



Machine Learning: Chenhao Tan University of Colorado Boulder

LECTURE 21: REVIEW SESSION

## **Precision**

## Confusion matrix:

true labels

	predicted labels		
	positive (1)	negative (0)	
positive (1)	true positive (TP)	false negative $(FN)$	
negative (0)	false positive (FP)	true negative $(TN)$	

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#### **Precision**

#### Confusion matrix:

Precision measures how accurate the predicted positive class are (exactness).

$$precision = \frac{TP}{TP + FP}$$

#### Recall

		predicted labels	
		1	0
true labels	1	TP	FN
	0	FP	TN

Recall measures the fraction of positives that are correctly identified (completeness).

#### Recall

		predicted labels	
		1	0
true labels	1	TP	FN
	0	FP	TN

Recall measures the fraction of positives that are correctly identified (completeness).

$$\mathsf{recall} = \frac{\mathit{TP}}{\mathit{TP} + \mathit{FN}}$$

F1 score strikes a balance between precision and recall.

$$F1 = 2 \frac{\mathsf{precision} \cdot \mathsf{recall}}{\mathsf{precision} + \mathsf{recall}}$$

F1 score of the minority class is usually used when evaluating classifiers on imbalanced datasets.

F1 is a special case of  $F_{\beta}=(1+\beta^2)\frac{\mathrm{precision\cdot recall}}{\beta^2\cdot\mathrm{precision+recall}}.$ 

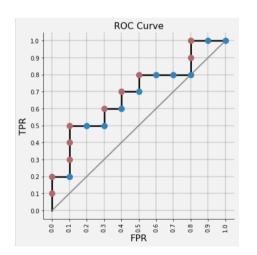
## Constructing a ROC curve

You need a classifier that is able to rank examples by predicted score.

- Order all examples by prediction confidence
- Move threshold to each point, one at a time
- If point is true positive, move vertically (1/NP)
- If point is true negative, move horizontally (1/NN)

#	c	$\hat{p}$	#	c	$\hat{p}$
1	P	0.90	11	P	0.40
2	P	0.80	12	N	0.39
3	N	0.70	13	P	0.38
4	P	0.60	14	N	0.37
5	P	0.55	15	N	0.36
6	P	0.54	16	N	0.35
7	N	0.53	17	P	0.34
8	N	0.52	18	P	0.33
9	P	0.51	19	N	0.30
10	N	0.50	20	N	0.10

## Constructing a ROC curve



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#### **ROC** curve

ROC cares both about TPR and FPR, so it values both positive examples and negative examples.

If only positive examples are important, one can plot precision and recall curve.

#### **Multi-class classification**

Assume training time is  $\mathcal{O}\left(m^{\alpha}\right)$  and test time is  $\mathcal{O}\left(c_{t}\right)$ 

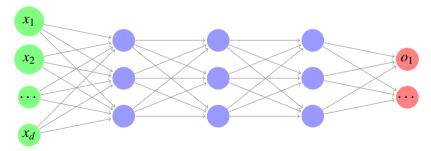
	Training	Testing
One-against-all	$\mathcal{O}\left(\mathit{Cm}^{lpha} ight)$	$\mathcal{O}\left(Cc_{t}\right)$
All-pairs	$\mathcal{O}\left(C^2\left(\frac{m}{C}\right)^{\alpha}\right)$	$\mathcal{O}\left(C^2c_t\right)$
All-pairs	$O(C^{2}(\frac{\pi}{C}))$	0

- One-against-all better for testing time
- All-pairs better for training
- All-pairs usually better for performance

## Forward propagation algorithm

How do we make predictions based on a multi-layer neural network? Store the biases for layer l in  $b^l$ , weight matrix in  $W^l$ 

 $W^1.b^1 W^2.b^2 W^3.b^3 W^4.b^4$ 



## Forward propagation algorithm

# Suppose your network has L layers Make prediction for an instance x

- 1: Initialize  $a^0 = x$
- 2: **for** l = 1 to L **do**
- 3:  $z^l = \boldsymbol{W}^l \boldsymbol{a}^{l-1} + \boldsymbol{b}^l$
- 4:  $a^l = g(z^l)$
- 5: end for
- 6: The prediction  $\hat{y}$  is simply  $a^L$

#### **Network architecture**

- Network architecture (a lot more then fully connected layers)
  - Convulutional layer
  - Recurrent layer

## **Back propagation**

Back propagation allows for computing the gradients of the parameters and watch out for unstable gradients!

$$\begin{split} \delta^L &= \frac{\partial \mathscr{L}}{\partial a_j^L} \odot g'(\mathbf{z}^L) \quad \text{\# Compute $\delta$'s on output layer} \\ \text{For } \ell &= L, \dots, 1 \\ &\frac{\partial \mathscr{L}}{\partial \mathbf{w}^\ell} = \boldsymbol{\delta}^\ell (\mathbf{a}^{l-1})^T \quad \text{\# Compute weight derivatives} \\ &\frac{\partial \mathscr{L}}{\partial \boldsymbol{b}^\ell} = \boldsymbol{\delta}^\ell \qquad \text{\# Compute bias derivatives} \\ &\boldsymbol{\delta}^{\ell-1} &= \left(W^\ell\right)^T \boldsymbol{\delta}^\ell \odot g'(\mathbf{z}^{\ell-1}) \quad \text{\# Back prop $\delta$'s to previous layer} \end{split}$$

#### **Practical issues**

- Unstable gradients
- Weight initialization
- Dropout
- Batch size

## Hard-margin SVM

## Primal problem

$$\min_{\mathbf{w},b} \frac{1}{2} ||\mathbf{w}||^2$$
s.t.  $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1, i \in [1, m]$ 

# Dual problem

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} (\mathbf{x}_{j} \cdot \mathbf{x}_{i})$$
s.t.  $\alpha_{i} \geq 0, i \in [1, m]$ 

$$\sum_{i} \alpha_{i} y_{i} = 0$$

## Karush-Kuhn-Tucker (KKT) conditions

# Primal and dual feasibility

$$y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i+b)\geq 1, \alpha_i\geq 0$$

# Stationarity

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i, \sum_{i=1}^{m} \alpha_i y_i = 0$$

# Complementary slackness

$$\alpha_i = 0 \vee y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$$

## **Soft-margin SVM**

# Primal problem

$$\min_{\mathbf{w},b,\xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{i=1} \xi_i$$
s.t.  $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1 - \xi_i, i \in [1, m]$ 
 $\xi_i \ge 0, i \in [1, m]$ 

# Dual problem

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} (\boldsymbol{x}_{j} \cdot \boldsymbol{x}_{i})$$
s.t.  $C \geq \alpha_{i} \geq 0, i \in [1, m]$ 

$$\sum_{i} \alpha_{i} y_{i} = 0$$

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#### Karush-Kuhn-Tucker (KKT) conditions

# Primal and dual feasibility

$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1 - \xi_i, \xi_i \ge 0, C \ge \alpha_i \ge 0, \beta_i \ge 0$$

# Stationarity

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i, \sum_{i=1}^{m} \alpha_i y_i = 0, \alpha_i + \beta_i = C$$

## Complementary slackness

$$\alpha_i[y_i(\mathbf{w}\cdot\mathbf{x}_i+b)-1+\xi_i]=0, \beta_i\xi_i=0$$

#### Kernels

$$\max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{i=1}^{m} \alpha_i \alpha_j y_i y_j (\mathbf{x_i} \cdot \mathbf{x_j}) \qquad \max_{\alpha} \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{i=1}^{m} \alpha_i \alpha_j y_i y_j K(\mathbf{x_i}, \mathbf{x_j})$$

- Replace all dot product with kernel evaluations  $K(x_1, x_2)$
- Makes computation more expensive, overall structure is the same
- K is a Gram matrix