A Support Vector Method for Multivariate Performance Measures

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Thanks to Rich Caruana, Alexandru Niculescu-Mizil, Pierre Dupont, Jérôme Callut

Supervised Learning

• Find function from input space X to output space Y

$$h: X \longrightarrow \{+1, -1\}$$

such that the prediction error is low.

Text Classification:

- F₁-Score
- Precision/Recall Break-Even (PRBEP)

Medical Diagnosis:

• ROC Area

Information Retrieval:

• Precision at 10

Related Work

- Approach "Estimate Probabilities"
 - E.g. [Platt, 2000] [Langford & Zadrozny, 2005] [Niculescu-Mizil & Caruana, 2005]
 - Potentially solve harder problem than required
- Approach "Optimize Substitute Loss, then Post-Process"
 - E.g. [Lewis, 2001] [Yang, 2001] [Abe et al. 2004] [Caruana & Niculescu-Mizil, 2004]
 - Typically multi-step approach, cross-validation
- Approach "Directly Optimize Desired Loss"
 - Linear cost models: e.g. [Morik et al., 1999] [Lin et al., 2002]
 - ROC-Area: e.g. [Herbrich et al. 2000] [Rakotomamonjy, 2004]
 [Cortes & Mohri, 2003] [Freund et al., 1998] [Yan et al., 2003]
 [Ferri et al., 2002]
 - F₁-Score: difficult [Musicant et al. 2003]

Overview

- Formulation of Support Vector Machine for
 - any loss function that can be computed from the contingency table.
 - F1-score, Error Rate, Linear Cost Models, etc.
 - any loss function that can be computed from contingency tables with cardinality constraints.
 - PRBEP, Prec@k, Rec@k, etc.
 - ROC-Area
- Polynomial Time Algorithm
- Conventional classification SVM is special case
 - New optimization problem
 - New representation and (extremely sparse) support vectors

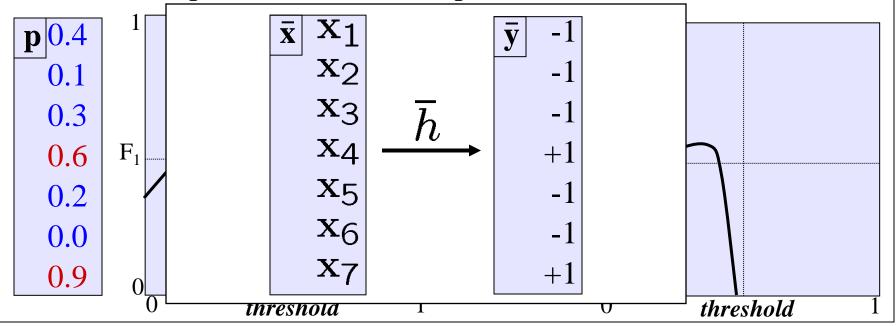
Optimizing F_1 -Score

• F_1 -score is non-linear function of example set

 $- F_I$ -score: harmonic average of precision and recall

$$F_1 = \frac{2 \operatorname{Prec} \operatorname{Rec}}{\operatorname{Prec} + \operatorname{Rec}}$$

- For example vector $\mathbf{x_1}$. Predict $y_1 = 1$, if $P(y_1 = 1/\mathbf{x_1}) = 0.4$? Depends on other examples!



Approach: Multivariate Prediction

- **Training Data:** $S = ((x_1, y_1), ..., (x_n, y_n)) \sim_{i.i.d} \Pr(x, y)$
- Conventional Setting: learn $h : X \longrightarrow \{-1, +1\}$

$$R^{\delta}(h) = \int \delta \left(h(\mathbf{x}'), y' \right) d \Pr(\mathbf{x}', y')$$
$$\hat{R}^{\delta}_{S}(h) = \frac{1}{n} \sum_{i=1}^{n} \delta \left(h(\mathbf{x}_{i}), y_{i} \right)$$

• Multivariate Setting: learn $\overline{h} : X^n \longrightarrow \{-1, +1\}^n$

$$R^{\Delta}(\bar{h}) = \int \Delta(\bar{h}(\mathbf{x}'_{1},...,\mathbf{x}'_{n'}), (y'_{1},...,y'_{n'})) d\Pr(S')$$
$$\hat{D}^{\Delta}(\bar{h}) = \Delta(\bar{h}(\mathbf{x}'_{1},...,\mathbf{x}'_{n'}), (y'_{1},...,y'_{n'}))$$

$$\widehat{R}_{S}^{\Delta}(\overline{h}) = \Delta\left(\overline{h}(\mathbf{x}_{1},...,\mathbf{x}_{n}),(y_{1},...,y_{n})\right)$$

Note:

If
$$\Delta(\bar{h}(\mathbf{x}_1, ..., \mathbf{x}_n), (y_1, ..., y_n)) = \frac{1}{n} \sum_{i=1}^n \delta(h(\mathbf{x}_i), y_i)$$

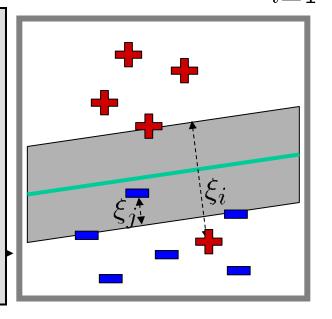
then both settings are equivalent.

Support Vector Machine [Vapnik et al.]

- Training Examples: $(x_1, y_1), ..., (x_n, y_n) \ x \in \Re^N \ y \in \{+1, -1\}$
- Hypothesis Space: $h(\mathbf{x}) = sgn[\mathbf{w}^T \mathbf{x} + b]$ with $\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i$
- **Training:** Find hyperplane $\langle \mathbf{w}, b \rangle$ with minimal $\frac{1}{\delta^2} + C \sum_{i=1}^{n} \xi_i$

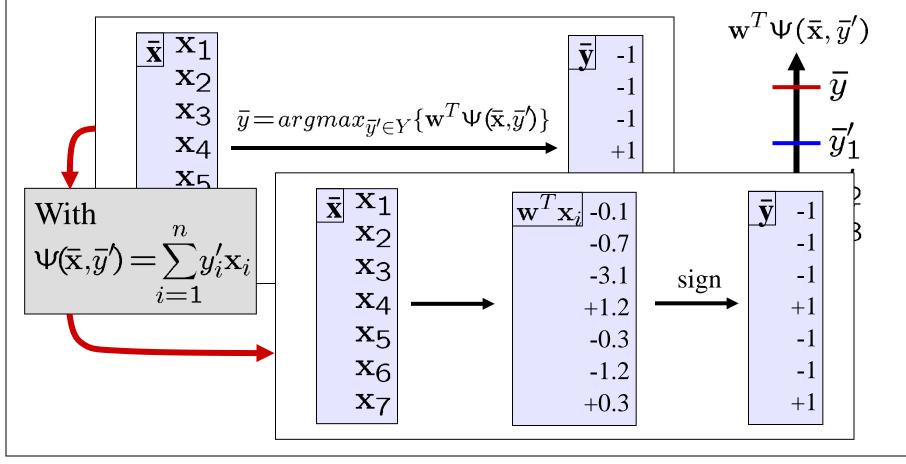
Optimization Problem:

$$\begin{array}{ll} \min_{\mathbf{w},\xi,b} & \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^n \xi_i \\ s.t. & y_1(\mathbf{w}^T\mathbf{x}_1 + b) \ge 1 - \xi_1 \\ & \cdots \\ & y_n(\mathbf{w}^T\mathbf{x}_n + b) \ge 1 - \xi_n \end{array}$$



Multivariate Support Vector Machine

- **Approach:** Linear Discriminant [Collins 2002] [Lafferty et al. 2002] [Taskar et al. 2004] [Tsochantaridis et al. 2004] etc.
 - "Learn weights w so that $\mathbf{w}^T \Psi(\bar{\mathbf{x}}, \bar{y})$ is max for correct \bar{y} ."



Multivariate SVM Optimization Problem

Approach: Structural SVM [Taskar et al. 04] [Tsochantaridis et al. 04]

 $\mathbf{w}^T \Psi(\mathbf{\bar{x}}, \mathbf{\bar{y}}')$

 $\mathbf{w}^T \Psi(\mathbf{\bar{x}}, \mathbf{\bar{y}}')$

 $\Delta(\bar{y},\bar{y}'_1)$

Hard-margin optimization problem:

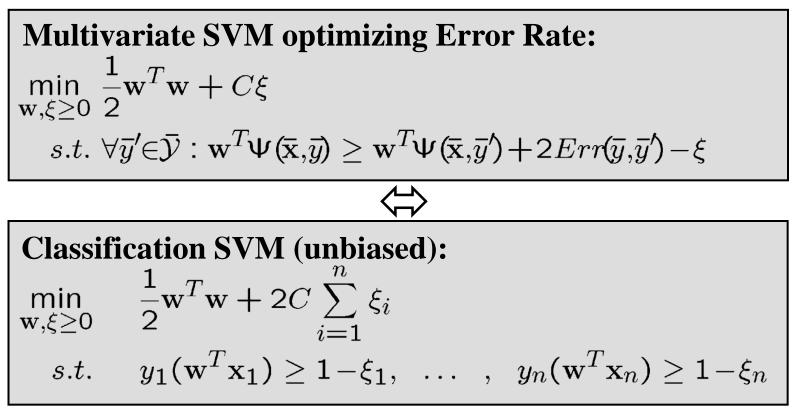
$$\min_{\mathbf{w}} \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ s.t. \ \forall \bar{y}' \in \bar{\mathcal{Y}} \setminus \{\bar{y}\} : \mathbf{w}^T \Psi(\bar{\mathbf{x}}, \bar{y}) \ge \mathbf{w}^T \Psi(\bar{\mathbf{x}}, \bar{y}') +$$

Soft-margin optimization problem: $\min_{\mathbf{w},\xi \ge 0} \frac{1}{2} \mathbf{w}^T \mathbf{w} + C\xi$ $s.t. \ \forall \overline{y}' \in \overline{\mathcal{Y}} : \mathbf{w}^T \Psi(\overline{\mathbf{x}}, \overline{y}) \ge \mathbf{w}^T \Psi(\overline{\mathbf{x}}, \overline{y}') + \Delta(\overline{y}, \overline{y}') - \xi$

Theorem: At the solution, the training loss is upper bounded by $\Delta(\bar{y}, \bar{h}(\bar{\mathbf{x}})) \leq \xi$.

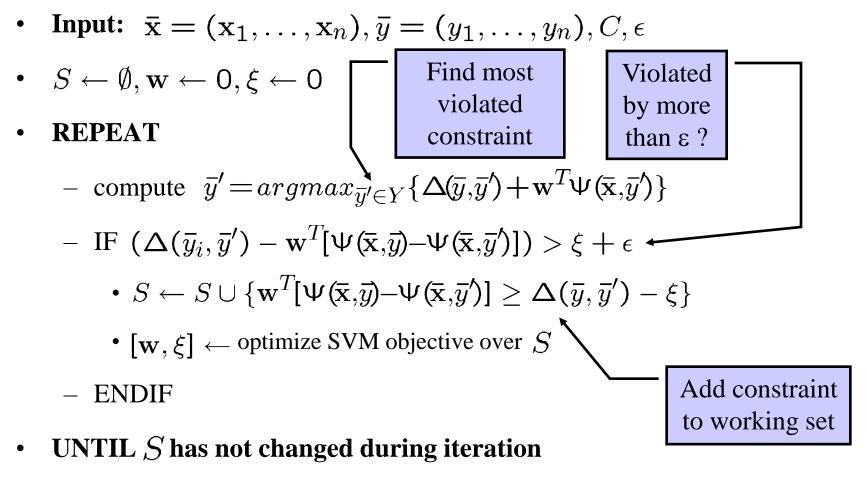
Multivariate SVM Generalizes Classification SVM

Theorem: The solutions of the multivariate SVM with number of errors as the loss function and an (unbiased) classification SVM are equal.



Cutting Plane Algorithm for Multivariate SVM

Approach: Sparse Approx. Structural SVM [Tsochantaridis et al. 04]



Polynomial Convergence Bound

• **Theorem [Tsochantaridis et al., 2004]:** The sparseapproximation algorithm finds a solution to the soft-margin optimization problem after adding at most

$$\max\left\{\frac{2L}{\epsilon}, \frac{8Cn^2R^2L}{\epsilon^2}\right\}$$

constraints to the working set S, so that the Kuhn-Tucker conditions are fulfilled up to a precision ϵ . The loss has to be bounded $0 \le \Delta(\bar{y}, \bar{y}') \le L$, and $R = \max_i ||\mathbf{x}_i||$.

ARGMAX for Contingency Table

- Problem:
 - $\operatorname*{argmax}_{\bar{y}' \in \{1,-1\}^n} \{ \Delta(\bar{y},\bar{y}') + \mathbf{w}^T \sum_{i=1}^n y_i' \mathbf{x}_i \}$
- Key Insight:
 - Only n² different contingency tables exist.
 - ARGMAX for each table easy to compute via sorting.
 - Time $O(n^2)$
- Applies to:
 - Errorrate, F₁, Prec@k, Rec@k, PRBEP, etc.

1: Input:
$$\bar{\mathbf{x}} = (\mathbf{x}_1, ..., \mathbf{x}_n), \ \bar{y} = (y_1, ..., y_n), \ \bar{y}$$

2: $(i_1^p, ..., i_{\#pos}^p) \leftarrow \text{sort}\{i : y_i = 1\}$ by $\mathbf{w}^T \mathbf{x}_i$
3: $(i_1^n, ..., i_{\#neg}^n) \leftarrow \text{sort}\{i : y_i = -1\}$ by $\mathbf{w}^T \mathbf{x}$
4: for $a \in [0, ..., \#pos]$ do
5: $c \leftarrow \#pos - a$
6: $\text{set } y'_{i_1}^p, ..., y'_{i_a}^p$ to 1
7: $\text{set } y'_{i_1}^p, ..., y'_{i_a}^p$ to -1
8: for $d \in [0, ..., \#neg]$ do
9: $b \leftarrow \#neg - d$
10: $\text{set } y'_{i_1}^n, ..., y'_{i_b}^n$ to 1
11: $\text{set } y'_{i_b+1}^n, ..., y'_{i_b}^n$ to -1
12: $v \leftarrow \Delta(a, b, c, d) + \mathbf{w}^T \sum_{i=1}^n y'_i \mathbf{x}_i$
13: if v is the largest so far then
14: $\bar{y}^* \leftarrow (y'_1, ..., y'_n)$
15: end if
16: end for
17: end for
18: return(\bar{y}^*)

ARGMAX for ROC-Area

- Problem:
 - $\operatorname*{argmax}_{\bar{y}' \in \{1,-1\}^n} \{ \Delta(\bar{y},\bar{y}') + \mathbf{w}^T \sum_{i=1}^n y'_i \mathbf{x}_i \}$
- Key Insight:
 - ROC Area is proportional to "swapped pairs"
 - Loss decomposes linearly over pairs
 - Find argmax via sort in time O(n log n)
 - Represent n^2 pairs as $\Psi(\bar{\mathbf{x}}, \bar{y}) = \sum_{i=1}^{n} c_i \mathbf{x}_i$ with $c_i =$

1: Input:
$$\bar{\mathbf{x}} = (\mathbf{x}_1, \dots, \mathbf{x}_n), \ \bar{y} = (y_1, \dots, y_n)$$

2: for $i \in \{i : y_i = 1\}$ do $s_i \leftarrow -0.25 + \mathbf{w}^T \mathbf{x}_i$
3: for $i \in \{i : y_i = -1\}$ do $s_i \leftarrow 0.25 + \mathbf{w}^T \mathbf{x}_i$
4: $(r_1, \dots, r_n) \leftarrow \text{sort } \{1, \dots, n\}$ by s_i
5: $s_p = \#pos, \ s_n = 0$
6: for $i \in \{1, \dots, n\}$ do
7: if $y_{r_i} > 0$ then
8: $c_{r_i} \leftarrow (\#neg - 2 s_n)$
9: $s_p \leftarrow s_p - 1$
10: else
11: $c_{r_i} \leftarrow (-\#pos + 2 s_p)$
12: $s_n \leftarrow s_n + 1$
13: end if
14: end for
15: return (c_1, \dots, c_n)

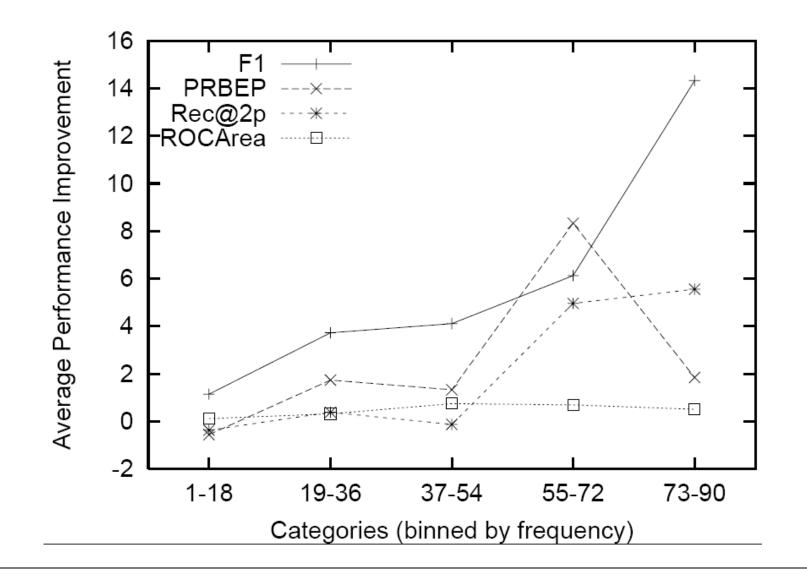
$$= \begin{cases} \sum_{j=1}^{\# neg} y_{ij}, & if(y_i = 1) \\ \sum_{j=1}^{\# pos} y_{ji}, & if(y_i = -1) \end{cases}$$

Experiment: Generalization Performance

- Experiment Setup
 - Macro-average over all classes in dataset
 - Baseline: classification SVM with linear cost model
 - Select *C* and cost ratio *j* via 2/3 1/3 holdout test
 - Two-tailed Wilcoxon (**=95%, *=90%)

Dataset	Method	F_1	PRBEP	Rec _{@2p}	ROCArea
Reuters (90 classes)	SVM^{Δ}_{multi}	62.0	68.2	78.3	99.1
Examples: 9603/3299	SVM _{org}	56.1	65.7	77.2	98.6
Features: 27658	win/lose		$(16/8)^{**}$	(14/8)	(43/33)*
ArXiv (14 classes)	SVM^{Δ}_{multi}	56.8	58.4	73.3	92.8
Examples: 1168/32487	SVM _{org}	49.6	57.9	74.4	92.7
Features: 13525	win/lose	(9/5)*	(9/4)	$(1/13)^{**}$	(8/6)
Optdigits (10 classes)	SVM^{Δ}_{multi}	92.5	92.7	98.4	99.4
Examples: 3823/1797	SVM _{org}	91.5	91.5	98.7	99.4
Features: 64	win/lose	(8/2)*	$(5/1)^{*}$	(1/5)	(6/4)
Covertype (7 classes)	SVM^{Δ}_{multi}	73.8	72.1	93.1	94.6
Examples: 1000/2000	SVM _{org}	73.9	71.0	94.7	94.1
Features: 54	win/lose	(3/4)	(5/2)	(2/5)	(4/3)

Experiment: Unbalanced Classes in Reuters



Experiment: Number of Iterations

- Numbers averaged over
 - all binary classification tasks within dataset
 - all parameter settings

Dataset	Method	F_1	PRBEP	Rec _{@2p}	ROCArea
Reuters (90 classes)	# Iter	119.6	65.6	81.4	30.8
Examples: 9603/3299					
Features: 27658					
ArXiv (14 classes)	# Iter	215.2	45.9	53.7	56.4
Examples: 1168/32487					
Features: 13525					
Optdigits (10 classes)	# Iter	130.5	81.5	86.8	21.6
Examples: 3823/1797					
Features: 64					
Covertype (7 classes)	# Iter	94.3	79.8	63.7	40.2
Examples: 1000/2000					
Features: 54					

Experiment: Number of SV

Corollary: For error rate as the loss function, the hard-margin solution after the first iteration is equal to Rocchio Algorithm.

$$\mathbf{w}_1 \sim \sum_{\{pos: y_{pos}=1\}} \mathbf{x}_{pos} - \sum_{\{neg: y_{neg}=-1\}} \mathbf{x}_{neg}$$

Dataset	Method	F_1	PRBEP	Rec _{@2p}	ROCArea	Err
Reuters (90 classes)	SVM^{Δ}_{multi}	62.0	45.0	46.3	5.1	86.3
Examples: 9603/3299	SVM _{org}					371.4
Features: 27658						
ArXiv (14 classes)	SVM^{Δ}_{multi}	129.5	43.4	45.3	26.8	177.7
Examples: 1168/32487	SVM _{org}					645.3
Features: 13525						
Optdigits (10 classes)	SVM^{Δ}_{multi}	19.6	14.6	14.0	3.9	25.0
Examples: 3823/1797	SVM _{org}					556.9
Features: 64						
Covertype (7 classes)	SVM^{Δ}_{multi}	12.5	12.0	9.4	5.0	17.1
Examples: 1000/2000	SVM _{org}					372.8
Features: 54	5					

Implementation in SVM^{struct}

- Multivariate SVM implemented in SVM^{struct}
 - http://svmlight.joachims.org
 - Also implementations for CFG, Sequence Alignment, OMM
- Application specific
 - Loss function $\Delta(\bar{y}, \bar{y}')$
 - Representation $\Psi(\bar{\mathbf{x}}, \bar{y})$
 - Algorithms to compute

$$\hat{y} = argmax_{\bar{y}' \in Y} \{ \mathbf{w}^T \Psi(\bar{\mathbf{x}}, \bar{y}') \}$$
$$\hat{y} = argmax_{\bar{y}' \in Y} \{ \Delta(\bar{y}, \bar{y}') + \mathbf{w}^T \Psi(\bar{\mathbf{x}}, \bar{y}') \}$$

⇒ Generic structure that covers OMM, MPD, Finite-State Transducers, MRF, etc. (polynomial time inference)

Conclusions

- Generalization of SVM to multivariate loss functions
 - Classification SVMs are special case
- Polynomial time training algorithms for
 - any loss function based on contingency table.
 - ROC-Area.
- New representation of SVM optimization problem
 - Support Vectors represent vector of classifications
 - Can be extremely sparse
- Future work
 - Other performance measures, other methods (e.g. boosting)
 - Faster training algorithm exploiting special structure

Joint Feature Map

- Feature vector Φ(*x*, *y*) that describes match between *x* and *y*
- Learn single weight vector and rank by $\vec{w}^T \Phi(x, y)$

$$h(\vec{x}) = argmax_{y \in Y} \left[\vec{w}^T \Phi(x, y) \right]$$

 $\vec{w}^T \Phi(x, y_2)$

 $\vec{w}^T \Phi(x, y_{12})$

 $\vec{w}^T \Phi(x, y_{34})$

 $\vec{w}^T \Phi(x, y_{58})$

Problems

- How to predict efficiently?
- How to learn efficiently?

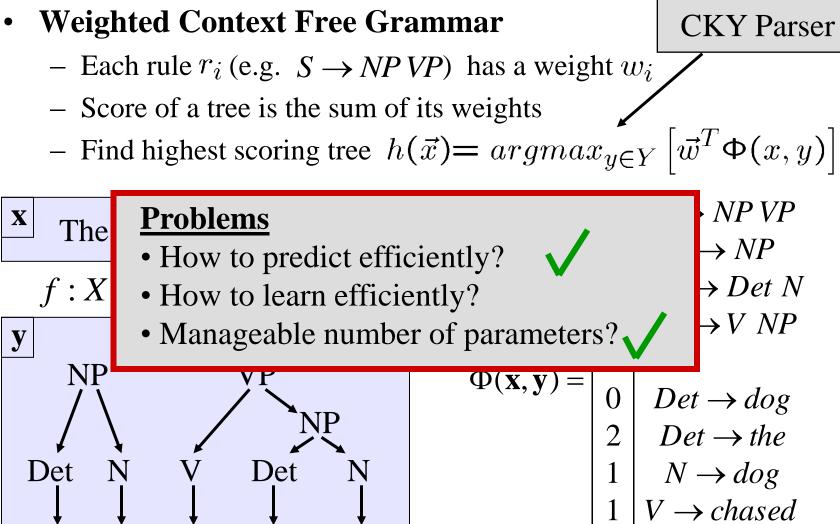
y⁵⁸

• Manageable number of parameters?

The dog chased the cat

Χ

Joint Feature Map for Trees



The dog chased the cat

 $\begin{pmatrix} 1 \\ 1 \end{pmatrix} V \to chase$ $N \to cat$

Experiment: Natural Language Parsing

• Implemention

- Implemented Sparse-Approximation Algorithm in SVM^{light}
- Incorporated modified version of Mark Johnson's CKY parser
- Learned weighted CFG with $\epsilon = 0.01, C = 1$
- Data
 - Penn Treebank sentences of length at most 10 (start with POS)
 - Train on Sections 2-22: 4098 sentences
 - Test on Section 23: 163 sentences

	Test Ac	ccuracy	Training Efficiency			
Method	Acc	$ $ F_1	CPU-h	Iter	Const	
PCFG with MLE	55.2	86.0	0	N/A	N/A	
SVM with $(1-F_1)$ -Loss	58.9	88.5	3.4	12	8043	

More Expressive Features

- Linear composition: $\Phi(x, \vec{y}) = \sum_{i=1}^{k} \phi(x, y_i)$
- So far: $\phi(x, y_i) = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ 1 \\ 0 \\ \cdots \\ c \end{pmatrix}$ if $y_i = 'S \leftarrow NP \vee P'$
 - **General:** $\phi(x, y_i) = \phi_{kernel}(\phi(x, [rule, start, end]))$ $K(a,b) = \phi_{kernel}(a)^T \phi_{kernel}(a)$

• Example:
$$\phi(x, y_i) = \begin{pmatrix} 1 & \text{if } x_{start} = \text{'while'} \land x_{end} = \text{'.'} \\ (start - end)^2 & \text{span contains } x_{start} = \text{'and'} \\ \dots & \end{pmatrix}$$

Experiment: Part-of-Speech Tagging

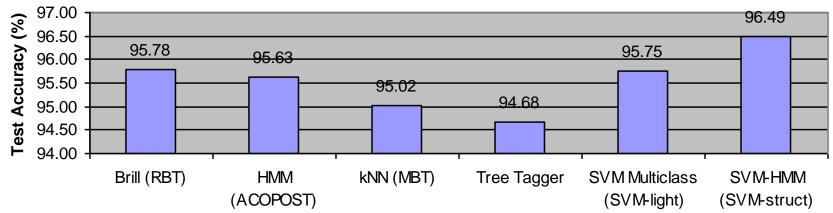
- Task
 - Given a sequence of words *x*, predict sequence of tags *y*.

 \mathbf{X} The dog chased the cat $\rightarrow \mathbf{Y}$ Det $\rightarrow N \rightarrow V \rightarrow Det \rightarrow N$

- Dependencies from tag-tag transitions in Markov model.
- Model
 - Markov model with one state per tag and words as emissions
 - Each word described by ~250,000 dimensional feature vector (all word suffixes/prefixes, word length, capitalization ...)

• Experiment (by Dan Fleisher)

- Train/test on 7966/1700 sentences from Penn Treebank



Overview

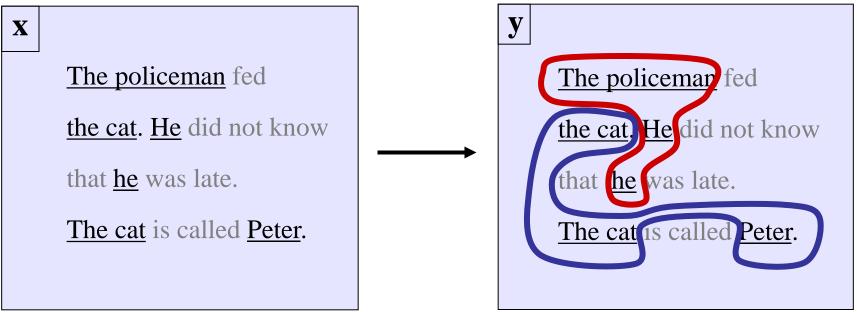
- Task: Discriminative learning with complex outputs
- Related Work
- SVM algorithm for complex outputs
 - Formulation as convex quadratic program
 - General algorithm
 - Sparsity bound
- Example 1: Learning to parse natural language
 - Learning weighted context free grammar
- Example 2: Optimizing F₁-score in text classification
 - Learn linear rule that directly optimizes F_1 -score
 - Example 3: Learning to cluster
 - Learning a clustering function that produces desired clusterings
 - Conclusions

Overview

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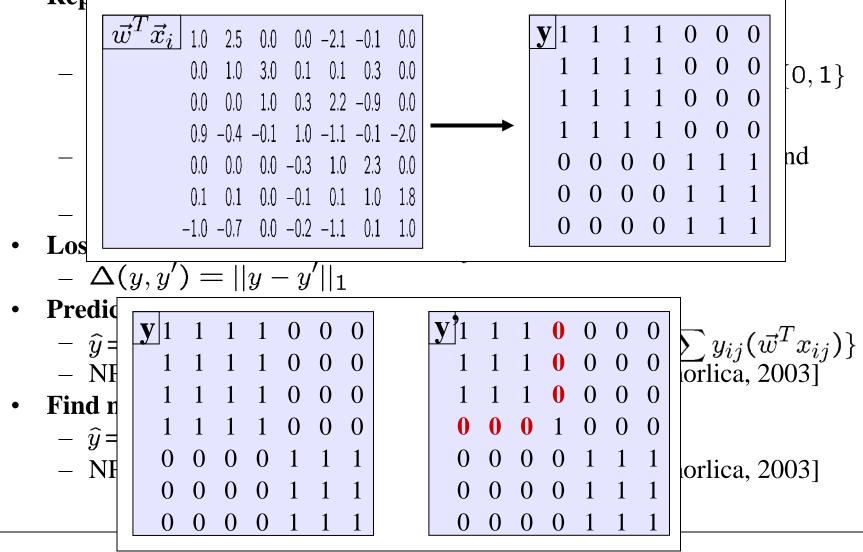
Learning to Cluster

- Noun-Phrase Co-reference
 - Given a set of noun phrases *x*, predict a clustering *y*.
 - Structural dependencies, since prediction has to be an equivalence relation.
 - Correlation dependencies from interactions.



Struct SVM for Supervised Clustering (by Thomas Finley)

Reprocontation



Conclusions

- Learning to predict complex output
 - Clean and concise framework for many applications
 - Discriminative methods are feasible and offer advantages
- An SVM method for learning with complex outputs
- Case Studies
 - Learning to predict trees (natural language parsing)
 - Optimize to non-standard performance measures (imbalanced classes)
 - Learning to cluster (noun-phrase coreference resolution)
- Software: SVM^{struct}
 - http://svmlight.joachims.org/
- Open questions
 - Applications with complex outputs?
 - Is it possible to extend other algorithms to complex outputs?
 - More efficient training algorithms for special cases?

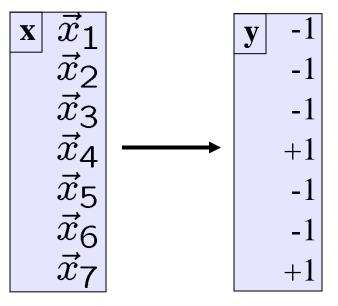
Examples of Complex Output Spaces

• Non-Standard Performance Measures (e.g. F₁-score, Lift)

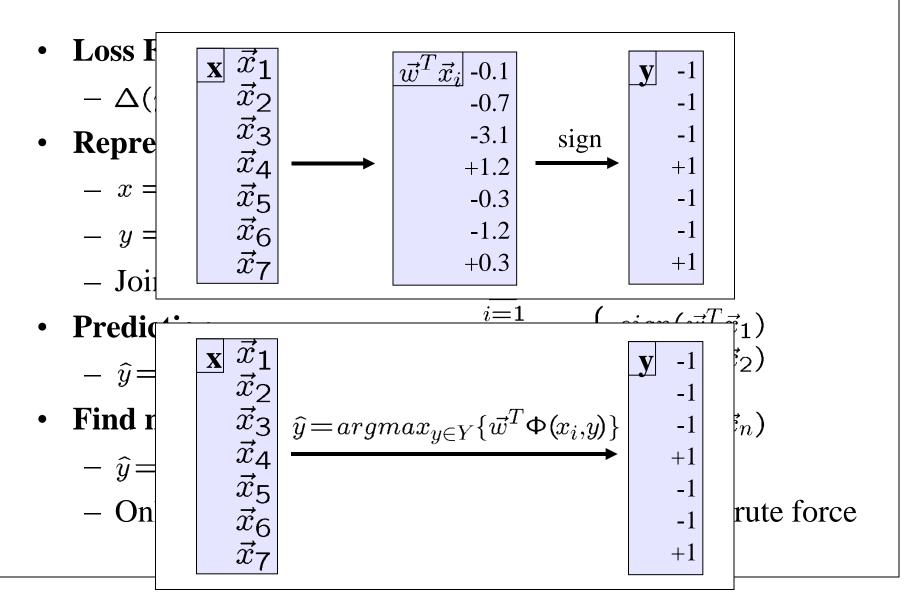
 $- F_I$ -score: harmonic average of precision and recall

$$F_1 = \frac{2 \operatorname{Prec} \operatorname{Rec}}{\operatorname{Prec} + \operatorname{Rec}}$$

- New example vector \vec{x}_8 . Predict $y_8 = 1$, if $P(y_8 = 1/\vec{x}_8) = 0.4$? \rightarrow Depends on other examples!



Struct SVM for Optimizing F₁-Score



Experiment: Text Classification

- Dataset: Reuters-21578 (ModApte)
 - 9603 training / 3299 test examples
 - 90 categories
 - TFIDF unit vectors (no stemming, no stopword removal)
- Experiment Setup
 - Classification SVM with optimal C in hindsight (C=8)
 - F_1 -loss SVM with C=0.0625 (via 2-fold cross-validation)

• Results

	Macroa	/eraged	Training Efficiency			
Method	Train F_1	Test F_1	CPU-min	Const	SV	
Classification SVM	98.4	52.8	0.1	N/A	264	
SVM with $(1-F_1)$ -Loss	91.8	61.8	32.2	173	93	