Multiclass Classification

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Overview

Motivation

- So far, most algorithms we've learned are designed for binary classification.
  - Sentiment analysis (positive vs. negative)
  - Spam filter (spam vs. non-spam)
- Many real-world problems have more than two classes.
  - Document classification (over 10 classes)
  - Object recognition (over 20k classes)
  - Face recognition (millions of classes)
- What are some potential issues when we have a large number of classes?
  - Computation cost
  - Class imbalance
  - Different cost of errors

Today's lecture

- How to *reduce* multiclass classification to binary classification?
  - We can think of binary classifier or linear regression as a black box. Naive ways:
  - E.g. multiple binary classifiers produce a binary code for each class (000, 001, 010)
  - E.g. a linear regression produces a numerical value for each class (1.0, 2.0, 3.0)
- How do we *generalize* binary classification algorithm to the multiclass setting?
  - We also need to think about the loss function.
- Example of very large output space: structured prediction.
  - Multi-class: Mutually exclusive class structure.
  - Text: Temporal relational structure.

Reduction to Binary Classification

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train k binary classifiers, one for each class: $h_1, \ldots, h_k : \mathcal{X} \to \mathrm{R}$.
- Classifier h_i distinguishes class i (+1) from the rest (-1).

Prediction

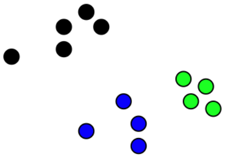
- Majority vote:

$$h(x) = \underset{i \in \{1,\ldots,k\}}{\arg\max}\, h_i(x)$$

- Ties can be broken arbitrarily.

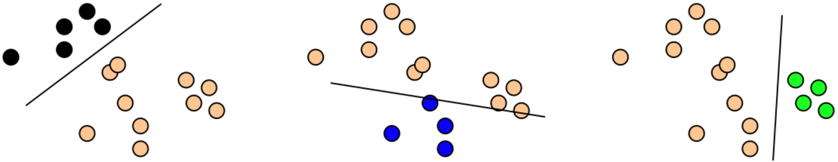
OvA: 3-class example (linear classifier)

Consider a dataset with three classes:



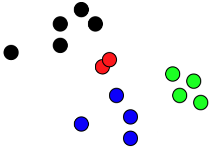
Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.

Train OvA classifiers:



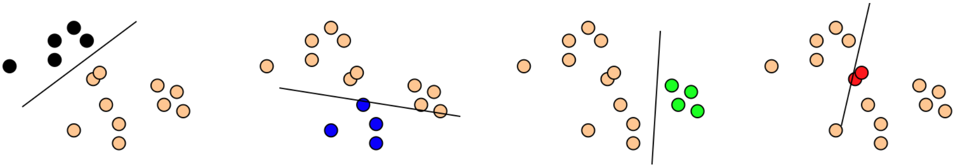
OvA: 4-class non linearly separable example

Consider a dataset with four classes:



Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

Prediction

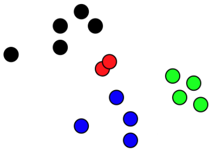
- Majority vote (each class gets $k-1$ votes)

$$h(x) = \underset{i \in \{1,\ldots,k\}}{\arg\max} \sum_{j \neq i} \underbrace{h_{ij}(x)\mathbb{I}\{i < j\}}_{\text{class } i \text{ is } +1} - \underbrace{h_{ji}(x)\mathbb{I}\{j < i\}}_{\text{class } i \text{ is -1}}$$

- Tournament
- Ties can be broken arbitrarily.

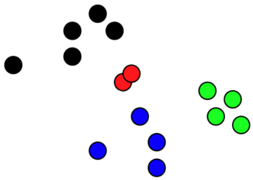
AvA: four-class example

Consider a dataset with four classes:



Assumption: each pair of classes are linearly separable.
More expressive than OvA.

What's the decision region for the red class?



OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$
challenges	train	class imbalance	small training set
	test	calibration / scale tie breaking	

Lack theoretical justification but simple to implement and works well in practice (when # classes is small).

Code word for labels

Using the reduction approach, can you train fewer than k binary classifiers?

Key idea: Encode labels as binary codes and predict the code bits directly.

OvA encoding:

class	h_1	h_2	h_3	h_4
1	1	0	0	0
2	0	1	0	0
3	0	0	1	0
4	0	0	0	1

OvA uses k bits to encode each label, what's the minimal number of bits you can use?

Error correcting output codes (ECOC)

Example: 8 classes, 6-bit code

class	h_1	h_2	h_3	h_4	h_5	h_6
1	0	0	0	1	0	0
2	1	0	0	0	0	0
3	0	1	1	0	1	0
4	1	1	0	0	0	0
5	1	1	0	0	1	0
6	0	0	1	1	0	1
7	0	0	1	0	0	0
8	0	1	0	1	0	0

Training Binary classifier h_i:

- +1: classes whose i-th bit is 1
- -1: classes whose i-th bit is 0

Prediction Closest label in terms of Hamming distance.

h_1	h_2	h_3	h_4	h_5	h_6
0	1	1	0	1	1

Code design Want good binary classifiers.

Error correcting output codes: summary

- Computationally more efficient than OvA (a special case of ECOC). Better for large k.
- Why not use the minimal number of bits ($\log_2 k$)?
  - If the minimum Hamming distance between any pair of code word is d, then it can correct $\left\lfloor \frac{d-1}{2} \right\rfloor$ errors.
  - In plain words, if rows are far from each other, ECOC is robust to errors.
- Trade-off between code distance and binary classification performance.
- Nice theoretical results [Allwein et al., 2000] (also incoporates AvA).

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design "natural" binary classification problems without large computation cost.

But,

- Unclear how to generalize to extremely large # of classes.
- ImageNet: >20k labels; Wikipedia: >1M categories.

Next, generalize previous algorithms to multiclass settings.

Multiclass Loss

Binary Logistic Regression

- Given an input x, we would like to output a classification between (0,1).

$$f(x) = sigmoid(z) = \frac{1}{1+\exp(-z)} = \frac{1}{1+\exp(-w^\top x - b)}. \tag{1}$$

- The other class is represented in $1 - f(x)$:

$$1 - f(x) = \frac{\exp(-w^\top x - b)}{1+\exp(-w^\top x - b)} = \frac{1}{1+\exp(w^\top x + b)} = sigmoid(-z). \tag{2}$$

- Another way to view: one class has $(+w, +b)$ and the other class has $(-w, -b)$.

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?

$$f_c(x) = \frac{\exp(w_c^\top x) + b_c}{\sum_c \exp(w_c^\top x + b_c)} \tag{3}$$

- Also called "softmax" in neural networks.
- Loss function: $L = \sum_i -y_c^{(i)} \log f_c(x^{(i)})$
- Gradient: $\frac{\partial L}{\partial z} = f - y$. Recall: MSE loss.

Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

- Intuitively, $h_i(x)$ scores how likely x is to be from class i.
- OvA objective: $h_i(x) > 0$ for x with label i and $h_i(x) < 0$ for x with all other labels.
- At test time, to predict (x, i) correctly we only need

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{4}$$

Multiclass Perceptron

- Base linear predictors: $h_i(x) = w_i^T x$ ($w \in \mathrm{R}^d$).
- Multiclass perceptron:

Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
    for $(x, y) \in \mathcal{D}$ **do**
        $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$;
        if $\hat{y} \neq y$ **then** `// We've made a mistake`
            $w_y \leftarrow w_y + x$; `// Move the target-class scorer towards` x
            $w_{\hat{y}} \leftarrow w_{\hat{y}} - x$; `// Move the wrong-class scorer away from` x
        end
    end
end

Rewrite the scoring function

- Remember that we want to scale to very large # of classes and reuse algorithms and analysis for binary classification
  - $\Longrightarrow$ a single weight vector is desired
- How to rewrite the equation such that we have one w instead of k?

$$w_i^T x = w^T \psi(x, i) \tag{5}$$

$$h_i(x) = h(x, i) \tag{6}$$

  - Encode labels in the feature space.
  - Score for each label $\rightarrow$ score for the "*compatibility*" of a label and an input.

The Multivector Construction

How to construct the feature map ψ?

- What if we stack w_i's together (e.g., $x \in \mathbb{R}^2, \mathcal{Y} = \{1,2,3\}$)

$$w = \left(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \right)$$

- And then do the following: $\Psi : \mathbb{R}^2 \times \{1,2,3\} \to \mathbb{R}^6$ defined by

$$\begin{aligned} \Psi(x,1) &:= (x_1, x_2, 0, 0, 0, 0) \\ \Psi(x,2) &:= (0, 0, x_1, x_2, 0, 0) \\ \Psi(x,3) &:= (0, 0, 0, 0, x_1, x_2) \end{aligned}$$

- Then $\langle w, \Psi(x,y) \rangle = \langle w_y, x \rangle$, which is what we want.

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in \mathcal{D}$ **do**
    $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w^T \psi(x, y')$; `// Equivalent to` $\arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w \leftarrow w + \psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$
      $w \leftarrow w - \psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$
    end
  end
end

Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,}\ldots\}$.
- Features of $x \in \mathcal{X}$: [The word itself], ENDS_IN_ly, ENDS_IN_ness, ...

How to construct the feature vector?

- Multivector construction: $w \in \mathrm{R}^{d \times k}$—doesn't scale.
- Directly design features for each class.

$$\Psi(x,y) = (\psi_1(x,y), \psi_2(x,y), \psi_3(x,y), \ldots, \psi_d(x,y)) \tag{7}$$

  - Size can be bounded by d.

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= 1(x = \text{apple AND } y = \text{NOUN}) \\
\psi_2(x,y) &= 1(x = \text{run AND } y = \text{NOUN}) \\
\psi_3(x,y) &= 1(x = \text{run AND } y = \text{VERB}) \\
\psi_4(x,y) &= 1(x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}) \\
&\ldots
\end{aligned}
$$

- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$
- After training, what's w_1, w_2, w_3, w_4?
- No need to include features unseen in training data.

Feature templates: implementation

- Flexible, e.g., neighboring words, suffix/prefix.
- "Read off" features from the training data.
- Often sparse—efficient in practice, e.g., NLP problems.
- Can use a hash function: template $\rightarrow \{1, 2, \ldots, d\}$.

Review

Ingredients in multiclass classification:

- Scoring functions for each class (similar to ranking).
- Represent labels in the input space $\implies$ single weight vector.

We've seen

- How to generalize the perceptron algorithm to multiclass setting.
- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

Next,

- How to generalize SVM to the multiclass setting.
- Concept check: Why might one prefer SVM / perceptron?

Margin for Multiclass

Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{8}$$

- Want margin to be large and positive ($w^T x^{(n)}$ has same sign as $y^{(n)}$)

Multiclass

- Class-specific margin for $(x^{(n)}, y^{(n)})$:

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{9}$$

- Difference between scores of the correct class and each other class
- Want margin to be large and positive for all $y \neq y^{(n)}$.

Multiclass SVM: separable case

Binary

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{10}$$

$$\text{s.t.} \quad \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}} \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D} \tag{11}$$

Multiclass As in the binary case, take 1 as our target margin.

$$m_{n,y}(w) \stackrel{\text{def}}{=} \underbrace{\left\langle w, \Psi(x^{(n)}, y^{(n)}) \right\rangle}_{\text{score of correct class}} - \underbrace{\left\langle w, \Psi(x^{(n)}, y) \right\rangle}_{\text{score of other class}} \tag{12}$$

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{13}$$

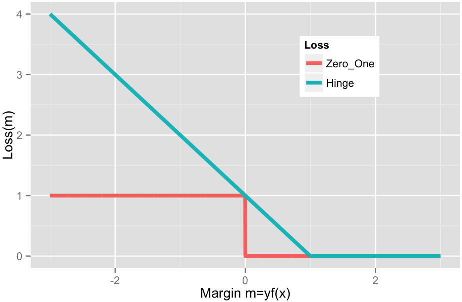
$$\text{s.t.} \quad m_{n,y}(w) \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D}, y \neq y^{(n)} \tag{14}$$

Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

- Hinge loss: a convex upperbound on the 0-1 loss

$$\ell_{\text{hinge}}(y,\hat{y}) = \max(0, 1 - yh(x)) \tag{15}$$



Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y,y') = \mathbb{I}\{y \neq y'\} \tag{16}$$

- In general, can also have different cost for each class.
- Upper bound on $\Delta(y,y')$.

$$\hat{y} \stackrel{\text{def}}{=} \underset{y' \in \mathcal{Y}}{\arg\max} \left\langle w, \Psi(x,y') \right\rangle \tag{17}$$

$$\implies \langle w, \Psi(x,y)\rangle \leqslant \langle w, \Psi(x,\hat{y})\rangle \tag{18}$$

$$\implies \Delta(y,\hat{y}) \leqslant \Delta(y,\hat{y}) - \langle w, (\Psi(x,y) - \Psi(x,\hat{y}))\rangle \qquad \text{When are they equal?} \tag{19}$$

- Generalized hinge loss:

$$\ell_{\text{hinge}}(y,x,w) \stackrel{\text{def}}{=} \max_{y' \in \mathcal{Y}} \left(\Delta(y,y') - \left\langle w, \left(\Psi(x,y) - \Psi(x,y')\right)\right\rangle\right) \tag{20}$$

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

$$\min_{w \in \mathrm{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max\left(0, 1 - \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}}\right).$$

- The multiclass objective:

$$\min_{w \in \mathrm{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max_{y' \in \mathcal{Y}}\left(\Delta(y, y') - \underbrace{\left\langle w, \left(\Psi(x, y) - \Psi(x, y')\right)\right\rangle}_{\text{margin}}\right)$$

  - $\Delta(y, y')$ as target margin for each class.
  - If margin $m_{n,y'}(w)$ meets or exceeds its target $\Delta(y^{(n)}, y')$ $\forall y \in \mathcal{Y}$, then no loss on example n.

Recap: What Have We Got?

- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$
- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathrm{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass loss
  - Train one model: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}$.
  - Prediction involves solving $\arg\max_{y \in \mathcal{Y}} h(x, y)$.

Does it work better in practice?

- Paper by Rifkin & Klautau: "In Defense of One-Vs-All Classification" (2004)
  - Extensive experiments, carefully done
    - albeit on relatively small UCI datasets
  - Suggests one-vs-all works just as well in practice
    - (or at least, the advantages claimed by earlier papers for multiclass methods were not compelling)
- Compared
  - many multiclass frameworks (including the one we discuss)
  - one-vs-all for SVMs with RBF kernel
  - one-vs-all for square loss with RBF kernel (for classification!)
- All performed roughly the same

Why Are We Bothering with Multiclass?

- The framework we have developed for multiclass
  - compatibility features / scoring functions
  - multiclass margin
  - target margin / multiclass loss
- Generalizes to situations where k is very large and one-vs-all is intractable.
- Key idea is that we can generalize across outputs y by using features of y.

Introduction to Structured Prediction

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
y	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

- $\mathcal{V} = \{\text{all English words}\} \cup \{\text{[START]}, \text{"."}\}$
- $\mathcal{X} = \mathcal{V}^n$, $n = 1, 2, 3, \ldots$ [Word sequences of any length]
- $\mathcal{P} = \{\text{START}, \text{Pronoun}, \text{Verb}, \text{Noun}, \text{Adjective}\}$
- $\mathcal{Y} = \mathcal{P}^n$, $n = 1, 2, 3, \ldots$[Part of speech sequence of any length]

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
  - Size depends on input x
- Base Hypothesis Space: $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}\}$
  - $h(x, y)$ gives compatibility score between input x and output y
- Multiclass hypothesis space

$$\mathcal{F} = \left\{ x \mapsto \operatorname*{arg\,max}_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$

- Final prediction function is an $f \in \mathcal{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.

Structured Prediction

- Part-of-speech tagging

x:	he	eats	apples
y:	pronoun	verb	noun

- Multiclass hypothesis space:

$$h(x, y) = w^T \Psi(x, y) \tag{21}$$

$$\mathcal{F} = \left\{ x \mapsto \arg\max_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\} \tag{22}$$

- A special case of multiclass classification
- How to design the feature map Ψ? What are the considerations?

Unary features

- A **unary feature** only depends on
  - the label at a single position, y_i, and x
- Example:

$$\begin{aligned}
\phi_1(x, y_i) &= 1(x_i = \text{runs})1(y_i = \text{Verb}) \\
\phi_2(x, y_i) &= 1(x_i = \text{runs})1(y_i = \text{Noun}) \\
\phi_3(x, y_i) &= 1(x_{i-1} = \text{He})1(x_i = \text{runs})1(y_i = \text{Verb})
\end{aligned}$$

Markov features

- A **markov feature** only depends on
  - two adjacent labels, y_{i-1} and y_i, and x
- Example:

$$
\begin{aligned}
\theta_1(x, y_{i-1}, y_i) &= 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Verb}) \\
\theta_2(x, y_{i-1}, y_i) &= 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Noun})
\end{aligned}
$$

- Reminiscent of Markov models in the output space
- Possible to have higher-order features

Local Feature Vector and Compatibility Score

- At each position i in sequence, define the **local feature vector** (unary and markov):

$$\begin{aligned}\Psi_i(x, y_{i-1}, y_i) &= (\phi_1(x, y_i), \phi_2(x, y_i), \ldots, \\ &\quad \theta_1(x, y_{i-1}, y_i), \theta_2(x, y_{i-1}, y_i), \ldots)\end{aligned}$$

- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.

- The compatibility score for (x, y) is the sum of local compatibility scores:

$$\sum_i \langle w, \Psi_i(x, y_{i-1}, y_i)\rangle = \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i)\right\rangle = \langle w, \Psi(x, y)\rangle, \tag{23}$$

  where we define the **sequence feature vector** by

$$\Psi(x, y) = \sum_i \Psi_i(x, y_{i-1}, y_i). \qquad \text{decomposable}$$

Structured perceptron

Given a dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in \mathcal{D}$ **do**
    $\hat{y} = \arg\max_{y' \in \mathcal{Y}(x)} w^T \psi(x, y')$;
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w \leftarrow w + \Psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$
      $w \leftarrow w - \Psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$
    end
  end
end

Identical to the multiclass perceptron algorithm except the $\arg\max$ is now over the structured output space $\mathcal{Y}(x)$.

Structured hinge loss

- Recall the generalized hinge loss

$$\ell_{\text{hinge}}(y,\hat{y}) \stackrel{\text{def}}{=} \max_{y' \in \mathcal{Y}(x)} \left(\Delta(y,y') + \left\langle w, \left(\Psi(x,y') - \Psi(x,y)\right)\right\rangle\right) \tag{24}$$

- What is $\Delta(y,y')$ for two sequences?
- **Hamming loss** is common:

$$\Delta(y,y') = \frac{1}{L}\sum_{i=1}^{L} 1(y_i \neq y_i')$$

where L is the sequence length.

Structured SVM

Exercise:

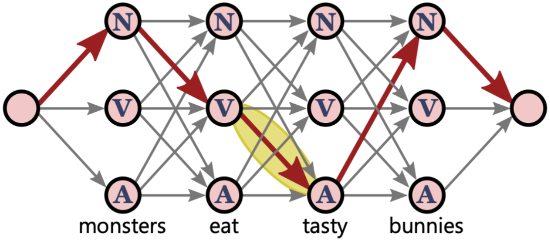
- Write down the objective of structured SVM using the structured hinge loss.
- Stochastic sub-gradient descent for structured SVM (similar to HW3 P3)
- Compare with the structured perceptron algorithm

The argmax problem for sequences

Problem To compute predictions, we need to find $\arg\max_{y \in \mathcal{Y}(x)} \langle w, \Psi(x, y) \rangle$, and $|\mathcal{Y}(x)|$ is exponentially large.

Observation $\Psi(x, y)$ decomposes to $\sum_i \Psi_i(x, y)$.

Solution Dynamic programming (similar to the Viterbi algorithm)



What's the running time?

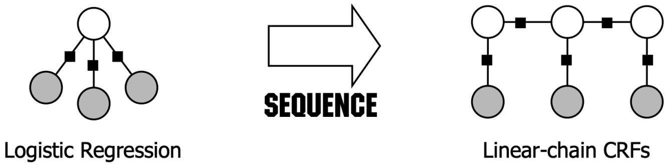
Figure by Daumé III. A course in machine learning. Figure 17.1.

Conditional random field (CRF)

- Recall that we can write logistic regression in a general form:

$$p(y|x) = \frac{1}{Z(x)} \exp(w^\top \psi(x, y)).$$

- Z is normalization constant: $Z(x) = \sum_{y \in Y} \exp(w^\top \psi(x, y))$.
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



Conditional random field (CRF)

- Compared to Structured SVM, CRF has a probabilistic interpretation.
- We can draw samples in the output space.
- How do we learn w? Maximum log likelihood, and regularization term: $\lambda \|w\|^2$
- Loss function:

$$
\begin{aligned}
l(w) &= -\frac{1}{N}\sum_{i=1}^{N} \log p(y^{(i)}|x^{(i)}) + \frac{1}{2}\lambda\|w\|^2 \\
&= -\frac{1}{N}\sum_{i}\sum_{t}\sum_{k} w_k \psi_k(y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_{i} \log Z(x^{(i)}) + \frac{1}{2}\sum_{k} \lambda w_k^2
\end{aligned}
$$

- Loss function:

$$l(w) = -\frac{1}{N}\sum_i \sum_t \sum_k w_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_i \log Z(x^{(i)}) + \frac{1}{2}\sum_k \lambda w_k^2$$

- Gradient:

$$\frac{\partial l(w)}{\partial w_k} = -\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) \tag{25}$$

$$+\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_t, y'_{t-1})) + \sum_k \lambda w_k \tag{26}$$

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})$?
- It is the expectation $\psi_k(x^{(i)}, y_t, y_{t-1})$ under the empirical distribution $\tilde{p}(x, y) = \frac{1}{N}\sum_i \mathbb{1}[x = x^{(i)}]\mathbb{1}[y = y^{(i)}]$.

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y'_t, y'_{t-1}))$?

$$
\begin{aligned}
&\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y'_t, y'_{t-1})) && (27)\\
&= \frac{1}{N}\sum_i \left[\sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y'_t, y'_{t-1}))\right]^{-1} && (28)\\
&\left[\sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y^{(i)}_t, y^{(i)}_{t-1})) \sum_t \psi_k(x^{(i)}, y'_t, y'_{t-1})\right] && (29)\\
&= \frac{1}{N}\sum_i \sum_t \sum_{y' \in Y} p(y'_t, y'_{t-1}|x)\psi_k(x^{(i)}, y'_t, y'_{t-1}) && (30)
\end{aligned}
$$

- It is the expectation of $\psi_k(x^{(i)}, y'_t, y'_{t-1})$ under the model distribution $p(y'_t, y'_{t-1}|x)$.

Conditional random field (CRF)

- To compute the gradient, we need to infer expectation under the model distribution $p(y|x)$.
- Compare the learning algorithms: in structured SVM we need to compute the argmax, whereas in CRF we need to compute the model expectation.
- Both problems are NP-hard for general graphs.

CRF Inference

- In the linear chain structure, we can use the forward-backward algorithm for inference, similar to Viterbi.
- Initiate $\alpha_j(1) = \exp(w^\top \psi(y_1 = j, x_1))$
- Recursion: $\alpha_j(t) = \sum_i \alpha_i(t-1)\exp(w^\top \psi(y_t = j, y_{t-1} = i, x_t))$
- Result: $Z(x) = \sum_j \alpha_j(T)$
- Similar for the backward direction.
- Test time, again use Viterbi algorithm to infer argmax.
- The inference algorithm can be generalized to belief propagation (BP) in a tree structure (exact inference).
- In general graphs, we rely on approximate inference (e.g. loopy belief propagation).

Examples

- POS tag Relationship between constituents, e.g. NP is likely to be followed by a VP.
- Semantic segmentation
  Relationship between pixels, e.g. a grass pixel is likely to be next to another grass pixel, and a sky pixel is likely to be above a grass pixel.
- Multi-label learning
  An image may contain multiple class labels, e.g. a bus is likely to co-occur with a car.

Conclusion

Multiclass algorithms

- Reduce to binary classification, e.g., OvA, AvA
  - Good enough for simple multiclass problems
  - They don't scale and have simplified assumptions
- Generalize binary classification algorithms using multiclass loss
  - Multi-class perceptron, multi-class logistics regression, multi-class SVM
- Structured prediction: Structured SVM, CRF. Data containing structure. Extremely large output space. Text and image applications.