



机器学习/模式识别基础

机器学习/模式识别基础



- 预测与识别
- 预测算法
- 特征提取

1 预测与识别



- 预测: 根据当前的观测, 预测未观测事件
- 识别: 根据当前的观测, 判断是否是预定模式
- 如何定义"事件"或"模式"?
- 机器学习方法: 基于数据的定义







color={0,1,2,3} weight={0,1,2,3,4}

color	weight	sweet?
3	4	yes
2	3	yes
0	3	no
3	2	no
1	4	no

机器学习/模式识别基础



- 预测与识别
- 预测算法
- 特征提取

Classification



Features: color, weight **Label**: taste is sweet (positive/+) or not (negative/-)



(color, weight) \rightarrow sweet ? $\mathcal{X} \rightarrow \{-1, +1\}$

ground-truth function f

examples/training data: $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_m, y_m)\}\$ $y_i = f(\boldsymbol{x}_i)$





Features: color, weight **Label**: sweetness [0,1]



(color, weight) \rightarrow sweetness $\mathcal{X} \rightarrow [-1, +1]$

ground-truth function f

examples/training data: $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_m, y_m)\}$ $y_i = f(\boldsymbol{x}_i)$





find a decision tree that matches the data?

Split-criterion: classification

for every possible split of every feature:









Split-criterion: classification



Split-criterion: classification

Gain ratio (C4.5):

Gain ratio(X) = $\frac{H(X) - I(X; \text{split})}{IV(\text{split})}$ IV(split) = H(split)







Gini index (CART): Gini: $Gini(X) = 1 - \sum_{i} p_i^2$ Gini after split: $\frac{\# \text{left}}{\# \text{all}} Gini(\text{left}) + \frac{\# \text{right}}{\# \text{all}} Gini(\text{right})$







Split-criterion: regression

Training error:



MSE: 8.75+22.83=31.583

MSE: 43.5833



Split-criterion: stop

Stop criterion: no feature to use

Classification: examples are pure of class

Regression: variance small enough



Make-leaf



Classification: major class

Regression: mean value



DT boundary visualization







decision stump

max depth=2

max depth=12

Neural networks







Neuron / perceptron

output a function of sum of input

linear function: $f(\sum_{i} w_{i} x_{i}) = \sum_{i} w_{i} x_{i}$

threshold function:

$$f(\sum_{i} w_i x_i) = I(\sum_{i} w_i x_i > 0)$$

sigmoid function:

$$f(\sum_{i} w_i x_i) = \frac{1}{1 + e^{-\Sigma}}$$





Limitation of single neuron





[Minsky and Papert, Perceptrons, 1969]



Marvin Minsky Turing Award 1969

AI Winter

Multi-layer perceptrons

feed-forward network



sigmoid network with one hidden layer can approximate arbitrary function [Cybenko 1989]



Back-propagation algorithm



 $\hat{y} = F(\boldsymbol{x})$ y gradient descent error: $E(w) = (F(x) - y)^2$ update one weight: $\Delta w_{i,j} = -\eta \frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}}$ weight of the laster layer $\frac{\partial E(\boldsymbol{w})}{\partial E(\boldsymbol{w})} = \frac{\partial E(\boldsymbol{w})}{\partial E(\boldsymbol{x})} \frac{\partial F(\boldsymbol{x})}{\partial E(\boldsymbol{x})}$ $\overline{\partial w_{i,j}} = \overline{\partial F(\boldsymbol{x})} \overline{\partial w_{i,j}}$ weight of the first layer \checkmark $\frac{\partial E(\boldsymbol{w})}{\partial w_{i,j}} = \frac{\partial E(\boldsymbol{w})}{\partial F(\boldsymbol{x})} \frac{\partial F(\boldsymbol{x})}{\partial \text{HL2}} \frac{\partial \text{HL2}}{\partial \text{HL1}} \frac{\partial \text{HL1}}{\partial w_{i,j}}$



[Rumelhart, Hinton, Williams, Nature 1986]

Back-propagation algorithm

For each given training example (x, y), do

- 1. Input the instance **x** to the NN and compute the output value o_u of every output unit *u* of the network
- 2. For each network output unit k, calculate its error term δ_k

$$\delta_k \leftarrow o_k (1 - o_k) (y_k - o_k)$$

3. For each hidden unit k, calculate its error term δ_h

$$\delta_h \leftarrow o_k(1-o_k) \sum_{k \in outputs} w_{kh} \delta_k$$

4. Update each network weight w_{ji} which is the weight associated with the *i*-th input value to the unit *j*



[Rumelhart, Hinton, Williams, Nature 1986]



Advantage and disadvantages

Smooth and nonlinear decision boundary





Slow convergence

Many local optima

Best network structure unknown

Hard to handle nominal features



Deep network

autoencoder:





[Hinton and Salakhutdinov, Science 2006]





classification using posterior probability

for binary classification

$f(x) = \begin{cases} +1, & P(y = +1 \mid x) > P(y = -1 \mid x) \\ -1, & P(y = +1 \mid x) < P(y = -1 \mid x) \\ \text{random, otherwise} \end{cases}$

in general $f(x) = \arg \max_{y} P(y \mid \boldsymbol{x})$ $= \arg \max_{y} P(\boldsymbol{x} \mid y) P(y) / P(\boldsymbol{x})$ $= \arg \max_{y} P(\boldsymbol{x} \mid y) P(y)$

how the probabilities be estimated

Naive Bayes

$$f(x) = \arg \max_{y} P(x \mid y) P(y)$$

estimation the a priori by frequency:
$$P(y) \leftarrow \tilde{P}(y) = \frac{1}{m} \sum_{i} I(y_i = y)$$

assume features are conditional independence given
the class (naive assumption):
$$P(\boldsymbol{x} \mid y) = P(x_1, x_2, \dots, x_n \mid y)$$

 $= P(x_1 \mid y) \cdot P(x_2 \mid y) \cdot \dots P(x_n \mid y)$

decision function:

$$f(x) = \arg\max_{y} \tilde{P}(y) \prod_{i} \tilde{P}(x_i \mid y)$$



Naive Bayes



color={0,1,2,3} weight={0,1,2,3,4}

color	weight	sweet?
3	4	yes
2	3	yes
0	3	no
3	2	no
1	4	no

$$P(y = yes) = 2/5$$

$$P(y = no) = 3/5$$

$$P(color = 3 \mid y = yes) = 1/2$$

$$f(y \mid color = 3, weight = 3) \rightarrow P(color = 3 \mid y = yes)P(weight = 3 \mid y = yes)P(y = yes) = 0.5 \times 0.5 \times 0.4 = 0.1$$
$$P(color = 3 \mid y = no)P(weight = 3 \mid y = no)P(y = no) = 0.33 \times 0.33 \times 0.6 = 0.06$$

$$f(y \mid color = 0, weight = 1) \rightarrow$$

$$P(color = 0 \mid y = yes)P(weight = 1 \mid y = yes)P(y = yes) = 0$$

$$P(color = 0 \mid y = no)P(weight = 1 \mid y = no)P(y = no) = 0$$

Naive Bayes



color={0,1,2,3} weight={0,1,2,3,4}

color	weight	sweet?			
				color	sweet?
3	4	yes		0	VOS
2	3	yes		0	yes
0	2		Ŧ	1	yes
0	3	no		2	yes
3	2	no		2	
1	4	no		3	yes
T	4	no			

smoothed (Laplacian correction) probabilities:

 $P(color = 0 \mid y = yes) = (0+1)/(2+4)$ P(y = yes) = (2+1)/(5+2)

for counting frequency, assume every event has happened once.

$$f(y \mid color = 0, weight = 1) \rightarrow$$

$$P(color = 0 \mid y = yes)P(weight = 1 \mid y = yes)P(y = yes) = \frac{1}{6} \times \frac{1}{7} \times \frac{3}{7} = 0.01$$

$$P(color = 0 \mid y = no)P(weight = 1 \mid y = no)P(y = no) = \frac{2}{7} \times \frac{1}{8} \times \frac{4}{7} = 0.02$$

Nearest neighbor classifier



k-nearest neighbor:



- asymptotically less than 2 times of the optimal Bayes error
- naturally handle multi-class
- no training time
- nonlinear decision boundary
- slow testing speed for a large training data set
- have to store the training data
- sensitive to similarity function



model space: \mathbb{R}^{n+1}

$$f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b$$

we sometimes omit the bias

 $f(\boldsymbol{x}) = \boldsymbol{w}^{\top} \boldsymbol{x}$

w with a constant element
 practically as good as with bias (centered data)

Least square regression





Least square regression

m

$$L(\boldsymbol{w}, b) = \frac{1}{m} \sum_{i=1}^{m} (\boldsymbol{w}^{\top} \boldsymbol{x}_i + b - y_i)^2$$

$$\frac{\partial L(\boldsymbol{w}, b)}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} 2(\boldsymbol{w}^{\top} \boldsymbol{x}_{i} + b - y_{i}) = 0$$
$$\frac{\partial L(\boldsymbol{w}, b)}{\partial \boldsymbol{w}} = \frac{1}{m} \sum_{i=1}^{m} 2(\boldsymbol{w}^{\top} \boldsymbol{x}_{i} + b - y_{i}) \boldsymbol{x}_{i} = 0$$

$$b = \frac{1}{m} \sum_{i=1}^{m} (y_i - \boldsymbol{w}^{\top} \boldsymbol{x}_i) = \bar{y} - \boldsymbol{w}^{\top} \bar{\boldsymbol{x}}$$

$$closed$$

$$form$$

$$w = \left(\frac{1}{m} \sum_{i=1}^{m} \boldsymbol{x}_i \boldsymbol{x}_i^{\top} - \bar{\boldsymbol{x}} \bar{\boldsymbol{x}}^{\top}\right)^{-1} \left(\frac{1}{m} \sum_{i=1}^{m} (y_i \boldsymbol{x}_i) - \bar{y} \bar{\boldsymbol{x}}\right)$$

$$solution$$

$$= var(\boldsymbol{x})^{-1} cov(\boldsymbol{x}, y) = (X^{\top} X)^{-1} X^{\top} Y$$





I.I.D. assumption

all training examples and future (test) examples are drawn *independently* from an *identical distribution*



Hypothesis class





box hypothesis class \mathcal{H} contains all boxes

 $h \in \mathcal{H}$ is a hypothesis $h(\boldsymbol{x}) = \begin{cases} +1, \text{ if } x \text{ is inside the box} \\ -1, \text{ if } x \text{ is outside the box} \end{cases}$
Training and generalization errors





training error

$$\epsilon_t = \frac{1}{m} \sum_{i=1}^m I(h(\boldsymbol{x}_i) \neq y_i)$$

generalization error

$$\epsilon_g = \mathbb{E}_x [I(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))]$$
$$= \int_{\mathcal{X}} p(x) I(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))] dx$$

find a hypothesis minimizes the generalization error



assume i.i.d. examples, and the ground-truth hypothesis is a box



the error of picking a consistent hypothesis:

with probability at least $1 - \delta$ $\epsilon_g < \frac{1}{m} \cdot \left(\ln |\mathcal{H}| + \ln \frac{1}{\delta} \right)$

smaller generalization error:

more examplessmaller hypothesis space

for one *h*

What is the probability of

h is consistent $\epsilon_g(h) \ge \epsilon$

assume *h* is **bad**: $\epsilon_g(h) \ge \epsilon$

h is consistent with 1 example:

 $P \leq 1-\epsilon$

h is consistent with *m* example:

 $P \le (1 - \epsilon)^m$



h is consistent with m example:

There are \boldsymbol{k} consistent hypotheses \cdot

Probability of choosing a bad one: h_1 is chosen and h_1 is bad $P \le (1 - \epsilon)^m$ h_2 is chosen and h_2 is bad $P \le (1 - \epsilon)^m$

 h_k is chosen and h_k is bad $P \leq (1-\epsilon)^m$

overall:

 $\exists h: h \text{ can be chosen (consistent) but is bad}$





 h_1 is chosen and h_1 is bad $P \le (1 - \epsilon)^m$ h_2 is chosen and h_2 is bad $P \le (1 - \epsilon)^m$... h_k is chosen and h_k is bad $P \le (1 - \epsilon)^m$

overall:

 $\exists h: h \text{ can be chosen (consistent) but is bad}$

Union bound: $P(A \cup B) \le P(A) + P(B)$

 $P(\exists h \text{ is consistent but bad}) \leq k \cdot (1-\epsilon)^m \leq |\mathcal{H}| \cdot (1-\epsilon)^m$





 $P(\exists h \text{ is consistent but bad}) \leq k \cdot (1 - \epsilon)^m \leq |\mathcal{H}| \cdot (1 - \epsilon)^m$ $\bigvee P(\epsilon_g \geq \epsilon) \leq |\mathcal{H}| \cdot (1 - \epsilon)^m$ δ

with probability at least $1 - \delta$ $\epsilon_g < \frac{1}{m} \cdot (\ln |\mathcal{H}| + \ln \frac{1}{\delta})$

Inconsistent hypothesis

What if the ground-truth hypothesis is NOT a box: non-zero training error









机器学习/模式识别基础



- 预测与识别
- 预测算法
- 特征提取



disclosure the inner structure of the data to support a better mining performance

> feature extraction construct new features commonly followed by a feature selection usually used for low-level features

> > digits bitmap:





Principal components analysis (PCA)

rotate the data to align the directions of the variance



 $z = w^T x$



Principal components analysis (PCA)

- the first dimension = the largest variance direction
 - $\operatorname{Var}(z_1) = \boldsymbol{w}_1^T \boldsymbol{\Sigma} \boldsymbol{w}_1$

find a unit *w* to maximize the variance

$$\max_{\boldsymbol{w}_1} \boldsymbol{w}_1^T \boldsymbol{\Sigma} \boldsymbol{w}_1 - \boldsymbol{\alpha} (\boldsymbol{w}_1^T \boldsymbol{w}_1 - 1)$$

$$2\Sigma w_1 - 2\alpha w_1 = 0$$
, and therefore $\Sigma w_1 = \alpha w_1$
 $w_1^T \Sigma w_1 = \alpha w_1^T w_1 = \alpha$
w is the eigenvector with the largest eigenvalue





Principal components analysis (PCA)

the second dimension = the largest variance direction orthogonal to the first dimension

$$\max_{\boldsymbol{w}_2} \boldsymbol{w}_2^T \boldsymbol{\Sigma} \boldsymbol{w}_2 - \boldsymbol{\alpha} (\boldsymbol{w}_2^T \boldsymbol{w}_2 - 1) - \boldsymbol{\beta} (\boldsymbol{w}_2^T \boldsymbol{w}_1 - 0)$$

$$2\boldsymbol{\Sigma}\boldsymbol{w}_2 - 2\boldsymbol{\alpha}\boldsymbol{w}_2 - \boldsymbol{\beta}\boldsymbol{w}_1 = 0$$

$$\boldsymbol{\beta} = \boldsymbol{0} \qquad \boldsymbol{\Sigma} \boldsymbol{w}_2 = \boldsymbol{\alpha} \boldsymbol{w}_2$$

w's are the eigenvectors sorted by the eigenvalues









Multidimensional Scaling (MDS)

keep the distance into a lower dimensional space

for linear transformation, W is an n*k matrix

$$rg\min_W \sum_{i,j} (\|oldsymbol{x}_i^ op W - oldsymbol{x}_j^ op W\| - \|oldsymbol{x}_i - oldsymbol{x}_j\|)^2$$





from [Intro. ML]

Linear Discriminant Analysis (LDA)

find a direction such that the two classes are well separated *

$$z = w^T x$$

m be the mean of a class s^2 be the variance of a class

maximize the criterion

$$J(\boldsymbol{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$



 X_1



Linear Discriminant Analysis (LDA)

$$(m_{1} - m_{2})^{2} = (w^{T}m_{1} - w^{T}m_{2})^{2}$$

$$= w^{T}(m_{1} - m_{2})(m_{1} - m_{2})^{T}w$$

$$= w^{T}S_{B}w$$

$$s_{1}^{2} = \sum_{t} (w^{T}x^{t} - m_{1})^{2}r^{t}$$

$$= \sum_{t} w^{T}(x^{t} - m_{1})(x^{t} - m_{1})^{T}wr^{t}$$

$$= w^{T}S_{1}w$$

$$s_{1}^{2} + s_{2}^{2} = w^{T}S_{W}w$$

$$S_{W} = S_{1} + S_{2}$$
The objective becomes:

$$J(w) = \frac{(m_{1} - m_{2})^{2}}{s_{1}^{2} + s_{2}^{2}} = \frac{w^{T}S_{B}w}{w^{T}S_{W}w} = \frac{|w^{T}(m_{1} - m_{2})|^{2}}{w^{T}S_{W}w}$$





Linear Discriminant Analysis (LDA)

The objective becomes:

$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{|\mathbf{w}^T (m_1 - m_2)|^2}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

$$\frac{\boldsymbol{w}^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)}{\boldsymbol{w}^T \mathbf{S}_W \boldsymbol{w}} \left(2(\boldsymbol{m}_1 - \boldsymbol{m}_2) - \frac{\boldsymbol{w}^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)}{\boldsymbol{w}^T \mathbf{S}_W \boldsymbol{w}} \mathbf{S}_W \boldsymbol{w} \right) = 0$$

Given that $w^T (m_1 - m_2) / w^T S_W w$ is a constant, we have

$$w = c \mathbf{S}_{W}^{-1}(\boldsymbol{m}_{1} - \boldsymbol{m}_{2})$$
just take $c = 1$ and find \boldsymbol{w}









Lighting direction

Left-right pose



A low intrinsic dimensional data embedded in a high dimensional space

cause a bad distance measure



ISOMAP

1. construct a neighborhood graph (kNN and ϵ -NN)

2. calculate distance matrix as the shortest path on the graph

3. apply MDS on the distance matrix









from [Intro. ML]



Local Linear Embedding (LLE):

1. find neighbors for each instance

2. calculate a linear reconstruction for an instance $\sum_{r} \|\mathbf{x}^{r} - \sum_{s} \mathbf{W}_{rs} \mathbf{x}_{(r)}^{s}\|^{2}$ 3. find low dimensional instances preserving the

3. find low dimensional instances preserving the reconstruction







from [Intro. ML]

more manifold learning examples







more manifold learning examples

Top arch articulation

Bottom bop articulation

机器学习/模式识别基础

小结

- •预测与识别
 - 用数据定义"模式"
- •预测算法

●特征提取

