Introduction to Machine Learning (67577)
Lecture 9

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Multiclass, Ranking, and Complex Prediction Problems

Outline

Multiclass Categorization

- So far, we mainly dealt with binary problems $h : \mathcal{X} \to \{\pm 1\}$ or regression problems, $h : \mathcal{X} \to \mathbb{R}$

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- E.g.: $x \in \mathcal{X}$ is an image and $\{1, \ldots, k\}$ represents k possible objects
- We'll later consider problems in which k is extremely large, E.g., in translation, $x \in \mathcal{X}$ is a sentence in Hebrew and $\{1, \ldots, k\}$ is all possible sentences in English

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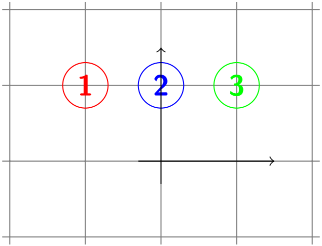
- In case of ties (more than one h_i predicts 1), and if h_i outputs a confidence as well (e.g. SVM), we can use the confidence of h_i to break ties

All-Pairs reduction

- All pairs of classes are compared to each other.
- For every $1 \le i < j \le k$, construct a binary sample, $S_{i,j}$, containing examples from class i against examples from class j.
- Call the binary learner to get $h_{i,j}$
- Output the multiclass classifier by predicting the class which had the highest number of "wins"

Sub-optimality of reductions

- One-vs-All over halfspace binary classifier will fail on the sample below, although it is separable by the resulting hypothesis class



Linear Multiclass Predictors

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- The immediate question, how to construct Ψ ?

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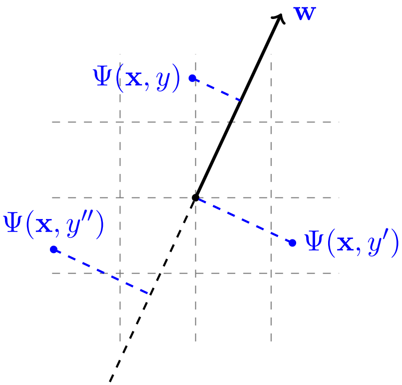

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  - Intuitively, $\Psi_j(\mathbf{x}, y)$ should be large if word j appears a lot in $\mathbf{x}$ but does not appear at all in documents that are not on topic y
    In such case, we tend to believe that the document $\mathbf{x}$ is on topic y

The Multi-vector Construction

$$h(\mathbf{x}) = \underset{y \in [k]}{\operatorname{argmax}} (W\mathbf{x})_y = \underset{y \in [k]}{\operatorname{argmax}} \langle \mathbf{w}_y, \mathbf{x} \rangle$$

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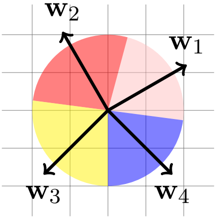

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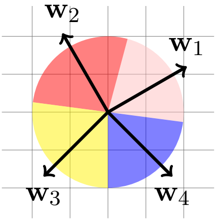

Can be written as $\operatorname{argmax}_y \langle \mathbf{w}, \Psi(\mathbf{x}, y) \rangle$ for

$$\Psi(\mathbf{x}, y) = [\ \underbrace{0, \ldots, 0}_{\in \mathbb{R}^{(y-1)n}}, \underbrace{x_1, \ldots, x_n}_{\in \mathbb{R}^n}, \underbrace{0, \ldots, 0}_{\in \mathbb{R}^{(k-y)n}}\ ] \ .$$

Cost-sensitive losses

Which prediction is worse?

$h_1($  $) = \text{cat}$

$h_2($  $) = \text{whale}$

Cost-sensitive losses

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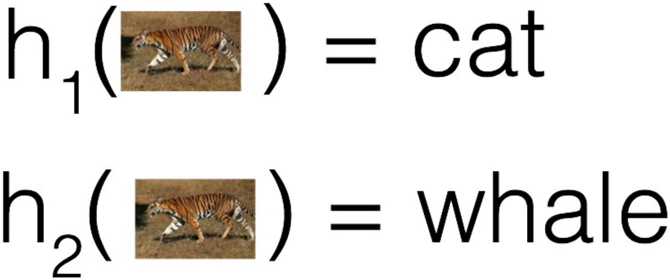

- Cost function: $\Delta : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$
- Zero-one loss is a special case: $\Delta(y, y') = \mathbb{1}_{[y' \neq y]}$

ERM

- ERM problem: find $\mathbf{w}$ that minimizes

$$L_S(h_{\mathbf{w}}) = \frac{1}{m}\sum_{i=1}^{m} \Delta(h_{\mathbf{w}}(\mathbf{x}_i), y_i) \ .$$

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$$\forall i \in [m],\ \forall y \in \mathcal{Y} \setminus \{y_i\},\quad \langle \mathbf{w}, \Psi(\mathbf{x}_i, y_i)\rangle > \langle \mathbf{w}, \Psi(\mathbf{x}_i, y)\rangle$$

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- NP hard in the non-realizable case so we'll use a surrogate convex loss

Generalized Hinge Loss

Multiclass predictor:

$$h_{\mathbf{w}}(\mathbf{x}) = \operatorname*{argmax}_{y' \in \mathcal{Y}} \langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y'}) \rangle \ .$$

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Therefore,

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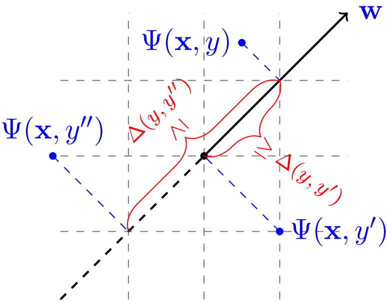
\end{aligned}$$

- The generalized hinge loss is convex and ρ-Lipschitz, for $\rho = \max_{y' \in \mathcal{Y}} \|\Psi(\mathbf{x}, y') - \Psi(\mathbf{x}, y)\|$.

Generalized Hinge Loss

The generalized hinge loss equals zero when:

$$\forall y' \in \mathcal{Y} \setminus \{y\}, \quad \langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y}) \rangle \geq \langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y}') \rangle + \Delta(y', y) \ .$$



Multiclass SVM

Parameters:

- class sensitive feature mapping, Ψ
- cost function $\Delta : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$
- regularization parameter $\lambda > 0$

Solve:

$$\underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \left(\lambda \|\mathbf{w}\|^2 + \frac{1}{m} \sum_{i=1}^{m} \max_{y' \in \mathcal{Y}} \left(\Delta(y', y_i) + \langle \mathbf{w}, \Psi(\mathbf{x}_i, y') - \Psi(\mathbf{x}_i, y_i) \rangle \right) \right)$$

Output:

$$h_{\mathbf{w}}(\mathbf{x}) = \underset{y \in \mathcal{Y}}{\operatorname{argmax}} \langle \mathbf{w}, \Psi(\mathbf{x}, y) \rangle$$

SGD implementation

- Loss function:

$$\ell(\mathbf{w},(\mathbf{x},y)) = \max_{y' \in \mathcal{Y}} \left(\Delta(y',y) + \langle \mathbf{w}, \Psi(\mathbf{x},y') - \Psi(\mathbf{x},y) \rangle \right)$$

- Sub-gradient calculation
  - find $\hat{y} \in \operatorname{argmax}_{y' \in \mathcal{Y}} \left(\Delta(y',y) + \langle \mathbf{w}^{(t)}, \Psi(\mathbf{x},y') - \Psi(\mathbf{x},y) \rangle \right)$
  - set $\mathbf{v}_t = \Psi(\mathbf{x},\hat{y}) - \Psi(\mathbf{x},y)$

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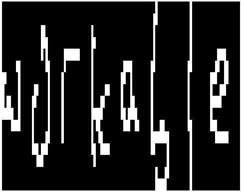
Example — Optical Character Recognitio (OCR):

- $\mathcal{X}$ = set of images
- $\mathcal{Y}$ all possible words in English



$\longrightarrow$ workable

Structured Output Prediction

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However, the huge size of $\mathcal{Y}$ poses computational challenges:

1. To apply the multiclass prediction we need to solve a maximization problem over $\mathcal{Y}$. How can we predict efficiently when $\mathcal{Y}$ is so large?
2. How do we train $\mathbf{w}$ efficiently? In particular, to apply the SGD rule we again need to solve a maximization problem over $\mathcal{Y}$.

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Solution:

- Endow Ψ and Δ with structure that allows fast maximization over $\mathcal{Y}$

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- Type 2 features: (capture "it is likely to see the pair 'qu' in a word")

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- Claim: The problem $\operatorname{argmax}_{\mathbf{y}\in\mathcal{Y}} \langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y})\rangle$ can be solved efficiently using dynamic programming

Dynamic Programming

- Can rewrite the problem as:

$$h_{\mathbf{w}}(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^{r} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, y_t, y_{t-1}) \rangle \ .$$

Dynamic Programming

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$$h_{\mathbf{w}}(\mathbf{x}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^{r} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, y_t, y_{t-1}) \rangle \ .$$

- Maintain a matrix $M \in \mathbb{R}^{q,r}$ such that

$$M_{s,\tau} = \max_{(y_1,\ldots,y_\tau):y_\tau = s} \sum_{t=1}^{\tau} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, y_t, y_{t-1}) \rangle$$

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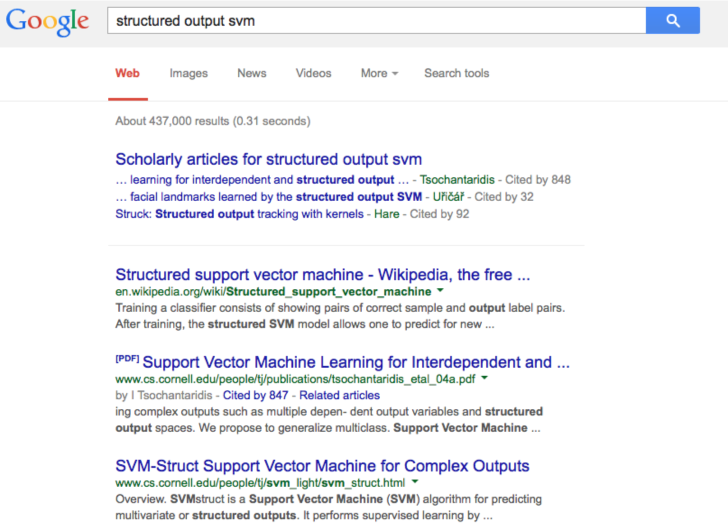
  and observe: Maximum of $\langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y}) \rangle$ equals to $\max_s M_{s,r}$
- Calculate M in a recursive manner:

$$M_{s,\tau} \ = \ \max_{s'} \ \left(M_{s',\tau-1} + \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, s, s') \rangle \right) \ .$$

Outline

Ranking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About 437,000 results (0.31 seconds)
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Structured support vector machine - Wikipedia, the free …
en.wikipedia.org/wiki/Structured_support_vector_machine
Training a classifier consists of showing pairs of correct sample and output label pairs. After training, the structured SVM model allows one to predict for new …
[PDF] Support Vector Machine Learning for Interdependent and …
www.cs.cornell.edu/people/tj/publications/tsochantaridis_etal_04a.pdf
by I Tsochantaridis - Cited by 847 - Related articles
ing complex outputs such as multiple depen- dent output variables and structured output spaces. We propose to generalize multiclass. Support Vector Machine …
SVM-Struct Support Vector Machine for Complex Outputs
www.cs.cornell.edu/people/tj/svm_light/svm_struct.html
Overview. SVMstruct is a Support Vector Machine (SVM) algorithm for predicting multivariate or structured outputs. It performs supervised learning by …

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- E.g.

$\mathbf{y}$	sorted $\mathbf{y}$	$\pi(\mathbf{y})$
2	-1	4
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- $\pi(\mathbf{y})_i$ is the position of y_i in the sorted vector. Top-ranked instances are those that achieve the highest values in $\pi(\mathbf{y})$.

Loss functions for Ranking

Kendall-tau loss:

- Count the number of pairs (i, j) that are in different order in the two permutations:

$$\Delta(\mathbf{y}', \mathbf{y}) = \frac{2}{r(r-1)} \sum_{i=1}^{r-1} \sum_{j=i+1}^{r} \mathbb{1}_{[\mathrm{sign}(y'_i - y'_j) \neq \mathrm{sign}(y_i - y_j)]} \ .$$

  More useful than the 0-1 loss as it reflects the level of similarity between the two rankings.

Loss functions for Ranking

Normalized Discounted Cumulative Gain (NDCG):

- Emphasizes correctness at the top of the list by using a discount
- Define a discounted cumulative gain measure:

$$G(\mathbf{y}', \mathbf{y}) = \sum_{i=1}^{r} D(\pi(\mathbf{y}')_i) \; y_i$$

  where D is a decreasing function
- Normalized discounted cumulative gain

$$\Delta(\mathbf{y}', \mathbf{y}) = 1 - \frac{G(\mathbf{y}', \mathbf{y})}{G(\mathbf{y}, \mathbf{y})}$$

- NDCG is often used to evaluate the performance of search engines since in such applications it makes sense to completely ignore elements which are not at the top of the ranking.

Discounted cumulative gain — example

$$G(\mathbf{y}',\mathbf{y}) = \sum_{i=1}^{r} D(\pi(\mathbf{y}')_i)\ y_i$$

$\mathbf{y}'$	sorted $\mathbf{y}'$	$\pi(\mathbf{y}')$	$D(\pi(\mathbf{y}'))$	$\mathbf{y}$	$D(\pi(\mathbf{y}))$	$\pi(\mathbf{y})$	sorted $\mathbf{y}$
2	-1	4	1	5	1	4	-2
1	0.5	3	0	-2	0	1	1
6	1	5	2	6	2	5	3
-1	2	1	0	1	0	2	5
0.5	6	2	0	3	0	3	6

$$\Delta(\mathbf{y}',\mathbf{y}) = 1 - \frac{G(\mathbf{y}',\mathbf{y})}{G(\mathbf{y},\mathbf{y})} = 1 - \frac{17}{17} = 0$$

Linear Predictors for Ranking

- Linear predictor

$$h_{\mathbf{w}}((\mathbf{x}_1, \ldots, \mathbf{x}_r)) = (\langle \mathbf{w}, \mathbf{x}_1 \rangle, \ldots, \langle \mathbf{w}, \mathbf{x}_r \rangle) \ .$$

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- Therefore, with $\Psi(\bar{\mathbf{x}}, \mathbf{v}) = \sum_{i=1}^{r} v_i \mathbf{x}_i$, we have

$$\begin{aligned} \pi(h_{\mathbf{w}}(\bar{\mathbf{x}})) &= \operatorname*{argmax}_{\mathbf{v} \in V} \sum_{i=1}^{r} v_i \langle \mathbf{w}, \mathbf{x}_i \rangle \\ &= \operatorname*{argmax}_{\mathbf{v} \in V} \langle \mathbf{w}, \sum_{i=1}^{r} v_i \mathbf{x}_i \rangle \\ &= \operatorname*{argmax}_{\mathbf{v} \in V} \langle \mathbf{w}, \Psi(\bar{\mathbf{x}}, \mathbf{v}) \rangle \ . \end{aligned}$$

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- Each step of SGD for the resulting learning problem boils down to "the assignment problem" and can be solved efficiently using the "Hungarian method"

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  - But, it's a poor predictor ...

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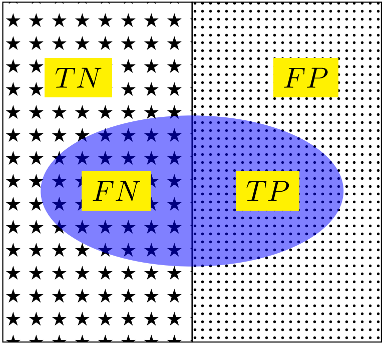
- θ controls the tradeoff between precision and recall

Multivariate Performance Measures

Example:

- y' predicts by the halfspace ('dots' $=$ positive, 'stars' $=$ negative)
- y predicts by the ellipse (within $=$ positive, outside $=$ negative)

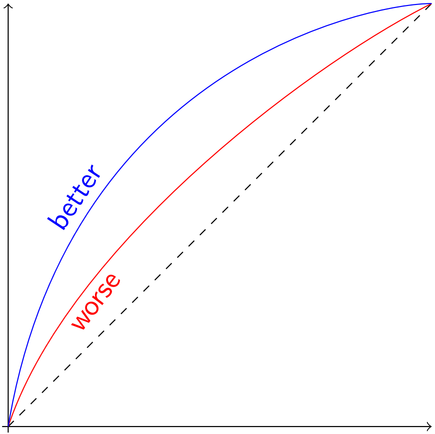


$$\text{Precision} = \frac{TP}{TP+FP}$$

$$\text{Recall} = \frac{TP}{TP+FN}$$

Receiver operating characteristic (ROC) curve

Recall=TPR=$\frac{TP}{TP+FN}$



1-sensitivity=FPR=$\frac{FP}{FP+TN}$

Multivariate Performance Measures

For every θ we can define a single number that measures the performance.

- Averaging sensitivity and specificity: $\frac{1}{2}\left(\frac{TP}{TP+FN}+\frac{TN}{TN+FP}\right)$. This is the accuracy on positive examples averaged with the accuracy on negative examples.
- F_1-score: The F_1 score is the harmonic mean of the precision and recall: $\frac{2}{\frac{1}{\text{Precision}}+\frac{1}{\text{Recall}}}$.
- Recall at k: We measure the recall while the prediction must contain at most k positive labels. That is, we should set θ so that $TP+FP \le k$. E.g., convenient for fraud detection
- Precision at k: We measure the precision while the prediction must contain at least k positive labels. That is, we should set θ so that $TP+FP \ge k$.

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- Conclusion: we need to train our predictor with an appropriate loss function for the problem

Linear Predictors for Multivariate Measures

- Linear predictor:

$$h_{\mathbf{w}}(\bar{\mathbf{x}}) = (\langle \mathbf{w}, \mathbf{x}_1 \rangle, \ldots, \langle \mathbf{w}, \mathbf{x}_r \rangle) \ .$$

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- E.g., for recall at k take V to be all vectors in $\{\pm 1\}^r$ that has at most k pluses

Linear Predictors for Multivariate Measures

- Hinge loss for multivariate:

$$\begin{aligned}
\Delta(h_{\mathbf{w}}(\bar{\mathbf{x}}), \mathbf{y}) &= \Delta(\mathbf{b}(h_{\mathbf{w}}(\bar{\mathbf{x}})), \mathbf{y}) \\
&\le \Delta(\mathbf{b}(h_{\mathbf{w}}(\bar{\mathbf{x}})), \mathbf{y}) + \sum_{i=1}^{r} (b_i(h_{\mathbf{w}}(\bar{\mathbf{x}})) - y_i) \langle \mathbf{w}, \mathbf{x}_i \rangle \\
&\le \max_{\mathbf{v} \in V} \left[\Delta(\mathbf{v}, \mathbf{y}) + \sum_{i=1}^{r} (v_i - y_i) \langle \mathbf{w}, \mathbf{x}_i \rangle \right]
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SGD for Multivariate Measures

- Applying SGD involves solving the maximization problem in the definition of the loss

$$\operatorname*{argmax}_{\mathbf{v}\in V} \left[\Delta(\mathbf{v},\mathbf{y}) + \sum_{i=1}^{r}(v_i - y_i)\langle \mathbf{w}, \mathbf{x}_i\rangle\right]$$

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- Key idea, suppose Δ only depends on $a = TP, b = FP$ and partition V into sets of the form

$$\bar{\mathcal{Y}}_{a,b} = \{\mathbf{v} \;:\; |\{i : v_i = 1 \wedge y_i = 1\}| = a \,\wedge\, |\{i : v_i = 1 \wedge y_i = -1\}| = b\}$$

SGD for Multivariate Measures

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$$\underset{\mathbf{v}\in V}{\operatorname{argmax}} \left[\Delta(\mathbf{v},\mathbf{y}) + \sum_{i=1}^{r}(v_i - y_i)\left\langle \mathbf{w}, \mathbf{x}_i \right\rangle\right]$$

- Key idea, suppose Δ only depends on $a = TP, b = FP$ and partition V into sets of the form

$$\bar{\mathcal{Y}}_{a,b} = \{\mathbf{v} \ : \ |\{i : v_i = 1 \wedge y_i = 1\}| = a \ \wedge \ |\{i : v_i = 1 \wedge y_i = -1\}| = b\}$$

- Withint each $\bar{\mathcal{Y}}_{a,b}$ the value of Δ is constant, so we only need to maximize the expression

$$\max_{\mathbf{v}\in\bar{\mathcal{Y}}_{a,b}} \sum_{i=1}^{r} v_i \langle \mathbf{w}, \mathbf{x}_i \rangle \ .$$

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$$\underset{\mathbf{v} \in V}{\operatorname{argmax}} \left[\Delta(\mathbf{v}, \mathbf{y}) + \sum_{i=1}^{r} (v_i - y_i) \langle \mathbf{w}, \mathbf{x}_i \rangle \right]$$

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$$\max_{\mathbf{v} \in \bar{\mathcal{Y}}_{a,b}} \sum_{i=1}^{r} v_i \langle \mathbf{w}, \mathbf{x}_i \rangle \; .$$

- This can be done efficiently by sorting the examples according to $\langle \mathbf{w}, \mathbf{x}_i \rangle$

Summary

- Multiclass problems
- Simple reductions
- Linear predictors and Multiclass SVM
- Structured Output Prediction
- Ranking
- Bipartite Ranking and Multivariate Performance Measures
- Efficient sub-gradient calculations using combinatorial optimization (dynamic programming, assignment problems, sorting)