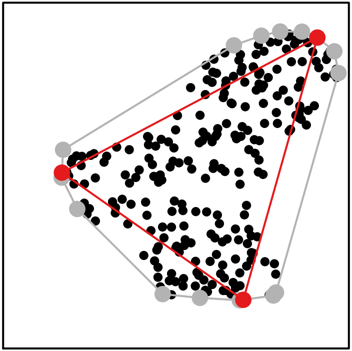




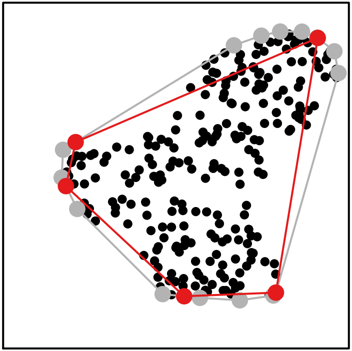
$k = 1$



$k = 2$



$k = 3$

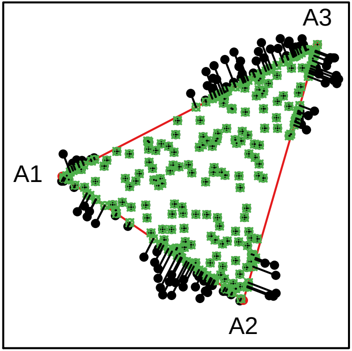


$k = 5$

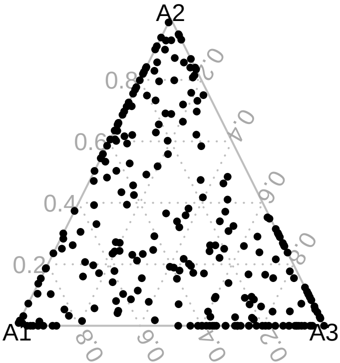
Approximation of the data:

Every observation can either be exactly represented or approximated by a convex combination of the archetypes.

Since $\alpha_{ij} \geq 0$ and $\sum_{j=1}^{k} \alpha_{ij} = 1$, the coefficients α_{ij} of an observation x_i can be interpreted as probabilities $p(x_i|z_j)$ indicating membership to classes represented by the archetypes.



Data approximation, $k = 3$



α coefficients, $k = 3$

Archetypal algorithm

Cutler and Breiman (1994) present an alternating constrained least squares algorithm: it alternates between finding the best α for given archetypes Z and finding the best archetypes Z for given α.

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- In each iteration $n + k$ convex least squares problems are solved (each of $O(n^2)$).
- The algorithm converges, but not necessarily against the global minimum; use different initializations.
- There is no rule for the correct number of archetypes k; use the "elbow criterion" to find an appropriate value k.

Given the number of archetypes k:

1. Data preparation and initialization of archetypes Z, and coefficients α, β
2. Loop until RSS reduction is sufficiently small or the number of maximum iterations is reached:

   2.1 Find best α for the given set of archetypes Z: solve n convex least squares problems ($i = 1, \dots, n$)

   $$\min_{\alpha_i} \frac{1}{2}\|X_i - Z\alpha_i\|_2 \text{ subject to } \alpha_i \geq 0 \text{ and } \sum_{j=1}^{k} \alpha_{ij} = 1.$$

   2.2 Recalculate archetypes $\tilde{Z}$: solve system of linear equations $X = \alpha\tilde{Z}^\top$.

   2.3 Find best β for the given set of archetypes $\tilde{Z}$: solve k convex least squares problems ($j = 1, \dots, k$)

   $$\min_{\beta_j} \frac{1}{2}\|\tilde{Z}_j - X\beta_j\|_2 \text{ subject to } \beta_j \geq 0 \text{ and } \sum_{i=1}^{n} \beta_{ji} = 1.$$

   2.4 Recalculate archetypes Z: $Z = X\beta$.

   2.5 Calculate residual sum of squares RSS.

3. Post-processing

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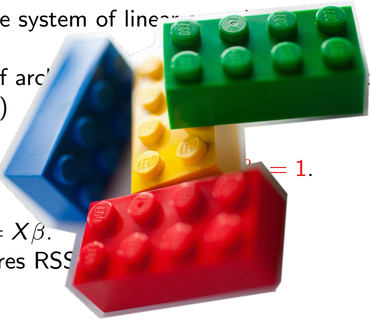
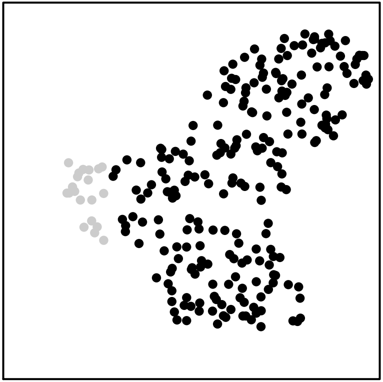


3. Post-processing

Weighted archetypes



Weighted archetypal problem:

Let W be a $n \times n$ diagonal matrix of weights for the observations. The weighted archetypal problem is then

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Weighting the residuals is equivalent to weighting the data set:

$$\begin{aligned} W(X - \alpha Z^\top) &= W(X - \alpha\beta^\top X) = \\ &\qquad WX - (W\alpha)(\beta^\top W^{-1})(WX) = \tilde{X} - \tilde{\alpha}\tilde{Z}^\top \end{aligned}$$

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Therefore the problem can be reformulated as minimizing

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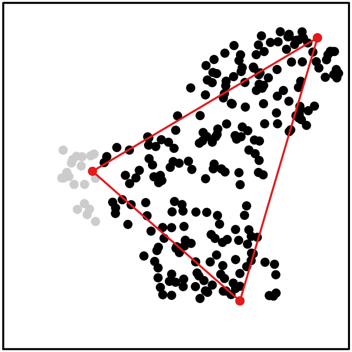
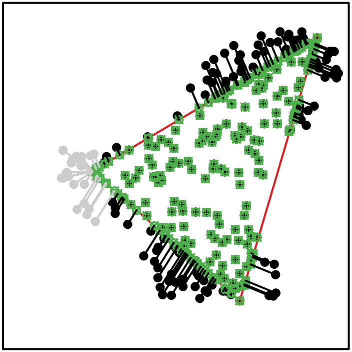
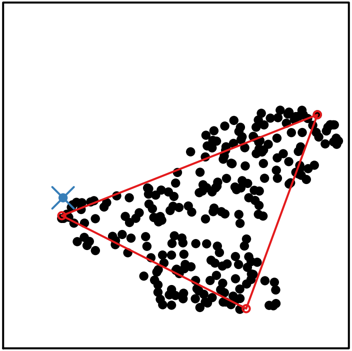
**:** change data preparation (Step 1) and post-processing (Step 3)





Robust archetypes



Breakdown point of 0%

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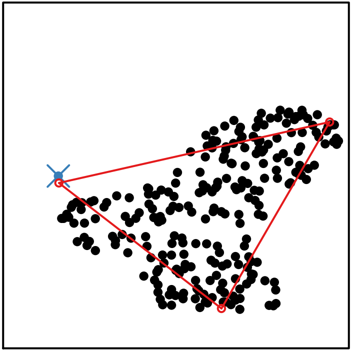

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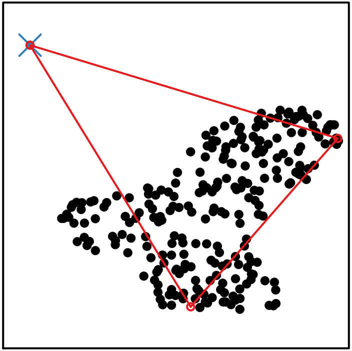

Breakdown point of 0%

M-estimator:

Let $R = (X - \alpha Z^\top)$ be the matrix of the residuals. In the standard archetypal problem,

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M-estimators try to reduce the effect of outliers by replacing the squared residuals by another function $\rho(\cdot)$,

$$\rho(R) \quad \rightarrow \quad \min_{\alpha,\beta}, \qquad Z = X^\top \beta$$

which is less increasing than the square.

Iterated reweighted least squares problem:

The problem can be reformulated as an iterated reweighted least squares one: in the i-th iteration

$$\mathrm{R}^{i} = \|w(R^{(i-1)})R\|_2$$

is solved with $w(\cdot)$ a weight function depending on $\rho(\cdot)$ and the residuals of the $(i-1)$-th iteration.

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We use the generalized *Bisquare* function: Let R_j be the j-th row of R, and $w(R) = \mathrm{diag}(\tilde{w}(R_i))$

$$\tilde{w}(R_j) = \begin{cases} (1 - \|R_j/t\|_2^2)^2, & \|R_i\|_1 < t \\ 0, & \|R_i\|_1 \geq t \end{cases}$$

with tuning parameter t. Following Cleveland we use $t = 6s$ with s the median of the residuals unequal to zero.

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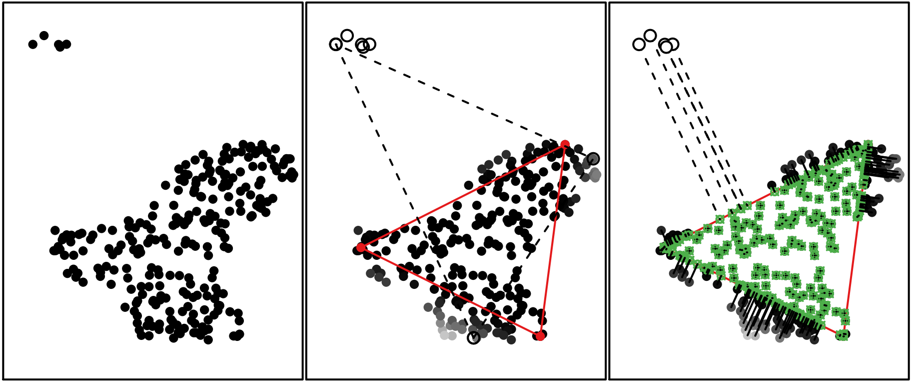
**:** change data reweighting (Step 2.1) and post-processing (Step 3)



Implementation

```
> library("archetypes")
```

```
> archetypesFamily("original")  # or "weighted", "robust", etc.
...
 $ undummyfn   :function (x, zs, ...)
 $ initfn      :function (x, p, ...)
 $ alphasfn    :function (coefs, C, d, ...)
 $ betasfn     :function (coefs, C, d, ...)
 $ zalphasfn   :function (alphas, x, ...)
 $ globweightfn:function (x, weights)
 $ weightfn    :function (x, weights)
...
```

```
> archetypes(data, k, family = archetypesFamily("original"), ...)
> stepArchetypes(data, ..., k, nrep)
```

Application example

Sports analytics is "*the management of structured historical data, the application of predictive analytic models that utilize that data, and the use of information systems to inform decision makers and enable them to help their organizations in gaining a competitive advantage on the field of play.*" (Alamar and Mehrotra, 2011)

In sports analytics, performance analysis, talent analytics, etc., usually the extreme performances are the most interesting aspect.

Archetypal soccer players:

Determine the archetypal soccer players and performance profiles of soccer player playing in four European top leagues.

The skill ratings are from the PES Stats Database, a community-based approach to create a database with accurate statistics and skill ratings for soccer players (originally for the video game "Pro Evolution Soccer" by Konami).

The extracted data set consists of 25 skills of 1658 players (all positions—Defender, Midfielder, Forward—except Goalkeepers) from the German Bundesliga, the English Premier League, the Italian Serie A, and the Spanish La Liga.


PSD – PES STATS DATABASE
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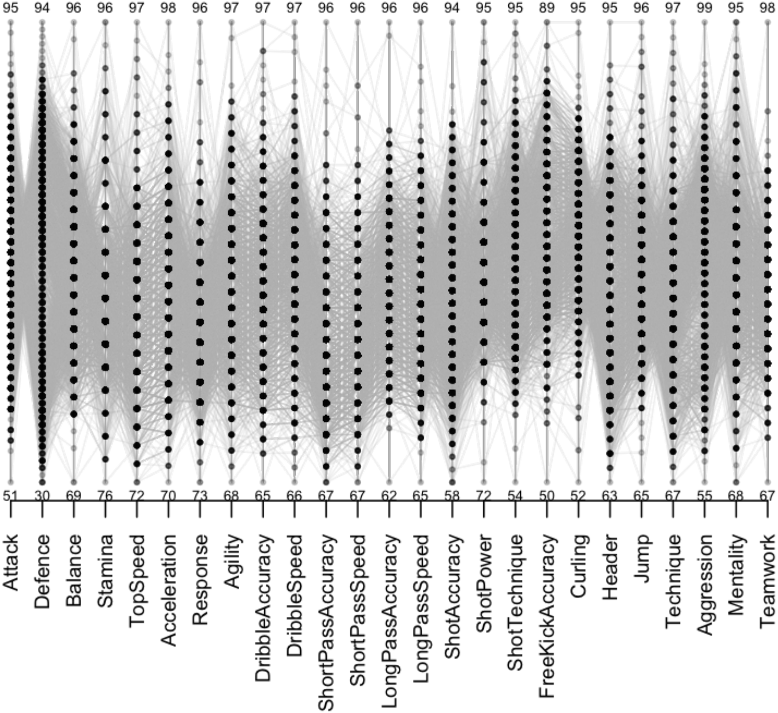
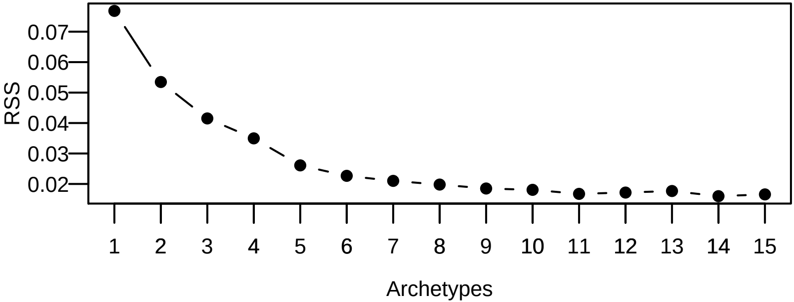
pesstatsdatabase.com/PSD/Player_old.php?Id=602&Club=25
Leo MESSI
Club: FC Barcelona
Name: Leo MESSI
Shirt Name: MESSI
Number: 10
Positions: SS*, AMF
Nationality: Argentinian
Age: 24 (24/06/1987)
Height: 169 cm
Weight: 67 kg
Injury Tolerance: A
Foot: L
Side: B
Attack: 98
Defence: 44
Balance: 83
Stamina: 82
Top Speed: 82
ATT
SPD
TEC
POW
STA
DEF
PLAYER INDEX CARDS:
P05 – Mazing Run
P10 – Incisive Run
P18 – Talisman
S01 – Marauding
S02 – Passer
S03 – 1-on-1 Finish
zotero


95 94 96 96 97 98 96 97 97 97 96 96 96 96 94 95 95 89 95 95 96 97 99 95 98
51 30 69 76 72 70 73 68 65 66 67 67 62 65 58 72 54 50 52 63 65 67 55 68 67
Attack
Defence
Balance
Stamina
TopSpeed
Acceleration
Response
Agility
DribbleAccuracy
DribbleSpeed
ShortPassAccuracy
ShortPassSpeed
LongPassAccuracy
LongPassSpeed
ShotAccuracy
ShotPower
ShotTechnique
FreeKickAccuracy
Curling
Header
Jump
Technique
Aggression
Mentality
Teamwork

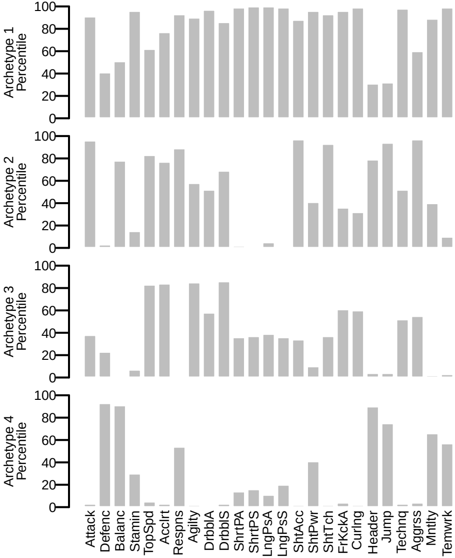
Model fitting and selection:



Model diagnostics:

Outliers, residuals, etc.

Model interpretation:



Archetypes:

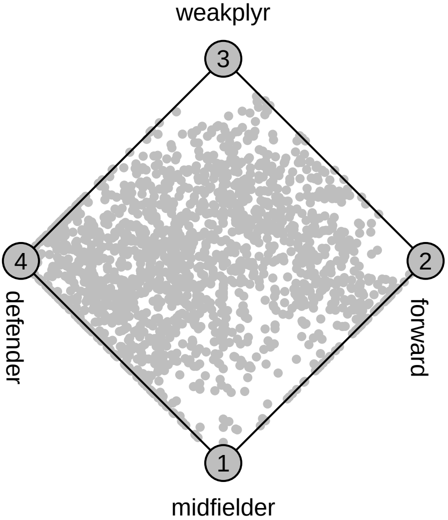
A1 is the archetypal midfielder with all skills high except the defense, balance, header, and jump.

A2 is the archetypal center forward with high skills in attack, shot, acceleration, header and jump, and low passing skills.

A3 is the archetypal weak player with high skills in running, but low skills in most ball related skills.

A4 is the archetypal defender with high skills in defense, balance, header, and jump.

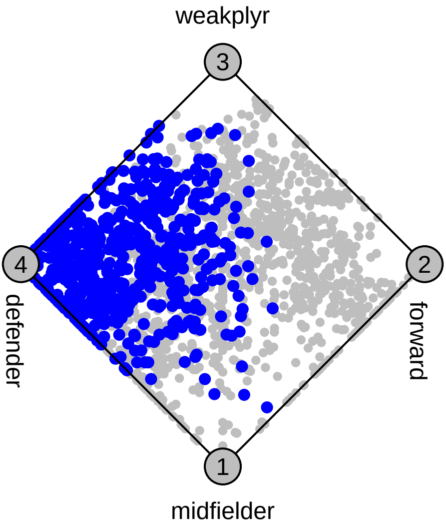
Model interpretation:



Archetypal soccer players:

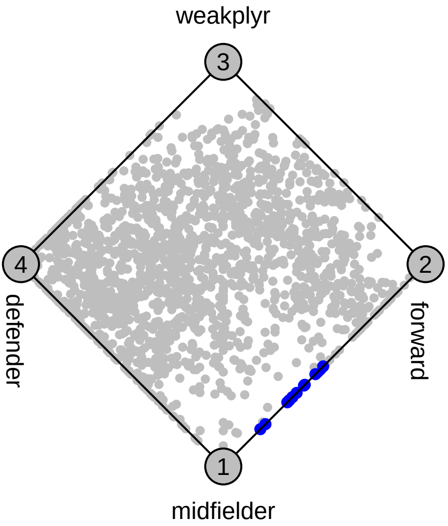
A1: Xavi Hernandez
A2: Filippo Inzaghi
A3: Florin Matei
A4: Massimo Paci

Model interpretation:



Talent scouting:
Find a new defender with offensive qualities.

Model interpretation:



Best soccer players:
A combination of Archetype 1 and Archetype 2 with Archetype 1 contributing more than Archetype 2.

1. Wayne Rooney
2. Leo Messi
3. Cristiano Ronaldo
4. Antonio Di Natale

...

Model deployment:

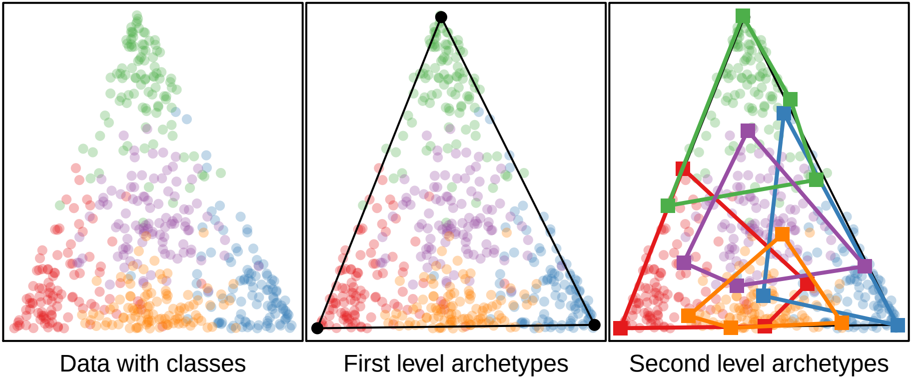
Enable end users to use the model without R; e.g., export the prediction model as standalone software component (as compiled C code).

```
$ sccratypes -i new_players.csv
     A1;      A2;      A3;      A4
0.42517; 0.57495; 0.00000; 0.00000
0.39257; 0.13046; 0.44863; 0.02833
0.08466; 0.01386; 0.04016; 0.86132
0.28616; 0.39076; 0.32318; 0.00000
0.00000; 0.30894; 0.62645; 0.06464
```

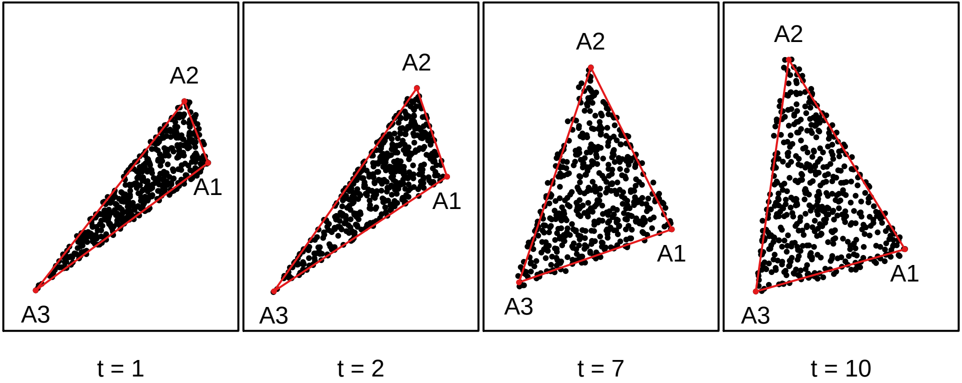
Outlook

Archetypal analysis is "*a promising unsupervised learning tool for many machine learning problems and as the representation is unique in general we believe the method holds particularly great promise for data mining application.*" (Mørup and Hansen, 2012)

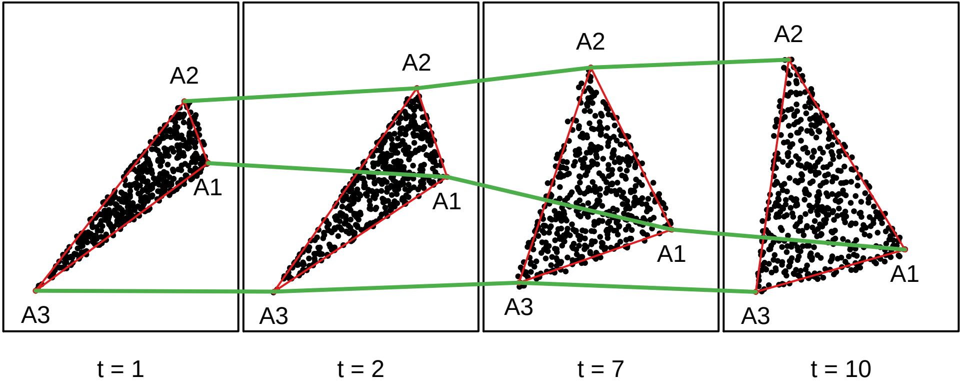
Hierarchical or multilevel archetypal analysis:



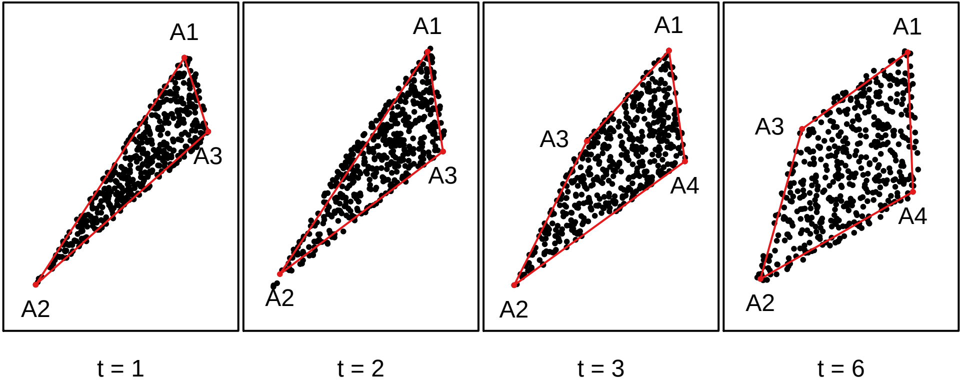
Evolutionary archetypal analysis:



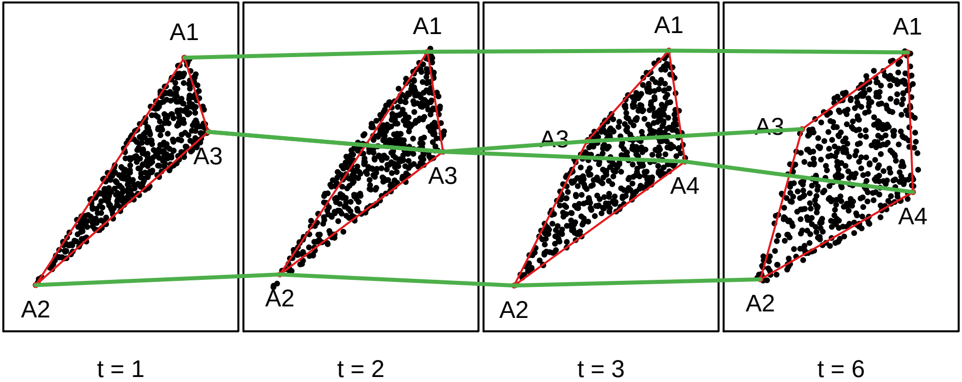
Evolutionary archetypal analysis:



Evolutionary archetypal analysis:



Evolutionary archetypal analysis:



Summary

- Archetypal analysis estimates data-driven (multivariate) extreme values which are easily interpretable by human experts.
- Application in a variety of areas, e.g., in performance analysis (economics), gene analysis (biology), and collaborative filtering (pattern recognition).
- Expertise from different areas, i.e., statistics, machine learning, and computer science.

`http://archetypes.r-forge.r-project.org/`

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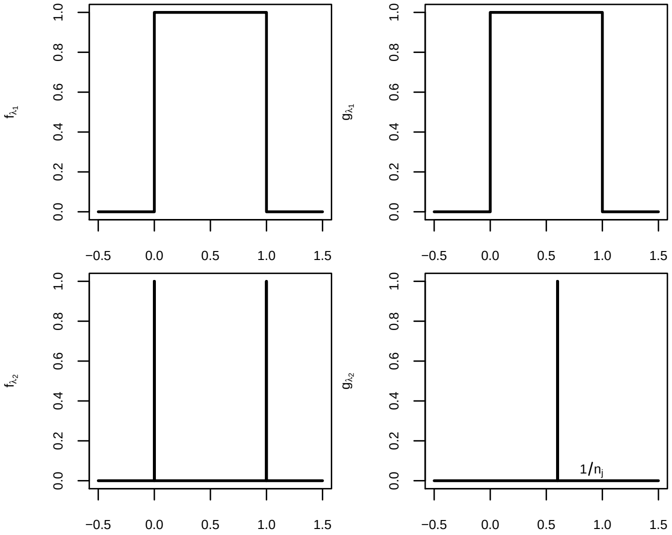
Prototypes problem I

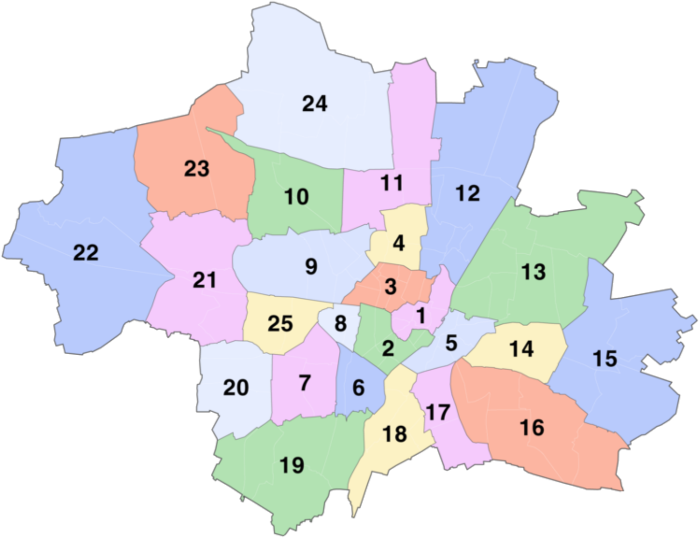
Given is an $n \times m$ matrix X representing a multivariate data set with n observations and m attributes. For a given k, the matrix Z of k m-dimensional prototypes are calculated according to:

$$
\begin{aligned}
& w\|X - \alpha Z^T\| \rightarrow \min \\
& \text{with } \sum_{j=1}^{k} \alpha_{ij} = 1 \text{ and } f_\lambda(\alpha_{ij}) > 0 \\
& Z = X^T \beta \\
& \text{with } \sum_{i=1}^{n} \beta_{ij} = 1 \text{ and } g_\lambda(\beta_{ij}) > 0
\end{aligned}
$$

whereas $i = 1, \ldots, n$, $j = 1, \ldots, k$; α, the coefficients of the prototypes, is an $n \times k$ matrix; β, the coefficients of the observations, is an $n \times k$ matrix; w, the weighting vector, is an n vector; $\| \cdot \|$ is an appropriate matrix norm; f and g are evaluation functions of the coefficients for a specific constraint controlled by the parameter λ.

Prototypes problem II

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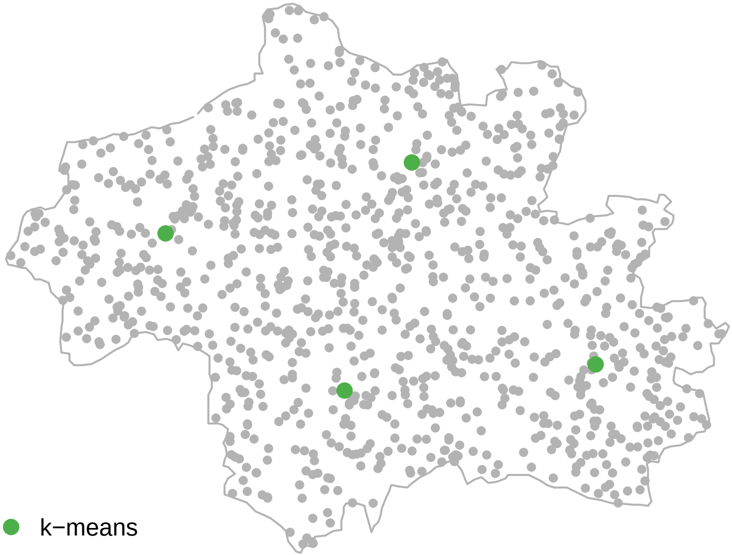
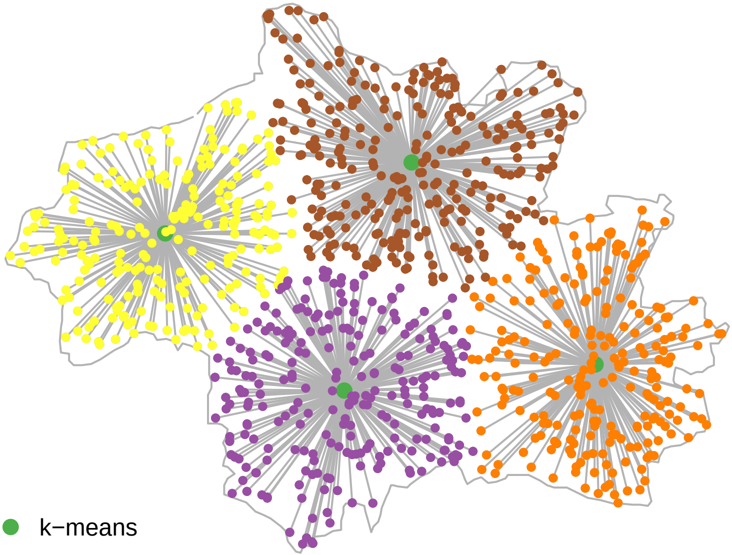
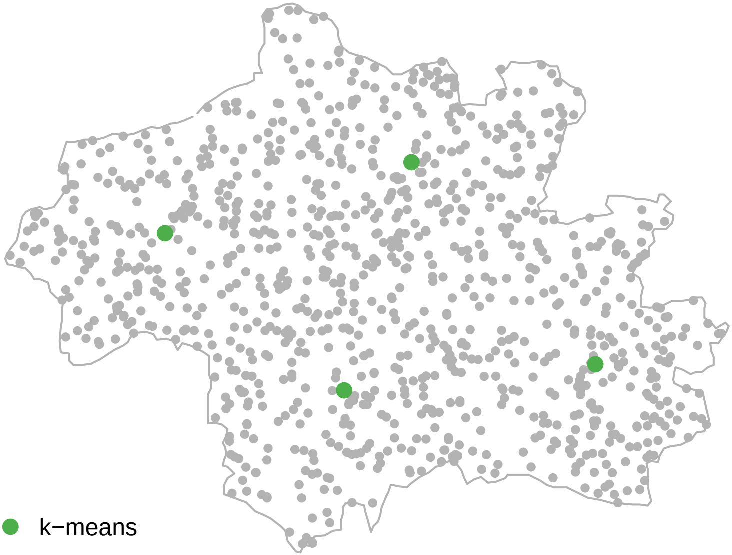
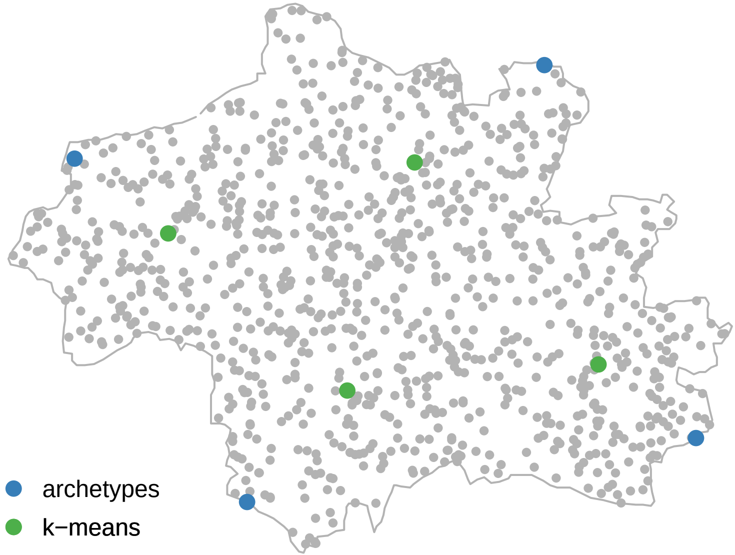
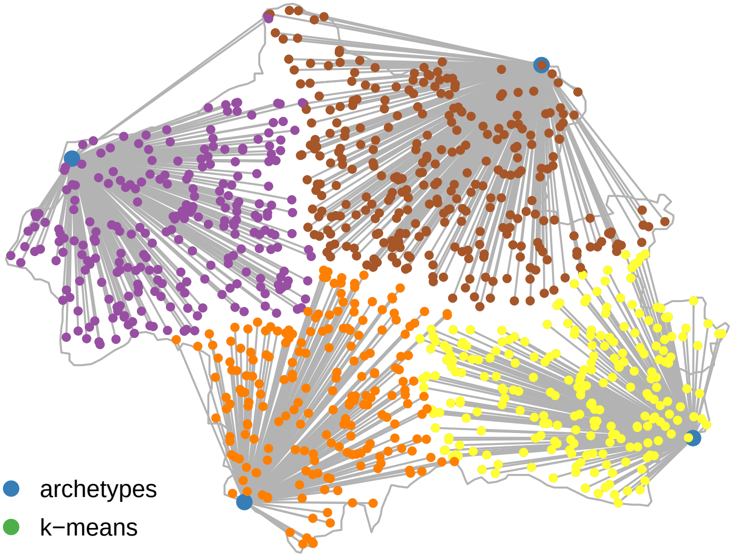

k−means


k−means


k−means


archetypes
k−means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