Feature selection methods

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Summary

Feature selection

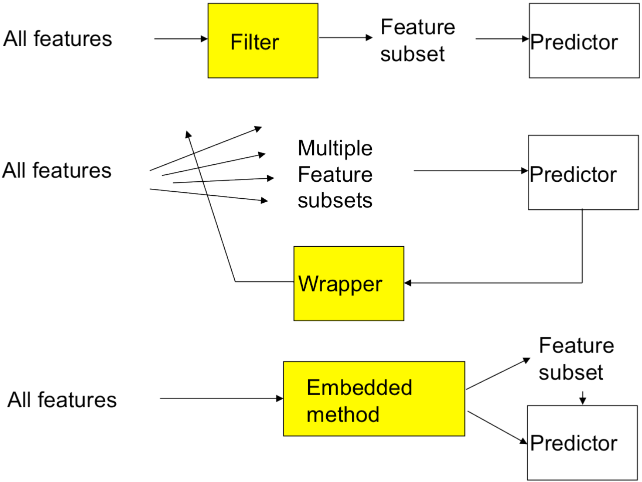
Goal

Find the subset of those feature which are relevant (informative) and needed to solve the task.

Advantages

- Training purposes:
  - Computational cost reduction
  - Performance improvement
- New data extraction
- Interpretation gain

Classification of FS methods



Filters

- Relevance criteria are considered to analyze the importance of a single feature (or a subset of them)
- They are independent of the subsequent classification stage
- They can be applied:
  - In a isolated way, providing a feature ranking.
  - Combined with a search procedure (forward/backward searchs) to find subsets of features.

Relevance criteria

Univariate

Evaluate feature by feature (independently) its relevance

- Variance (unsupervised)
- Correlation coefficient (regression)
- Statistical tests: t-test (binary), ANOVA F-test (multiclass), chi-square (categorical feat)

Multivariate

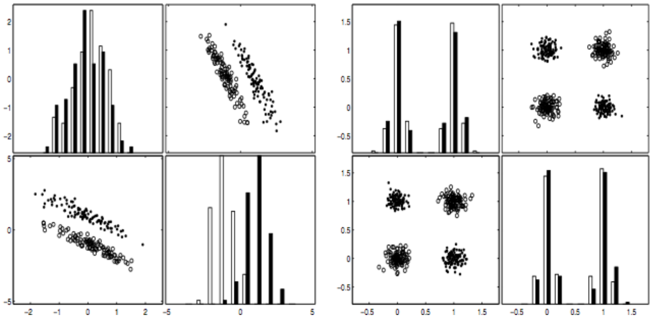
Evaluate the relevance of subsets of features

- Multidimensional relevance criteria: Mutual Information, HSIC,...
- Classification capability: gini (random forest), error, AUC (ROC),...
- Multivariate strategies: Minimum Redundancy Maximal Relevance (mRMR)

Univariate vs. Multivariate criteria

Is good univariate analysis?

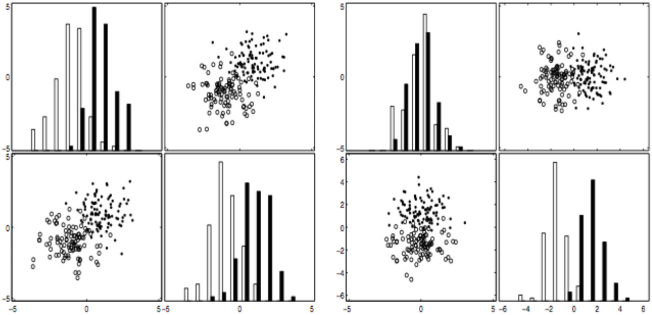
- Useless (isolated) features can be relevant when are combines with other ones



Univariate vs. Multivariate criteria

Is good univariate analysis?

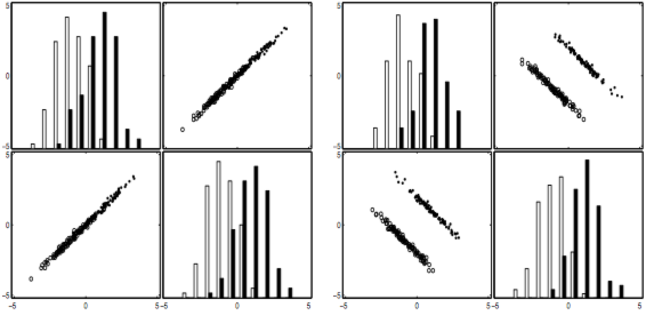
- Let's generate gaussian i.i.d. variables.
- (Presumably) redundant features can be more useful to classify (left plot) than no redundant ones (right).



Univariate vs. Multivariate criteria

Is good univariate analysis?

- Let's generate correlated gaussian variables.
- (Actually) redundant features can be useful to classify (right plot) or completely useless (left).



Anova F-test

- It analyzes if the expected values of a feature/variable differ from one class to other.
- It considers all $p(\mathbf{x}|H_j)$ are gaussian with same standard deviation.
- Are their means equal?
- F-statistic is

$$F = \frac{\text{between group variability}}{\text{within} - \text{group variability}}$$

where

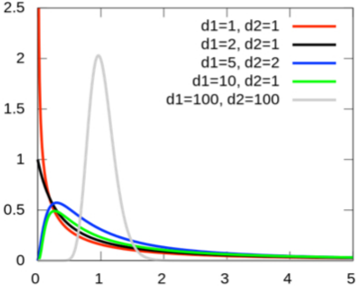
$$\text{between group variability} = \sum_{j=1}^{J} N_j \left(\bar{X}_j - \bar{X}\right)^2 / (J-1)$$

$$\text{within group variability} = \sum_{j=1}^{J} \sum_{i \in C_j} \left(X_{ij} - \bar{X}_j\right)^2 / (L-J)$$

being $\bar{X}$ the overall mean, $\bar{X}_j$ the mean of the data in the class j, N_J the number of data in the j-th class and X_{ij} is the i-th data of class j.

Anova F-test

- F-statistic follows the F-distribution with $J-1$, $L-J$ degrees of freedom under the null hypothesis (equal means).
- The statistic will be large if the between-group variability is large relative to the within-group variability
- This is unlikely to happen if the group means have the same value.



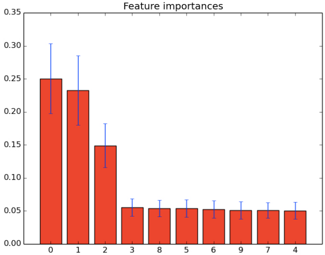
If F is in the tail of the distribution, we can:

- reject the null hypothesis
- claim that the analyzed feature is relevant

RF for Feature Selection

- The relative rank (i.e. depth) of a feature used as a decision node in a tree can be used to assess the relative importance of that feature.
- Features used at the top of the tree are used contribute to the final prediction decision of a larger fraction of the input samples.

- Average those expected activity rates over several randomized trees
- You would be reducing the variance of such an estimate
- Use it for feature selection.



Mutual Information (MI)

- It is able to measure no linear relationships in high dimensional spaces:

$$MI(X,Y) = \int\int p_{X,Y}(x,y) \log \frac{p_{X,Y}(x,y)}{p_X(x)p_Y(y)}$$

- You need to know the probability distributions (usually unknown).
- Otherwise, you can use MI estimators:
  - Histogram based
  - Parzen window based
  - K-NN based

Hilbert-Schmidt Independence Criterion (HSIC)

- The covariance let us measure linear relationships between two variables:

$$\mathcal{C}_{xy} = \mathbb{E}_{xy}(\mathbf{x}\mathbf{y}^\top) - \mathbb{E}_x(\mathbf{x})\mathbb{E}_y(\mathbf{y}^\top)$$

- We can extend the covariance definition to the Hilbert space by means of kernel functions:

$$\mathcal{C}_{xy} = \mathbb{E}_{xy}[(\phi(\mathbf{x}) - \mu_x) \otimes (\psi(\mathbf{y}) - \mu_y)]$$

where $\mu_x = \mathbb{E}_x[\boldsymbol{\phi}(\mathbf{x})]$, and $\mu_y = \mathbb{E}_y[\boldsymbol{\psi}(\mathbf{y})]$.

Hilbert-Schmidt Independence Criterion (HSIC)

- The 2 norm over the covariance matrix computed in the Hilbert space, $\|\mathcal{C}_{xy}\|^2_{\text{HS}}$, provides the Hilbert-Schmidt Independence Criterion.
- It can be expressed in terms of kernel matrices as:

$$\text{HSIC}(\mathbf{X}, \mathbf{Y}) = \frac{1}{m^2}\text{Tr}(\tilde{K}_x \tilde{K}_y)$$

where $\tilde{K}_x$ y $\tilde{K}_y$ are the centered kernel matrices corresponding to variables $\mathbf{X}$ and $\mathbf{Y}$.

  - A. Gretton, O. Bousquet, A. J. Smola, and B. Schölkopf. *"Measuring statistical dependence with Hilbert-Schmidt norms"*, in Proceedings Algorithmic Learning Theory, 2005.
  - Gustavo Camps-Valls, Joris Mooij and Bernhard Schölkopf. *"Remote Sensing Feature Selection by Kernel Dependence Estimation"*, IEEE Geoscience and Remote Sensing Letters, 2009

A variable ranking

- A first approach to find he subset with the most relevant features is ranking them according to their individual relevances.
- It is fast and effective, mainly when $N >> K$ (more variables than data), since exhaustive searchs tend to overfit.
- It presents the same disadvantages as univariate measurements:
  - Variables which are irrelevant can become relevant when they are combine with other ones.
  - Variables which are relevant can become usefulness if they are also redundant.

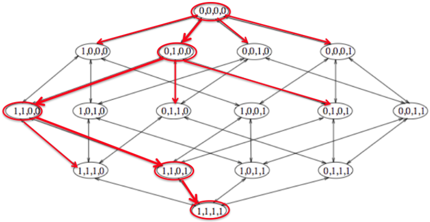
Exhaustive search

F_1	F_2	F_3	F_4	F_5	C
0	0	1	0	1	0
0	1	0	0	1	1
1	0	1	0	1	1
1	1	0	0	1	1
0	0	1	1	0	0
0	1	0	1	0	1
1	0	1	1	0	1

- Data set
  - 5 boolean features
  - $C = \mathrm{OR}(F_1, F_2)$
  - $F_3 = \mathrm{NOT}\ F_2$ y $F_5 = \mathrm{NOT}\ F_4$
  - Optimum set: $\{F_1, F_2\}$ ó $\{F_1, F_3\}$
- How can I find the optimum set?

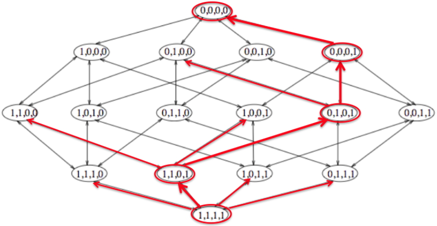
EXHAUSTIVE SEARCH: search in the space of all possible subsets $\Rightarrow$ $2^N - 1$ combinations!!!!!

"Forward search"



- Start with an empty set
- Iteratively, add new features according to a relevance criterion
- We have to evaluate $\frac{N+1}{2}$ subsets
- When can apply an early stopping criterion

"Backward search"



- Start considering all the features
- Iteratively, remove features according to a relevance criterion
- We have to evaluate $\frac{N+1}{2}$ subsets
- When can apply an early stopping criterion

Minimum Redundancy Maximal Relevance (mRMR)

- Extension of univariate scorings to a multivariate analysis.
- Select relevance and redundancy scorings (R_{REL}, R_{RED})
- $var_{\text{sel}} = \{\}$; $var_{\text{cand}} = \{X_1, \ldots, X_D\}$;
  - For i in var_{cand}:

$$\text{Relevance}^i = R_{\text{REL}}(X_i, Y)$$

$$\text{Redundancy}^i = \sum_{i' in var_{\text{sel}}} R_{\text{RED}}(X_i, X_{i'})$$

$$\text{mRMR}^i = \text{Relevance}^i - \text{Redundancy}^i$$

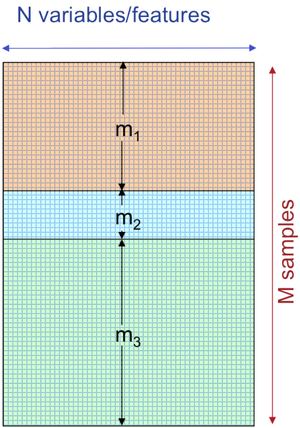
- Compute

$$i^* = \underset{i}{\operatorname{argmax}} \left\{\text{mRMR}^i\right\}$$

  and add i^* to var_{sel} and remove from var_{cand}.
- Repeat the process until any stopping criterion.

Wrappers

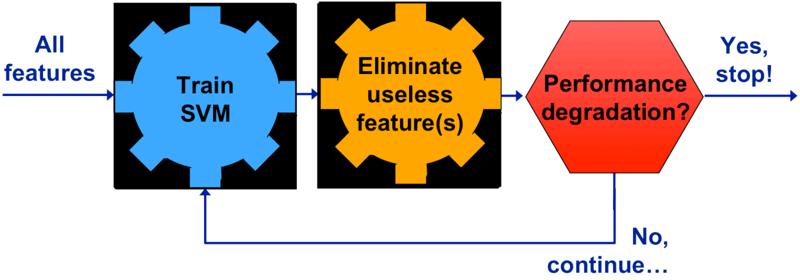
- Divide your data in training, validation and test. With the feature subset to analyze:
  - Train a classifier with the training data
  - Evaluate it with the validation partition
- Select the feature subset with the best validation accuracy
- With cross validation techniques the variance of the final result is reduced
- Final performance is computed over test data



Recursive Feature Elimination

Proposed by...

Isabelle Guyon, Jason Weston, Stephen Barnhill, M.D. and Vladimir Vapnik, "Gene Selection for Cancer Classification using Support Vector Machines". Machine Learning, vol. 46, n.1-3, pp. 389-422.



Recursive Feature Elimination

Procedure

- Start with all the variables selected: $\mathbf{X}_S = \{X_1, \dots, X_D\}$.
- For $1 = 1, \dots, D$
  - Train a SVM with $\mathbf{X}_S$
  - Compute $\|\mathbf{w}\|_2^2$ with the data in $\mathbf{X}_S$

$$\|\mathbf{w}_S\|_2^2 = \sum_{l=1}^{L} \sum_{l'=1}^{L} \alpha^{(l)} \alpha^{(l')} K(\mathbf{X}_S^{(l)}, \mathbf{X}_S^{(l')})$$

  - For each variable, built $\mathbf{X}_{S'} = \mathbf{X}_S \setminus X_i$ and compute $\|\mathbf{w}\|_2^2$ with the data in $\mathbf{X}_{S'}$

$$\|\mathbf{w}_{S'}\|_2^2 = \sum_{l=1}^{L} \sum_{l'=1}^{L} \alpha^{(l)} \alpha^{(l')} K(\mathbf{X}_S^{(l)}, \mathbf{X}_S^{(l')})$$

  - Compute

$$\Delta \mathbf{w}_i = \|\mathbf{w}_S\|_2^2 - \|\mathbf{w}_{S'}\|_2^2$$

- Remove the feature X_{i^*}, where $i^* = \underset{i}{\operatorname{argmin}} \{\Delta \mathbf{w}_i\}$
- Define $\mathbf{X}_S = \mathbf{X}_S \setminus X_i$

Embedded methods: L_1 SVM

Standard SVM formulation

In regularized problems, such as, a linear SVM, we find

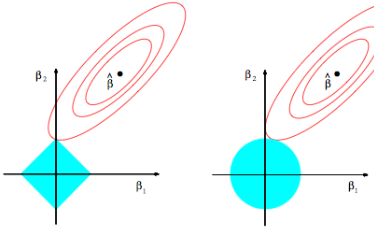
$$\begin{aligned} \min_{\mathbf{w},b,\xi_{(l)}} \quad & \|\mathbf{w}\|_{\mathbf{2}}^{\mathbf{2}} + \mathbf{C}\sum_{\mathbf{l=1}}^{\mathbf{L}} \xi^{(\mathbf{l})} \\ \text{st.} \quad & y^{(l)}\left(\mathbf{w}^T\mathbf{x}^{(l)} + b\right) \geq 1 - \xi^{(l)}; \quad \forall l \\ & \xi^{(l)} \geq 0; \quad \forall l \end{aligned}$$

L_1 SVM formulation

We could modify the regularization term in such a way that the L_1 norm is minimized

$$\begin{aligned} \min_{\mathbf{w},b,\xi_{(l)}} \quad & \|\mathbf{w}\|_{\mathbf{1}} + \mathbf{C}\sum_{\mathbf{l=1}}^{\mathbf{L}} \xi^{(\mathbf{l})} \\ \text{st.} \quad & y^{(l)}\left(\mathbf{w}^T\mathbf{x}^{(l)} + b\right) \geq 1 - \xi^{(l)}; \quad \forall l \\ & \xi^{(l)} \geq 0; \quad \forall l \end{aligned}$$

L_1 SVM



L_1 norm properties

- The lack of continuity in the origin causes most of the coefficients to fall into it, making them to be zero.
- It provides sparse solutions (over $\mathbf{w}$).
- In linear algorithms, this is an automatic **feature selection**.