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Feature evaluation and selection



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Contents

- why feature subset selection?
- filter, wrapper and embedded methods
- in classification: heuristic and optimization based methods
- extensions to supervised learning: multi-task, multi-view, and multi-label learning
- unsupervised and semi-supervised learning
- issues in feature subset selection: stability, redundancy, and higher order interactions.

Huge number of features

• text classification, \approx 50,000 words in a dictionary



- bioinformatics, ≈ 10,000 measurements of gene expression levels
- computer vision, \approx 1,000,000 pixels





Feature subset selection

- choose a small subset of the relevant features from the original features by removing irrelevant, redundant or noisy features
- the aim: better learning performance, i.e. higher learning accuracy, lower computational cost, or better model interpretability

Evaluation of attributes

attr. descriptionattributequalityof the problemevaluationevaluation

- numerical evaluation and ranking of the attributes
- the success of the evaluation procedure depends on the role it plays in learning:
 - feature subset selection
 - building of the tree-based models
 - constructive induction
 - discretization
 - attribute weighting
 - comprehension

• ...

Attribute description

color	weight	shape	size	sort	
red	12	round	middle	apple	
yellow	20	conic	large	pear	
red	15	round	tiny	apple	
green	8	round	small	pear	
yellow	22	conic	large	apple	
mixed	12	conic	small	apple	
green	15	round	middle	apple	
mixed	8	round	tiny	apple	
yellow	6	round	small	pear	

- nominal attributes: ordered and unordered
- numeric attributes

Feature evaluation

- in order to select attributes, we have to evaluate (rank) them
- the success of feature evaluation is measured through the success of learning
- an example: feature evaluation in decision tree building
 - in each interior node of the tree an attribute is selected which determines split of the instances
 - the attributes are evaluated to ensure useful split



Three types of feature selection methods

- filter methods: independent on learning algorithm, select the most discriminative features through a criterion based on the character of data, e.g. information gain and ReliefF
- wrapper methods: use the intended learning algorithm to evaluate the features, e.g., progressively add features to SVM while performance increases
- embedded method select features in the process of learning

Heuristic measures for attribute evaluation

- impurity based
 - information theory based (information gain, gain ratio, distance measure, J-measure)
 - probability based: Gini index, DKM, classification error on the training set
 - MDL
 - statistics G, \aleph^2
 - mean squared and mean absolute error (MSE, MAE)
 - assume conditional independence (upon label) between the attributes
- context sensitive measures:
 - Relief, Contextual Merit,
 - random forests or boosting based attribute evaluation,
 - affinity graph based

Information gain

- measure purity of labels before and after the split
- impurity = entropy

$$I(\tau) = -\sum_{i=1}^{c} p(\tau_i) \log_2 p(\tau_i)$$

$$I(\tau \mid A) = -\sum_{j=1}^{v_A} p(v_j) \sum_{i=1}^{c} p(\tau_i \mid v_j) \log_2 p(\tau_i \mid v_j)$$

$$IG(A) = I(\tau) - I(\tau \mid A)$$







 numeric: requires prior discretization



Attribute interactions



Relief algorithms

 criterion: evaluate attribute according to its power of separation between near instances



 values of good attribute should distinguish between near instances from different class and have similar values for near instances from the same class

Relief algorithms

- no assumption of conditional independence
- context sensitive
- reliable also in problems with strong conditional dependencies
- included in several machine learning systems (e.g., Weka, Orange, scikitlearn, R)
 - Relief (Kira in Rendell, 1992): two class classification
 - ReliefF (Kononenko, 1994): multi-class classification
 - RReliefF (Robnik Šikonja in Kononenko, 1997): regression

Marko Robnik-Šikonja, Igor Kononenko: Theoretical and Empirical Analysis of ReliefF and RReliefF. *Machine Learning Journal*, 53:23-69, 2003

Algorithm Relief

Input: set of instances $\langle x_i, \tau_i \rangle$ *Output*: the vector W of attributes' evaluations

```
set all weights W[A] := 0.0;
```

for i := 1 to m do begin

randomly select an instance R;

find nearest hit H and nearest miss M;

for A := 1 to #all_attributes **do**

W[A] := W[A] - diff(A,R,H)/m + diff(A,R,M)/m;end;

Function diff

for nominal attributes

diff
$$(A, I_1, I_2) = \begin{cases} 0; \text{value}(A, I_1) = \text{value}(A, I_2) \\ 1; otherwise \end{cases}$$

for numerical attributes

diff
$$(A, I_1, I_2) = \frac{\left| \text{value}(A, I_1) - \text{value}(A, I_2) \right|}{\max(A) - \min(A)}$$

- distance between two instances $\delta(I_1, I_2) = \sum_{i=1}^{a} \text{diff}(A, I_1, I_2)$
- unknown values of attributes

Extension ReliefF

- multi-class problems
- incomplete and noisy data
- robust
- uses with k nearest instances from all the classes

The algorithm ReliefF

Input: set of instances $\langle x_i, \tau_i \rangle$ Output: the vector W of attributes' evaluations for v:=1 to a do W_v := 0.0; **for** i := 1 **to** m **do begin** randomly select an instance R_i find k nearest hits H **for** each class $t \neq R_{i,\tau}$ **do** from class t find k nearest misses M(t)**for** v := 1 to a **do** update W_v according to update formula end;

Update formula

$$W_{v} = W_{v} - \frac{1}{m} \operatorname{con}(A_{v}, R_{i}, H) + \frac{1}{m} \sum_{\substack{t=1\\t \neq R_{i,\tau}}}^{c} \frac{p(\tau_{t}) \operatorname{con}(A_{v}, R_{i}, M(t))}{1 - p(R_{i,\tau})}$$
$$\operatorname{con}(A_{v}, R_{i}, S) = \frac{1}{k} \sum_{j=1}^{k} \operatorname{diff}(A_{v}, R_{i}, S_{j})$$

In regression: RReliefF

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W[A] := W[A] - diff(A,R,H)/m + diff(A,R,M)/m; W[A] = P(different value of A | nearest instances with different prediction) -P(different value of A | nearest instances with same prediction) $W[A] = P_{dA|dC} - P_{dA|\neg dC}$

• after applying the Bayesian rule: P(A|B) = P(A)P(B|A)/P(B)

$$W[A] = = \frac{P_{dC|dA}P_{dA}}{P_{dA}} - \frac{(1 - P_{dC|dA})P_{dA}}{1 - P_{dC}}$$

we approximate this formula

• unified view on attribute evaluation in classification and regression

Marko Robnik-Šikonja, Igor Kononenko: An adaptation of Relief for attribute estimation in regression. *Machine Learning, Proceedings of ICML 1997*

Algorithm RReliefF

Input: for each training instance a vector of attribute values x and predicted value $\tau(x)$

Output: vector W of estimations of the qualities of attributes

1. set all
$$N_{dC}$$
, $N_{dA}[A]$, $N_{dC\&dA}[A]$, $W[A]$ to 0;

- 2. for i := 1 to m do begin
- 3. randomly select instance R_i ;
- 4. select **k** instances I_j nearest to R_i ;
- 5. for j := 1 to k do begin
- 6. $N_{dC} := N_{dC} + \operatorname{diff}(\tau(\cdot), R_i, I_j) \cdot d(i, j);$
- 7. for A := 1 to a do begin

8.
$$N_{dA}[A] := N_{dA}[A] + \operatorname{diff}(A, R_i, I_j) \cdot d(i, j);$$

9.
$$N_{dC\&dA}[A] := N_{dC\&dA}[A] + \operatorname{diff}(\tau(\cdot), R_i, I_j) \cdot$$

10.

 $\operatorname{diff}(A, R_i, I_j) \cdot d(i, j);$

- 11. **end**;
- 12. **end**;
- 13. **end**;
- 14. **for** *A* := 1 **to** a **do**
- 15. $W[A] := N_{dC\&dA}[A]/N_{dC} (N_{dA}[A] N_{dC\&dA}[A])/(m N_{dC});$

Relief's interpretations

• probabilistic interpretation

 $W[A] = P(\text{different value of } A \mid \text{nearest instances with different prediction})$ - $P(\text{different value of } A \mid \text{nearest instances with same prediction})$

 ratio of the explained concept: in the limit, an attribute is assigned a weight interpreted as a ratio between the number of prediction values it helps to determine and the number of examined instances

Regularization for feature selection

- feature selection as part of learning (embedded method)
- loss function is composed of two components: prediction error and number/weight of included features

$$L(X, Y, f) = \sum_{i=1}^{n} I(y_i \neq f(x_i)) + \lambda \sum_{j=1}^{a} I(A_j \in X)$$

• in regression we get similar expressions for ridge regression and lasso

Ridge regression

• Ordinary Least Squares (OLS) estimates b's by minimizing

$$RSS = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2.$$

• Ridge regression minimizes a slightly different equation

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = \text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2,$$

Ridge regression adds a penalty on *b*'s !

• The effect of this equation is to add a penalty of the form

where the tuning parameter λ is a positive value.

- This has the effect of "shrinking" large values of b's towards zero.
- It turns out that such a constraint should improve the fit, because shrinking the coefficients can significantly reduce their variance

 $\lambda \sum_{j=1} \beta_j^2,$

• Notice that when $\lambda = 0$, we get the OLS!

Credit data: ridge regression

• As λ increases, the standardized coefficients shrinks towards zero.



Why can shrinking towards zero be a good thing to do?

- It turns out that the OLS estimates generally have low bias but can be highly variable. In particular when n and p are of similar size or when n < p, then the OLS estimates will be extremely variable.
- The penalty term makes the ridge regression estimates biased but can also substantially reduce variance
- Thus, there is a bias/ variance trade-off

Ridge regression bias / variance

- Black: Bias
- Green: Variance
- Purple: MSE
- Increase of λ increases bias but decreases variance



Bias / variance trade-off

 In general, the ridge regression estimates will be more biased than the OLS ones but have lower variance

 Ridge regression will work best in situations where the OLS estimates have high variance



Computational advantages of ridge regression

- If number of features p is large, then using the best subset selection approach requires searching through enormous numbers of possible models
- With ridge regression, for any given λ , we only need to fit one model and the computations turn out to be very simple
- Ridge regression can even be used when p > n, a situation where OLS fails completely!

The LASSO method

- Ridge regression isn't perfect
- One significant problem is that the penalty term will never force any of the coefficients to be exactly zero. Thus, the final model will include all variables, which makes it harder to interpret
- A more modern alternative is the LASSO
- The LASSO works in a similar way to ridge regression, except it uses a different penalty term

LASSO's Penalty Term

• Ridge Regression minimizes

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = \text{RSS} + \lambda \sum_{j=1}^{p} \beta_j^2,$$

• The LASSO estimates the b's by minimizing the

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| = \text{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|.$$

What's the difference between ridge regression and lasso?

• This seems like a very similar idea but there is a big difference.

• Using this penalty, it could be proven mathematically that some coefficients end up being set to exactly zero.

• With LASSO, we can produce a model that has high predictive power and it is simple to interpret.

Credit data: Ridge and LASSO





Selecting the tuning parameter λ

- We need to decide on a value for λ .
- Select a grid of potential values, use cross validation to estimate the error rate on test data (for each value of λ) and select the value that gives the least error rate.



Wrapper approach

start with an empty set of features *S*={} // forward selection **repeat**

add all unused features one by one to *S* train a prediction model with each set *S* evaluate each prediction model

keep the best added feature in *S* **until** all features are added to *S* **return** the best set of features encountered

- high computational load but effective for a given learning model; attention to data overfitting
- how would backward selection differ?

Model evaluation metrics

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Regression: MSE, MAE
- Classification: accuracy, sensitivity, specificity, AUC, precision, recall
- Comparing classifiers:
 - Confidence intervals
 - Cost-benefit analysis and ROC Curves
 - rank-based tests (Friedman/Nemenyi)
 - Bayesian (hierarchical) tests

Classifier evaluation metrics: confusion matrix aka missclassification matrix

Confusion Matrix:

Actual class\Predicted class	C ₁	¬ C ₁	
C ₁	True Positives (TP)	False Negatives (FN)	
– C ₁	False Positives (FP)	True Negatives (TN)	

Example of Confusion Matrix:

Actual class\Predicted	buy_computer	buy_computer	Total
class	= yes	= yes = no	
buy_computer = yes	6954	46	7000
buy_computer = no	412	2588	3000
Total	7366	2634	10000

- Given *m* classes, an entry, *CM*_{i,j} in a confusion matrix indicates # of tuples in class *i* that were labeled by the classifier as class *j*
- May have extra rows/columns to provide totals

Classification accuracy, error rate

A\P	С	¬C	
С	ТР	FN	Р
¬C	FP	TN	N
	P'	N′	All

 Classifier Accuracy, or recognition rate: percentage of test set tuples that are correctly classified

Accuracy = (TP + TN)/All

• Error rate: 1 – accuracy, or Error rate = (FP + FN)/All

Sensitivity and specificity

A\P	С	¬C	
С	ТР	FN	Р
¬C	FP	TN	N
	P'	N′	All

Class Imbalance Problem:

One class may be rare, e.g. fraud, or HIV-positive

Significant *majority of the negative class* and minority of the positive class

Sensitivity: True Positive recognition rate

Sensitivity = TP/P

Specificity: True Negative recognition rate

Specificity = TN/N

Precision, recall and F-measures

- **Precision**: exactness what % of tuples that the classifier labeled as positive are actually positive **Precision = TP/P'** TPprecision $\overline{TP + FP}$
- Recall: completeness what % of positive tuples did the classifier label as positive? **Recall = TP / P** (the same as sensitivity) recall
- Perfect score is 1.0
- Inverse relationship between precision & recall

F measure (F₁ or **F-score)**: harmonic mean of precision and recall,

F_β: weighted measure of precision and recall
 F assigns ß times as much weight to recall as to precision

$$= \frac{(1+\beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$$

 $2 \times precision \times recall$

precision + recall

Example: precision and recall

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	90	210	300	30.00 (sensitivity)
cancer = no	140	9560	9700	98.56 (specificity)
Total	230	9770	10000	96.40 (<i>accuracy</i>)

Precision = 90/230 = 39.13%

Recall = 90/300 = 30.00%

Error depends on decision threshold

• Example: False positive and false negative rate are computed based on probabilities returned by classifier

P(Class=True $|X_1, X_2, ...) ≥ 0.5$

 We can change the two error rates by changing the threshold from 0.5 to some other value in [0, 1]: P(Class=True |X₁, X₂,) ≥ threshold

Varying the threshold



• To reduce false negative rate, we would chose threshold other than 0.5, e.g., threshold ≤ 0.1

ROC curve

- ROC curve shows both TP rate and FP rate simultaneously
- To summarize overall performance we also use area under the ROC curve (AUC)
- The larger the AUC the better is the classifier. Why? What would be an ideal ROC curve?



ROC Curve

False positive rate

Issues affecting model selection

• Accuracy

- classifier accuracy: predicting class label
- regression: MSE, MAE
- Speed
 - time to construct the model (training time)
 - time to use the model (classification/prediction time)
- Robustness: handling noise and missing values
- **Scalability**: efficiency in disk-resident databases
- Interpretability
 - understanding and insight provided by the model
 - other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules

Unsupervised feature selection

- criterion: preserve similarity between instances
- SPEC: spectral feature selection
- take instance similarity matrix and compute its eigenvectors and eigenvalues of graph Laplacian matrix L
- according to spectral clustering theories, the eigenvalues of L measure the separability of the components of the graph and the eigenvectors are the corresponding soft cluster indicators
- rank features according to their consistency with the graph structure
 - a feature that is *consistent* with the graph structure assigns similar values to instances that are near each other in the graph

Zhao Z, Liu H. Spectral feature selection for supervised and unsupervised learning. In Proceedings of ICML 2007, pp. 1151-1157.

Laplacian matrix

• Given a simple graph G with *n* vertices, its Laplacian matrix $L_{n \times n}$ is defined as:

L = D - A

where D is the degree matrix and A is the adjacency matrix of the graph. A only contains 1s or 0s and its diagonal elements are all 0s. For D, a diagonal matrix, in the case of directed graphs, either the indegree or outdegree might be used, depending on the application.

• The elements of L are given by

$$L_{i,j} \begin{cases} \deg(v_i) & ; \ i = j \\ -1 & ; \ i \neq j \text{ and } i \text{ is adjacent to } j \\ 0 & \text{otherwise} \end{cases}$$

- where deg(v_i) is the degree of the vertex i
- in feature selection, the adjacency matrix is weighted by the distance between instances (and class membership)
- the degree serves as an estimation of density around instance (vertex) x

SPEC – spectral feature selection

- compute f^T L f to measure how feature f is consistent with graph
- smaller values indicate better consistency
- both f and L have to be normalized in order not to affect the score



Unsupervised FS with clustering

- Nonnegative Discriminative Feature Selection (NDFS)
- perform spectral clustering to learn the cluster labels of the input samples
- simultaneously optimize for cluster labels and feature selection matrix

Li, Z., Yang, Y., Liu, J., Zhou, X. and Lu, H., 2012, Unsupervised feature selection using nonnegative spectral analysis. In *Proceedings of AAAI*, vol. 2, pp. 1026-1032.

Semi-supervised feature selection

- typically a small sample of labelled and a large sample of unlabeled data is available
- principle: use the label information of labeled data and data distribution or local structure of both labeled and unlabeled data to evaluate feature relevance



image by Techerin, Wikipedia

Laplacian score for semi-supervised feature selection

- Build two graphs:
 - W (within class): labeled instances are connected if from the same class, unlabeled instances are connected if near each other
 - B (between): labelled instances are connected if from different class
- proceed similarly as in unsupervised case, compute eigenvectors of Laplacian graph for W and optimize for soft cluster membership, use degree graph of B for normalization

Cheng, H., Deng, W., Fu, C., Wang, Y. and Qin, Z., 2011. Graph-based semi-supervised feature selection with application to automatic spam image identification. In Computer Science for Environmental Engineering and EcoInformatics (pp. 259-264).

Stability of feature selection

- for high dimensional small sample data, the stability of feature selection is a pressing issue, e.g., in microarray data we might get similar classification accuracy with different sets of features
- Solution: ensemble approach:
 - 1. produce diverse feature sets
 - different feature selection techniques,
 - instance-level perturbation
 - feature-level perturbation
 - stochasticity in the feature selector,
 - Bayesian model averaging
 - combinations of the above techniques
 - 2. aggregate them
 - weighted voting
 - counting



Big data issues

- distributed feature selection, e.g., use Statistical Query model in MapReduce architecture
- procedure
 - 1. decompose the feature selection process into summation forms over training samples,
 - 2. divide data and store data partitions on nodes of the cluster,
 - 3. compute local feature selection results in parallel on nodes of the cluster, and
 - 4. calculate the final feature selection result by integrating the local results.

Janez Kranjc, Roman Orač, Vid Podpečan, Nada Lavrač, Marko Robnik-Šikonja: ClowdFlows: online workflows for distributed big data mining. *FGCS*, 68:38-58, 2017



Multi-view learning

- information from different sources, e.g., measurements from a series of medical examinations for each subject, including clinical, imaging, immunologic, serologic, and cognitive measures.
- some measurements are irrelevant, noisy, or conflicting
- different views typically provide complementary information
- approaches:
 - baseline: concatenate all views
 - construct tensor space from views, preserve relations between views, use feature selection in tensor space
 - use ReliefF like approach, where different views contribute to the distances between objects
 - multi-view clustering and feature selection

Magajna T., Robnik-Šikonja M. (2018) Feature Selection for Multi-View Clustering.



Multi-label learning

- each instance may have more than one label, e.g., purchased items, items on the picture
- approaches
 - transform to single label case (does not take correlations between labels into account)
 - select-max, select-min, select-random
 - copy all, copy weighted
 - label the power set
 - treat multiple labels directly e.g., binary relevance or via graph of correlations between labels
 - Relief like approaches:
 - using multi-label approach to difference of labels (hits, misses) by comparing sets of instance labels (similarly as RReliefF compares different values of response in regression)

Spolaôr, N., Cherman, E.A., Monard, M.C. and Lee, H.D., 2013. A comparison of multi-label feature selection methods using the problem transformation approach. *Electronic Notes in Theoretical Computer Science*, 292, pp.135-151.



Hierarchical multi-label learning

- labels appear in hierarchies, e.g., biological processes or image labelling
- Relief like approach:
 - compute distances between two label as the distance in the hierarchy
 - using multi-label approach to difference of labels (hits, misses) by comparing sets of instance labels (similarly as RReliefF compares different values of response in regression)

Slavkov, I., Karcheska, J., Kocev, D., Džeroski, S. (2017) HMC-ReliefF: Feature ranking for hierarchical multi-label classification. Computer Science and Information Systems. 15. 43-43.



Multitask learning

- learn several related tasks simultaneously with the same model
- advantages:
 - the tasks share knowledge representation,
 - learning several related tasks prevents overfitting
- feature selection:
 - transform to several single tasks, aggregate the results
 - uses wrapper or embedded methods, e.g., multitask random forests where feature importance is estimated as the degradation of performance if feature values are randomly shuffled

Petković, M., Džeroski, S. and Kocev, D., 2017, October. Feature Ranking for Multi-target Regression with Tree Ensemble Methods. In *International Conference on Discovery Science*, pp. 171-185.

Multitask learning



Online feature selection

- in data stream scenario (e.g., financial trading, environmental monitoring, industrial processes)
 - instances arrive sequentially, potentially the learned concept changes (concept-drift problem)
 - detect failure of classifier, reassess features, or
 - continuously asses features, measure their stability
 - new features may appear, e.g., new acronyms or hashtags on Twitter
 - asses new features, potentially replace some of the old chosen ones
 - both the above scenarios appear simultaneously

Wang, J., Zhao, P., Hoi, S.C. and Jin, R., 2014. Online feature selection and its applications. IEEE Transactions on Knowledge and Data Engineering, 26(3), pp.698-710.



Feature selection for graphs

- graphs are useful to represent relations, e.g., in biology
- Linked Open Data: huge graphs of relations for different areas, e.g. Bio2RDF
- GeneOntology a hierarchical description of knowledge about genes
- the graphs are often embedded into a vector space to enable learning
- graph reduction techniques enable relational learning



Jan Kralj, Marko Robnik-Šikonja, Nada Lavrač: NetSDM: Semantic Data Mining with Network Analysis, *Journal of Machine Learning Research*, 20(32):1–50, 2019

Things we did not cover

- cost-sensitive feature evaluation
- privacy preserving feature selection
- adaptations of feature selection approaches for specific important domains: bionformatics, image analysis, NLP, graphs
- etc

Conclusions



- feature selection is a well researched area with many successful approaches
- but: abundance of data, new types of structured data, and many new learning scenarios offer lots of opportunities for new developments
- E.g., combinations of scenarios, like multi-label feature selection in online scenario
- from feature rankings to feature subsets
- how to assure combinations of properties, e.g., scalability, stability, and security