Feature selection

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FEATURE SELECTION

Feature Selection

"is the process of reducing to subset of selected features (variables, predictors) for use in model construction

Informative / Relevant

Non redundant

Loss of information (A)
Irrelevance (B)

Redundance (C)

We assume that the dataset
is characterized by these issues

Reducing (B) (C)
without affecting (A)

Feature Selection

“ is the process of reducing to subset of selected features (variables, predictors) for use in model construction

Informative / Relevant

Non redundant

Loss of information
Irrelevance

Redundance

Reasons for performing a feature-selection step

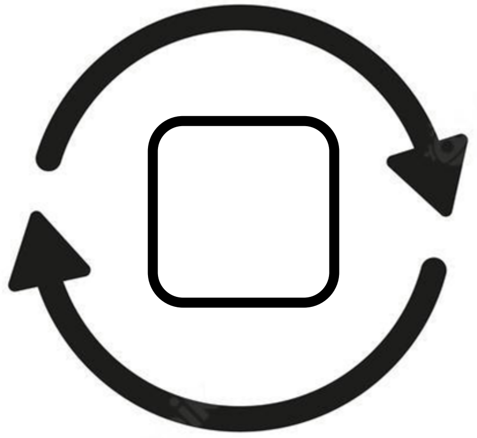
Improving explainability

Reducing training time
by
Reducing computational costs

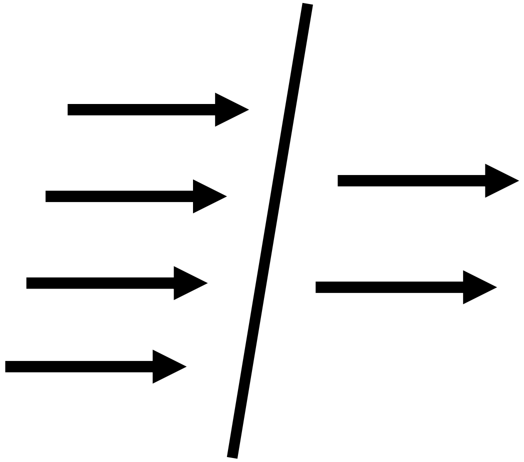
Improving generalization ability
by
Reducing model complexity

(Trying to) avoid the curse of dimensionality

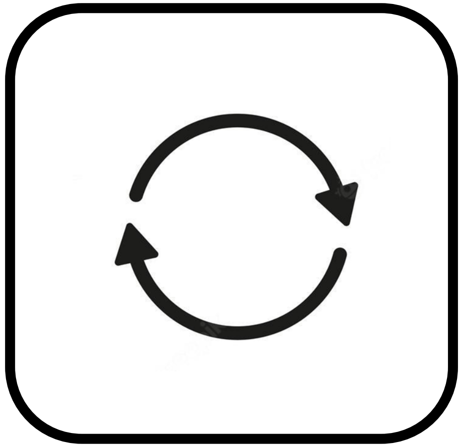
Feature Selection



WRAPPER



FILTER



EMBEDDED

Feature selection

	Feature #1	Feature #2	Feature #3	Feature #4
Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7
Sample #2	+ 0,03	+ 1,81	+ 0,02	- 8,2
Sample #3	- 0,91	+ 9,70	+ 0,01	+ 5,4
Sample #4	+ 1,20	- 1,71	+ 0,01	+ 3,2
…	…	…	…	…
Sample #n	- 0,87	+ 0,88	+ 0,02	- 1,7

Informative / relevant features

	Feature #1	Feature #2	Feature #3	Feature #4
Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7
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…	…	…	…	…
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Informative / relevant features

	Feature #1	Feature #2	Feature #3	Feature #4	Feature #5
Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7	+ 1
Sample #2	+ 0,03	+ 1,81	+ 0,02	- 8,2	+ 1
Sample #3	- 0,91	+ 9,70	+ 0,01	+ 5,4	+ 1
Sample #4	+ 1,20	- 1,71	+ 0,01	+ 3,2	+ 1
…	…	…	…	…	…
Sample #n	- 0,87	+ 0,88	+ 0,02	- 1,7	+ 1

How to capture this information?

Informative / relevant features

	Feature #1	Feature #2	Feature #3	Feature #4	Feature #5
Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7	+ 1
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Sample #3	- 0,91	+ 9,70	+ 0,01	+ 5,4	+ 1
Sample #4	+ 1,20	- 1,71	+ 0,01	+ 3,2	+ 1
…	…	…	…	…	…
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How to capture this information? $\Rightarrow$ $\mathrm{Var}(X) = \mathbf{E}\left[(X-\mu)^2\right]$

Near-Zero Variance

To remove constant and almost-constant predictors across samples

Zero variance

Near-zero variance

Near-Zero Variance

Usually performed following these two criteria: a feature is removed if

(1) the fraction of unique values over the whole set of samples is low (typically <10%)

(1) the ratio of the frequency of the most prevalent value to the frequency of the second most prevalent value is large (typically, around 20).

In our example…

Near-Zero Variance

(1) the fraction of unique values over the whole set of samples is low (typically <10%)

(2) the ratio of the frequency of the most prevalent value to the frequency of the second most prevalent value is large (typically, around 20).

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…	…	…	…	…	…
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(1) $\frac{2}{5} = 40\%$ $\frac{1}{5} = 20\%$

(2) $\frac{3}{5} / \frac{2}{5} = 1{,}5$ $5/5 / 0 > 20$

Non-redundant features

		Feature #1	Feature #2	Feature #3	Feature #4
CLASS 1	Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7
	Sample #2	+ 0,03	+ 1,81	+ 0,02	- 8,2
	Sample #3	- 0,91	+ 9,70	+ 0,01	+ 5,4
CLASS 2	Sample #4	+ 1,20	- 1,71	+ 0,01	+ 3,2
	…	…	…	…	…
	Sample #n	- 0,87	+ 0,88	+ 0,02	- 1,7

Is there a “best approach” to calculate the dependence between two variables?

Mutual Information

Mutual information is a way to calculate statistical dependence between two variables

(it is related to information gain, which will be introduced in classification trees)

$$I(X,Y) = H(X) - H(X|Y)$$

> *A quantity called mutual information measures the amount of information one can obtain from one random variable given another.*

Mutual Information

Mutual information is a way to calculate statistical dependence between two variables

(it is related to information gain, which will be introduced in classification trees)

$$I(X,Y) = H(X) - H(X|Y)$$

Mutual Information

Entropy

Conditional Entropy

> *A quantity called mutual information measures the amount of information one can obtain from one random variable given another.*

Mutual Information

$$I(X,Y) = H(X) - H(X|Y)$$

Mutual information is symmetric and non-negative (and it is measures in bits)

Which range does it span?

In our example...

Mutual Information

In our example…

	Feature #1	Feature #2	Feature #3	Feature #4
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…	…	…	…	…
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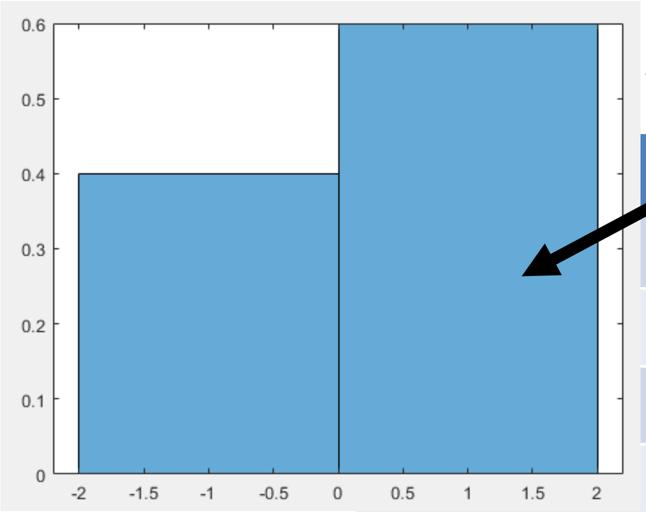
Entropy(feature #1) =
-sum(p.*log2(p))

where
P([0,25 0,03 -0,91 1,20 -0,87]) =
[0,40   0,60]

Entropy = 0,971

Conditional entropy(feature #1 | feature #2) =
sum [p(x,y) .* log2(p(x) / p(x,y))] =
$\boxed{\text{sum [p(y) .* H(X|Y=y)]}}$

Mutual Information



	Feature #1	Feature #2	Feature #3	Fe
	+ 0,25	+ 1,47	+ 0,02	- 5,
	+ 0,03	+ 1,81	+ 0,02	- 8,
	- 0,91	+ 9,70	+ 0,01	+ 5
	+ 1,20	- 1,71	+ 0,01	+ 3
…	…	…	…	…
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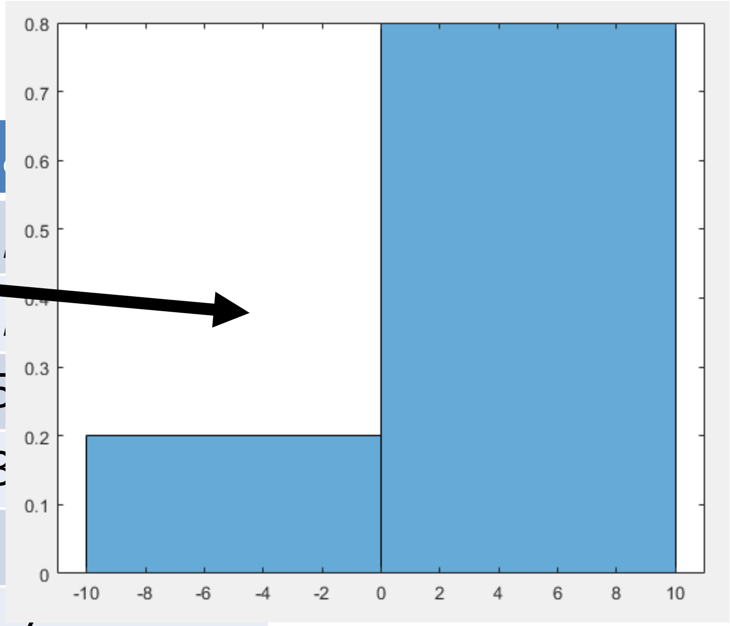

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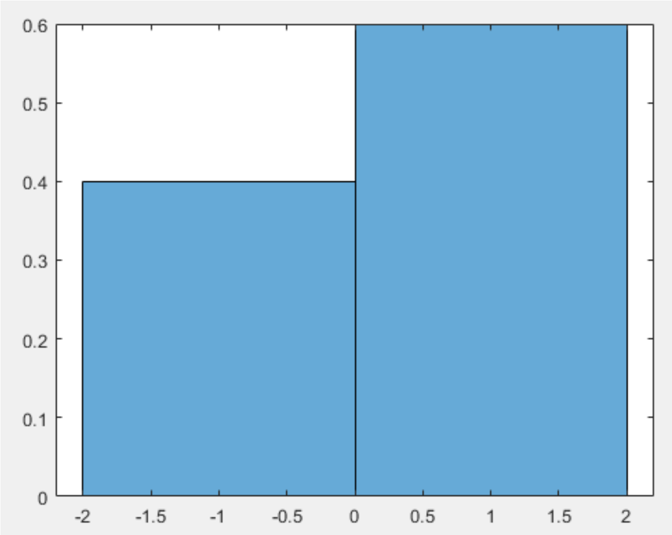
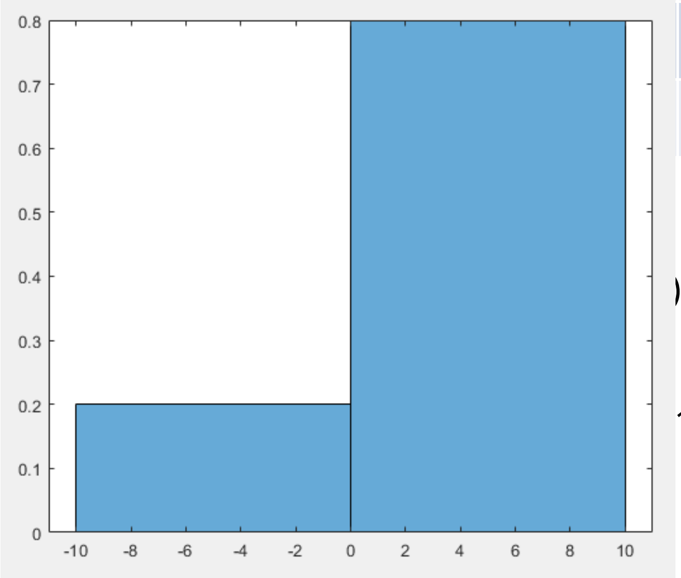
Mutual Information





Feature #1	Feature #2
+ 0,25	+ 1,47
+ 0,03	+ 1,81
- 0,91	+ 9,70
+ 1,20	- 1,71
…	…
- 0,87	+ 0,88

1 / 2	0	1
0	0	2/5
1	1/5	2/5

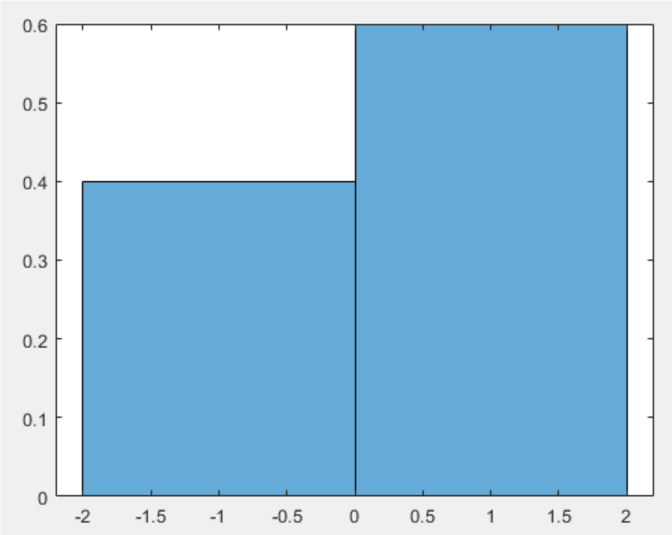
#1) =

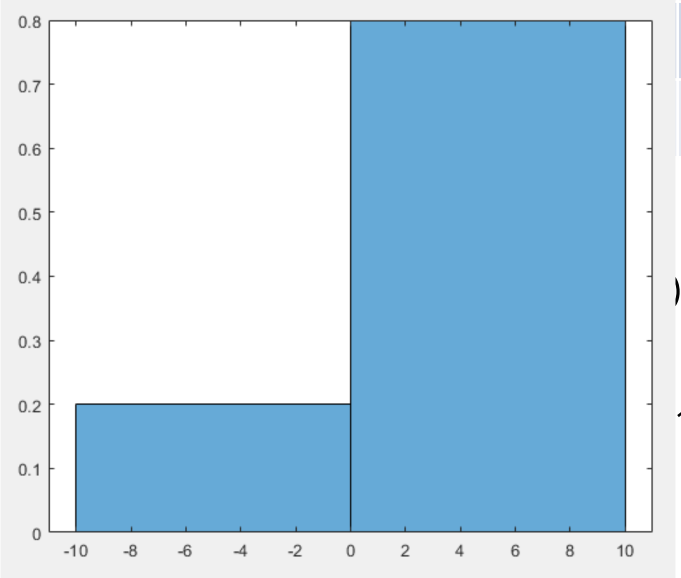
)

1 1,20 -0,87]) =

Conditional entropy(feature #1 | feature #2) =
sum [p(x,y) .* log2(p(x) / p(x,y))] =
sum [p(y) .* H(X|Y=y)]

Mutual Information





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- 0,87	+ 0,88

1 / 2	0	1
0	0	2/5
1	1/5	2/5

#1) =
)

1 1,20 -0,87]) =

Conditional entropy(feature #1 | feature #2) =
sum [p(x,y) .* log2(p(x) / p(x,y))] =
sum [p(y) .* H(X|Y=y)] =

0,4 * H(Y|X=0) + 0,6 * H(Y|X=1) =
0,4 * H(0 , 1) + 0,6 * H(1/3 , 2/3) =
0,6 * 0,918 =
0,55

Mutual Information

	Feature #1	Feature #2
Sample #1	+ 0,25	+ 1,47
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Sample #3	- 0,91	+ 9,70
Sample #4	+ 1,20	- 1,71
…	…	…
Sample #n	- 0,87	+ 0,88

$$I(X,Y) = H(X) - H(X|Y)$$

Entropy(feature #1) =
0,971

Conditional entropy(feature #1 | feature #2) =
0,55

MI = I(feature #1, feature #2) =
0,971 – 0,55 = 0,421

Mutual Information

Proof

$$
\begin{aligned}
\mathrm{H}(Y|X) &\equiv \sum_{x\in\mathcal{X}} p(x)\,\mathrm{H}(Y|X=x) \\
&= -\sum_{x\in\mathcal{X}} p(x) \sum_{y\in\mathcal{Y}} p(y|x)\ \log\ p(y|x) \\
&= -\sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x,y)\ \log\ p(y|x) \\
&= -\sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y) \log\ p(y|x) \\
&= -\sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y) \log \frac{p(x,y)}{p(x)}. \\
&= \sum_{x\in\mathcal{X},y\in\mathcal{Y}} p(x,y) \log \frac{p(x)}{p(x,y)}.
\end{aligned}
$$

Informative / Discriminant features

	Feature #1	Feature #2	Feature #3	Feature #4
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Fisher's Discriminant Ratio / Linear Discriminant Analysis

Linear and supervised reduction of dimensionality

Aim: maximizing the separation between (among) classes

In order to formulate the optimization criterion of maximum separation between (among) classes, we define the following scattering matrices:

- within-class
- between-class

The first says how much the vectors are scattered with respect to the centre of the corresponding classes (each set of data with respect to the corresponding -belonging- class)

The second says how the centres of the classes are scattered with respect to the centre of the entire distribution (it measures how much the classes are scattered)

Fisher's Discriminant Ratio / Linear Discriminant Analysis

Given a dataset containing n samples (x1,y1) … (xn,yn)
where xi are the multidimensional patterns and yi are the labels of the s classes,

let us assume that ni is the number of patterns
and x the mean vector of the i-th class

then the scattering matrices are defined as follows:

within-class

$$\mathbf{S}_w = \sum_{i=1\dots s} \mathbf{S}_i, \qquad \mathbf{S}_i = \sum_{\mathbf{x}_j \mid y_j = i} (\mathbf{x}_j - \overline{\mathbf{x}}_i)(\mathbf{x}_j - \overline{\mathbf{x}}_i)^t$$

covariance matrix
(without normalizing for the number of samples)

sample of the i-th class

between-class

$$\mathbf{S}_b = \sum_{i=1\dots s} n_i \cdot (\overline{\mathbf{x}}_i - \overline{\mathbf{x}_0})(\overline{\mathbf{x}}_i - \overline{\mathbf{x}_0})^t, \qquad \overline{\mathbf{x}_0} = \frac{1}{n} \sum_{i=1\dots s} n_i \cdot \overline{\mathbf{x}}_i$$

global mean

Fisher's Discriminant Ratio / Linear Discriminant Analysis

The criterion for the optimal solution is intuitive, as it tries to maximize the scattering between classes Sb, minimizing at the same time the within-class scattering Sw (within each class).

Thus, this means maximizing the following quantity:

$$J_1 = tr\left(\mathbf{S}_w{}^{-1}\mathbf{S}_b\right) = \sum\nolimits_{i=1\ldots d} \lambda_i$$

$$\frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

Between-class variance

Within-class variance

where *tr* is the trace of the matrix (sum of the eigenvalues).

It can be shown that in order to maximize J1, the LDA space is defined by the eigenvectors corresponding to the first k eigenvalues of the matrix $S_w^{-1} S_b$ (k<n, k<s, k<d) (analogy with PCA).

Maximum value of k = s-1

Fisher's Discriminant Ratio / Linear Discriminant Analysis

In our example…

		Feature #1	Feature #2	Feature #3	Feature #4
CLASS 1	Sample #1	+ 0,25	+ 1,47	+ 0,02	- 5,7
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$$\frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

Between-class variance

Within-class variance

$m_1 = -0,21$
$m_2 = 0,17$

$s_1^2 = 0,38$
$s_2^2 = 2,14$

0,057

0,898

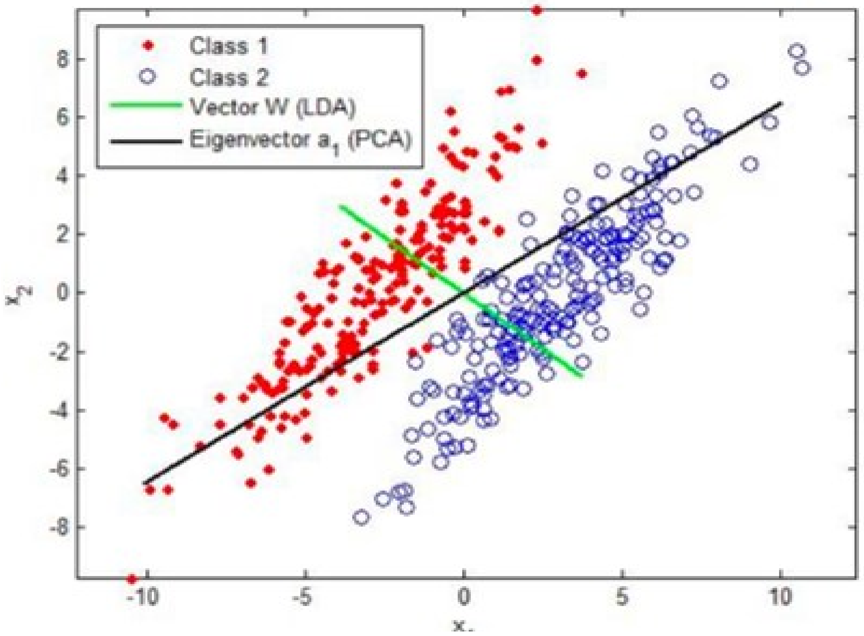
0,033

0,199

Linear Discriminant Analysis vs. Principal Components Analysis

Dimensionality reduction from d = 2 to k = 1

Linear mapping are performed in both cases, but the solution is different:



$$\frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

Between-class variance

Within-class variance

The black line identifies the PCA solution, that is, the hyperplane on which the projected data samples (independently from their belonging class) preserve the maximum information.

The green line identifies the LDA solution, that is, the hyperplane on which the projected data samples allow to best discriminating the two classes.

While PCA privileges the dimensions that best represent the distribution of the data samples, LDA privileges the dimensions that best discriminate them in the two considered classes.