Multiclass Classification

CDS, NYU

March 28, 2023

Overview

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  - Sentiment analysis (positive vs. negative)
  - Spam filter (spam vs. non-spam)

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- 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)
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- 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: $\mathcal{Y} = \{1, \ldots, k\}$

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Prediction

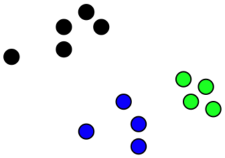
- Majority vote:

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

- Ties can be broken arbitrarily.

OvA: 3-class example (linear classifier)

Consider a dataset with three classes:



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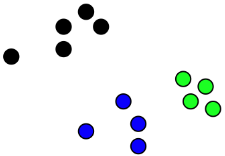

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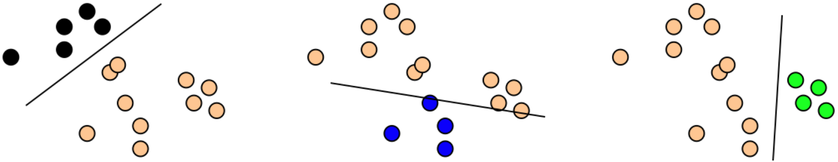

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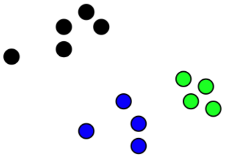

Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.

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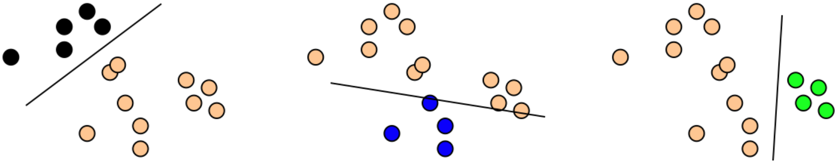

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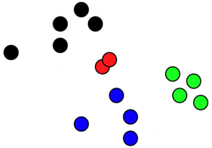

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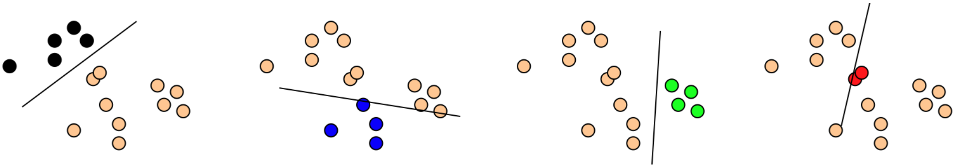

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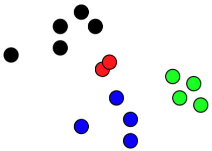

Cannot separate red points from the rest.
Which classes might have low accuracy?

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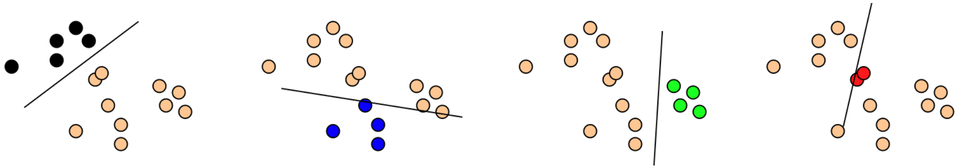

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- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
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Prediction

- 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

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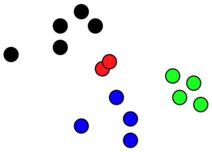
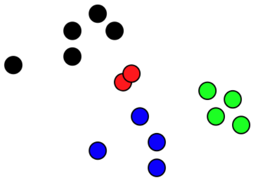


What's the decision region for the red class?



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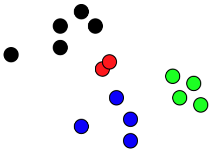
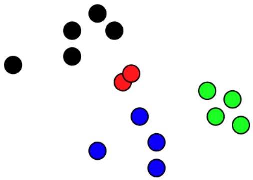


Assumption: each pair of classes are linearly separable.
More expressive than OvA.

What's the decision region for the red class?



OvA vs AvA

		OvA	AvA
computation	train	$O(k\quad)$	$O(k^2\quad)$
	test	$O(k\quad)$	$O(k^2\quad)$

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	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$

challenges

OvA vs AvA

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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).

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OvA encoding:

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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
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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
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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 ($\log_2 k$)?

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  - 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:

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- 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).

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

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

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

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

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- 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):

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

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- 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

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- 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

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  - $\implies$ a single weight vector is desired
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$$w_i^T x = w^T \psi(x, i) \tag{5}$$

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

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

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

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

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- And then do the following: $\Psi : \mathrm{R}^2 \times \{1,2,3\} \to \mathrm{R}^6$ 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) \\
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- 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 $\mathcal{D} = \{(x, y)\}$;
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for $iter = 1, 2, \ldots, T$ **do**
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Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,}\ldots\}$.

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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: $w \in \mathbf{R}^{d \times k}$—doesn't scale.

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

How to construct the feature vector?

- Multivector construction: $w \in \mathbb{R}^{d \times k}$—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 .
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- 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 $\to \{1, 2, \ldots, d\}$.

Review

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- Represent labels in the input space $\implies$ single weight vector.

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- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

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We've seen

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- 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 $y^{(n)}$)

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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

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

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

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

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

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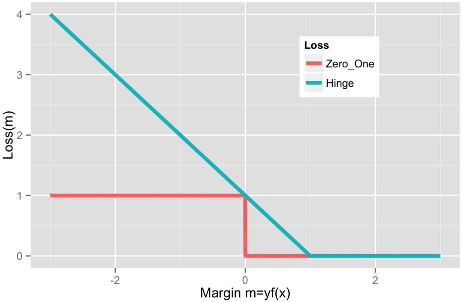
Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

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

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



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

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- Upper bound on $\Delta(y, y')$.

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

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

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- Generalized hinge loss:

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

Multiclass SVM with Hinge Loss

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

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

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- The multiclass objective:

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

  - $\Delta(y, y')$ 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?

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  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathrm{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
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  - 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: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}$.
  - 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
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    - (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
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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	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

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- $\mathcal{V} = \{\text{all English words}\} \cup \{\text{[START]}, ``."\}$
- $\mathcal{X} = \mathcal{V}^n$, $n = 1, 2, 3, \ldots$ [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)
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  - $h(x, y)$ gives compatibility score between input x and output y
- Multiclass hypothesis space

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

- 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):

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

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

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- 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
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    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?

Structured hinge loss

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- 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.

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

The argmax problem for sequences

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

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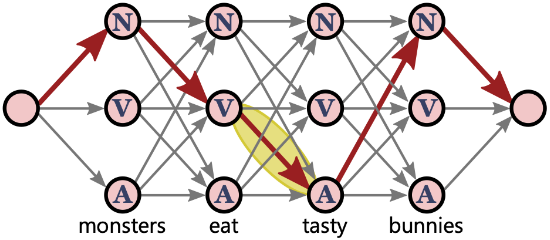
Solution Dynamic programming (similar to the Viterbi algorithm)



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:

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

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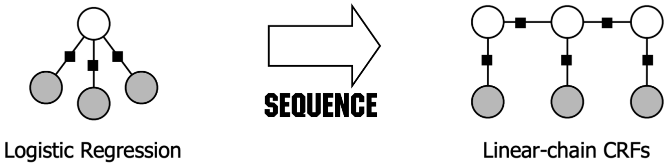
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



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- 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
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- Gradient:

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

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

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

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

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- 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.

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- In general graphs, we rely on approximate inference (e.g. loopy belief propagation).

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- 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

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  - They don't scale and have simplified assumptions
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- Structured prediction: Structured SVM, CRF. Data containing structure. Extremely large output space. Text and image applications.