

# Multiclass and Introduction to Structured Prediction

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# Introduction

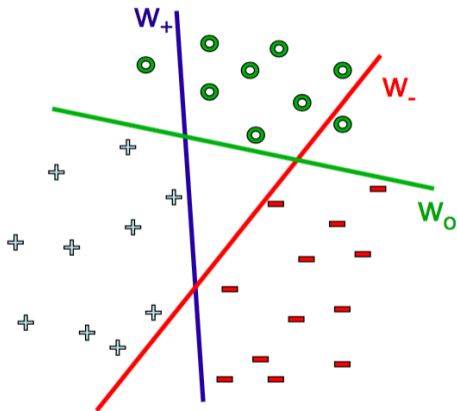
# Multiclass Setting

- Input space:  $\mathcal{X}$
- Output space:  $\mathcal{Y} = \{1, \dots, k\}$
- Our approaches to multiclass problems so far:
  - multinomial / softmax logistic regression
- Soon: trees and random forests
- Today we consider linear methods specifically designed for multiclass.
- But the main takeaway will be an approach that generalizes to situations where  $k$  is “exponentially large” – too large to enumerate.

## Reduction to Binary Classification

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# One-vs-All / One-vs-Rest



Plot courtesy of David Sontag.

# One-vs-All / One-vs-Rest

- Train  $k$  binary classifiers, one for each class.
- Train  $i$ th classifier to distinguish class  $i$  from rest
- Suppose  $h_1, \dots, h_k : \mathcal{X} \rightarrow \mathbf{R}$  are our binary classifiers.
  - Can output hard classifications in  $\{-1, 1\}$  or scores in  $\mathbf{R}$ .
- Final prediction is

$$h(x) = \arg \max_{i \in \{1, \dots, k\}} h_i(x)$$

- Ties can be broken arbitrarily.

## Linear Classifiers: Binary and Multiclass

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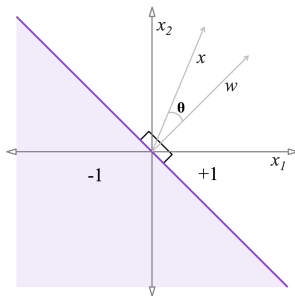
# Linear Binary Classifier Review

- Input Space:  $\mathcal{X} = \mathbf{R}^d$
- Output Space:  $\mathcal{Y} = \{-1, 1\}$
- Linear classifier score function:

$$f(x) = \langle w, x \rangle = w^T x$$

- Final classification prediction:  $\text{sign}(f(x))$
- Geometrically, when are  $\text{sign}(f(x)) = +1$  and  $\text{sign}(f(x)) = -1$ ?

# Linear Binary Classifier Review



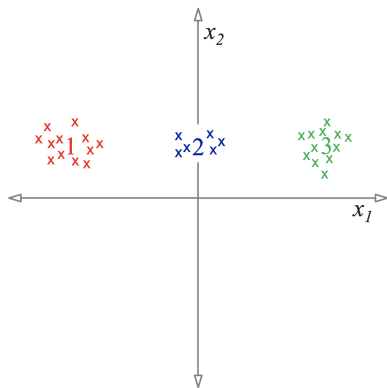
Suppose  $\|w\| > 0$  and  $\|x\| > 0$ :

$$f(x) = \langle w, x \rangle = \|w\| \|x\| \cos \theta$$

$$f(x) > 0 \iff \cos \theta > 0 \iff \theta \in (-90^\circ, 90^\circ)$$

$$f(x) < 0 \iff \cos \theta < 0 \iff \theta \notin [-90^\circ, 90^\circ]$$

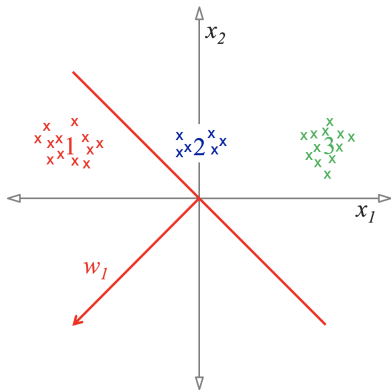
# Three Class Example



- Base hypothesis space  $\mathcal{H} = \{f(x) = w^T x \mid x \in \mathbf{R}^2\}$ .
- Note: Separating boundary always contains the origin.

Example based on Shalev-Schwartz and Ben-David's *Understanding Machine Learning*, Section 17.1

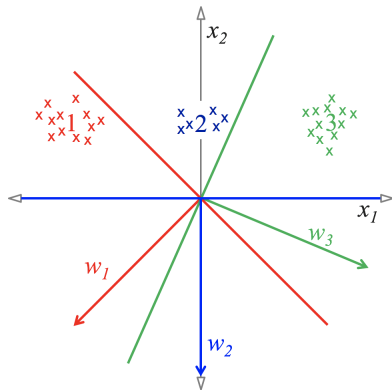
## Three Class Example: One-vs-Rest



- Class 1 vs Rest:

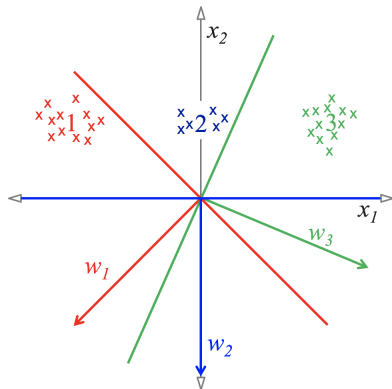
$$f_1(x) = w_1^T x$$

## Three Class Example: One-vs-Rest



- Examine “Class 2 vs Rest”
  - Predicts everything to be “Not 2”.
  - If it predicted some “2”, then it would get many more “Not 2” incorrect.

# One-vs-Rest: Predictions



- Score for class  $i$  is

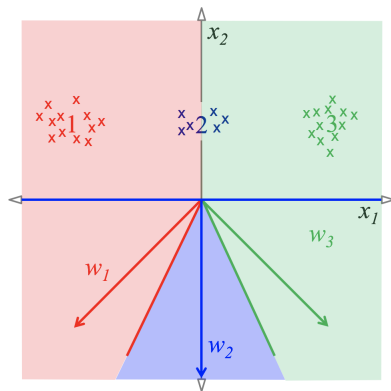
$$f_i(x) = \langle w_i, x \rangle = \|w_i\| \|x\| \cos \theta_i,$$

where  $\theta_i$  is the angle between  $x$  and  $w_i$ .

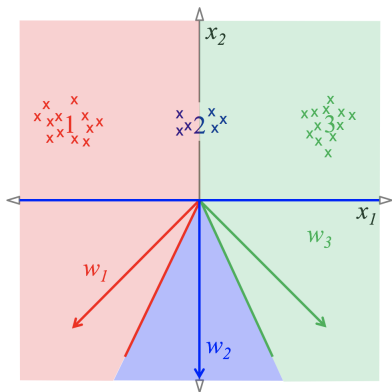
# One-vs-Rest: Class Boundaries

- For simplicity, we've assumed  $\|w_1\| = \|w_2\| = \|w_3\|$ .
- Then  $\|w_i\|$  and  $\|x\|$  are equal for all scores.

$\implies x$  is classified by whichever has largest  $\cos\theta_i$  (i.e.  $\theta_i$  closest to 0)



# One-vs-Rest: Class Boundaries



- This approach doesn't work well in this instance.
- How can we fix this?



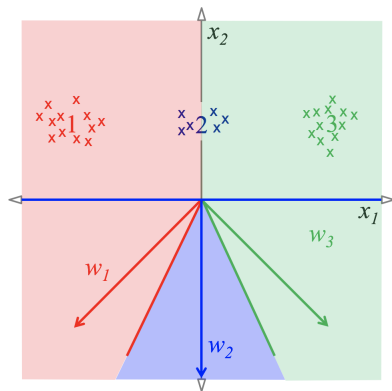
# The Linear Multiclass Hypothesis Space

- **Base Hypothesis Space:**  $\mathcal{H} = \{x \mapsto w^T x \mid w \in \mathbf{R}^d\}$ .
- **Linear Multiclass Hypothesis Space** (for  $k$  classes):

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

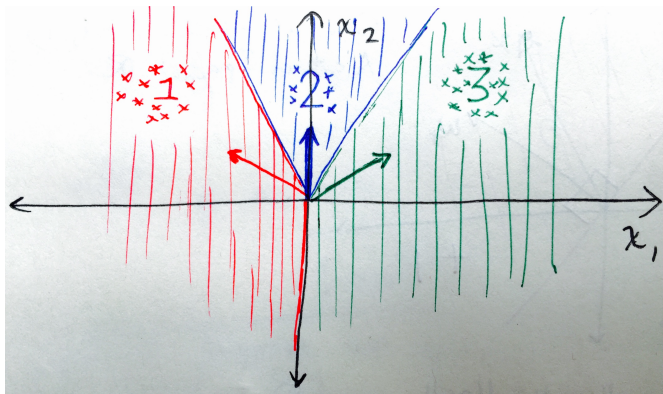
- What's the action space here?

# One-vs-Rest: Class Boundaries



- Recall: A **learning algorithm** chooses the hypothesis from the hypothesis space.
- Is this a failure of the hypothesis space or the learning algorithm?

# A Solution with Linear Functions



- This works... so the problem is not with the hypothesis space.
- How can we get a solution like this?

# Multiclass Predictors

# Multiclass Hypothesis Space

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

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

- $h_i(x)$  **scores** how likely  $x$  is to be from class  $i$ .

Issue: Need to learn (and represent)  $k$  functions. Doesn't scale to very large  $k$ .

# Multiclass Hypothesis Space: Reframed

- **General [Discrete] Output Space:**  $\mathcal{Y}$  (e.g  $\mathcal{Y} = \{1, \dots, k\}$  for multiclass)
- *New idea:* Rather than a score function for each class,
  - use one function  $h(x, y)$  that gives a **compatibility score** between input  $x$  and output  $y$
- Final **prediction** is the  $y \in \mathcal{Y}$  that is “most compatible” with  $x$ :

$$f(x) = \arg \max_{y \in \mathcal{Y}} h(x, y)$$

- This subsumes the framework with class-specific score functions.
- Given class-specific score functions  $h_1, \dots, h_k$ , we could define compatibility function as

$$h(x, i) = h_i(x), \quad i = 1, \dots, k.$$

# Multiclass Hypothesis Space: Reframed

- **General [Discrete] Output Space:**  $\mathcal{Y}$
- **Base Hypothesis Space:**  $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}\}$ 
  - $h(x, y)$  gives **compatibility score** between input  $x$  and output  $y$
- **Multiclass Hypothesis Space**

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

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

# Learning in a Multiclass Hypothesis Space: In Words

- **Base Hypothesis Space:**  $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}\}$
- Training data:  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Learning process chooses  $h \in \mathcal{H}$ .
- Want compatibility  $h(x, y)$  to be large when  $x$  has label  $y$ , small otherwise.



# Learning in a Multiclass Hypothesis Space: In Math

- $h(x, y)$  classifies  $(x_i, y_i)$  correctly iff

$$h(x_i, y_i) > h(x_i, y) \forall y \neq y_i$$

- $h$  should give higher score for correct  $y$  than for all other  $y \in \mathcal{Y}$ .
- An equivalent condition is the following:

$$h(x_i, y_i) > \max_{y \neq y_i} h(x_i, y)$$

- If we define

$$m_i = h(x_i, y_i) - \max_{y \neq y_i} h(x_i, y),$$

then classification is correct if  $m_i > 0$ . Generally want  $m_i$  to be large.

- Sound familiar?

## A Linear Multiclass Hypothesis Space

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# Linear Multiclass Prediction Function

- A **linear class-sensitive score function** is given by

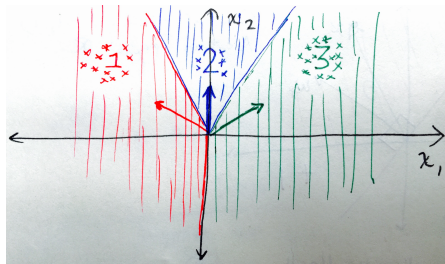
$$h(x, y) = \langle w, \Psi(x, y) \rangle,$$

where  $\Psi(x, y) : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}^d$  is a **class-sensitive feature map**.

- $\Psi(x, y)$  extracts features relevant to how compatible  $y$  is with  $x$ .
- Final compatibility score is a **linear** function of  $\Psi(x, y)$ .
- **Linear Multiclass Hypothesis Space**

$$\mathcal{F} = \left\{ x \mapsto \arg \max_{y \in \mathcal{Y}} \langle w, \Psi(x, y) \rangle \mid w \in \mathbf{R}^d \right\}$$

Example:  $\mathcal{X} = \mathbf{R}^2$ ,  $\mathcal{Y} = \{1, 2, 3\}$



- $w_1 = \left(-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right)$ ,  $w_2 = (0, 1)$ ,  $w_3 = \left(\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right)$
- Prediction function:  $(x_1, x_2) \mapsto \arg \max_{i \in \{1, 2, 3\}} \langle w_i, (x_1, x_2) \rangle$ .
- How can we get this into the form  $x \mapsto \arg \max_{y \in \mathcal{Y}} \langle w, \Psi(x, y) \rangle$

# The Multivector Construction

- What if we stack  $w_i$ 's together:

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

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

$$\Psi(x, 1) := (x_1, x_2, 0, 0, 0, 0)$$

$$\Psi(x, 2) := (0, 0, x_1, x_2, 0, 0)$$

$$\Psi(x, 3) := (0, 0, 0, 0, x_1, x_2)$$

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

## NLP Example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}.$
- $\mathcal{Y} = \{\text{NOUN, VERB, ADJECTIVE, ADVERB, ARTICLE, PREPOSITION}\}.$
- Features of  $x \in \mathcal{X}$ : [The word itself], ENDS\_IN\_ly, ENDS\_IN\_ness, ...
- $\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \dots, \psi_d(x, y)):$

$$\psi_1(x, y) = 1(x = \text{apple AND } y = \text{NOUN})$$

$$\psi_2(x, y) = 1(x = \text{run AND } y = \text{NOUN})$$

$$\psi_3(x, y) = 1(x = \text{run AND } y = \text{VERB})$$

$$\psi_4(x, y) = 1(x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB})$$

$$\vdots \quad \vdots \quad \vdots$$

- e.g.  $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \dots)$
- After training, what would you guess corresponding  $w_1, w_2, w_3, w_4$  to be?

## NLP Example: How does it work?

- $\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \dots, \psi_d(x, y)) \in \mathbf{R}^d$ :

$$\psi_1(x, y) = 1(x = \text{apple AND } y = \text{NOUN})$$

$$\psi_2(x, y) = 1(x = \text{run AND } y = \text{NOUN})$$

$$\vdots \quad \vdots \quad \vdots$$

- After training, we've learned  $w \in \mathbf{R}^d$ . Say  $w = (5, -3, 1, 4, \dots)$
- To predict label for  $x = \text{apple}$ ,
  - we compute compatibility scores for each  $y \in \mathcal{Y}$ :

$$\langle w, \Psi(\text{apple}, \text{NOUN}) \rangle$$

$$\langle w, \Psi(\text{apple}, \text{VERB}) \rangle$$

$$\langle w, \Psi(\text{apple}, \text{ADVERB}) \rangle$$

$$\vdots$$

- Predict class that gives highest score.

## Another Approach: Use Label Features

- What if we have a very large number of classes?
- Make features for the classes.
- Common in advertising
  - $\mathcal{X}$ : User and user context
  - $\mathcal{Y}$ : A large set of banner ads
- Suppose user  $x$  is shown many banner ads.
- We want to predict which one the user will click on.
- Possible compatibility features:

$$\psi_1(x, y) = 1(x \text{ interested in sports AND } y \text{ relevant to sports})$$

$$\psi_2(x, y) = 1(x \text{ is in target demographic group of } y)$$

$$\psi_3(x, y) = 1(x \text{ previously clicked on ad from company sponsoring } y)$$



# Linear Multiclass SVM

# The Margin for Multiclass

- Let  $h: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}$  be our **compatibility score function**.
- Define a “**margin**” between correct class and each other class:

## Definition

The [class-specific] **margin** of score function  $h$  on the  $i$ th example  $(x_i, y_i)$  for class  $y$  is

$$m_{i,y}(h) = h(x_i, y_i) - h(x_i, y).$$

- Want  $m_{i,y}(h)$  to be large and positive for all  $y \neq y_i$ .
- For our linear hypothesis space, margin is

$$m_{i,y}(w) = \langle w, \Psi(x_i, y_i) \rangle - \langle w, \Psi(x_i, y) \rangle$$

# Multiclass SVM with Hinge Loss

- Recall binary SVM (without bias term):

$$\min_{w \in \mathbf{R}^d} \frac{1}{2} \|w\|^2 + \frac{c}{n} \sum_{i=1}^n \max \left( 0, 1 - \underbrace{y_i w^T x_i}_{\text{margin}} \right).$$

- Multiclass SVM (Version 1):

$$\min_{w \in \mathbf{R}^d} \frac{1}{2} \|w\|^2 + \frac{c}{n} \sum_{i=1}^n \max_{y \neq y_i} [\max(0, 1 - m_{i,y}(w))]$$

where  $m_{i,y}(w) = \langle w, \Psi(x_i, y_i) \rangle - \langle w, \Psi(x_i, y) \rangle$ .

- As in SVM, we've taken the value 1 as our “target margin” for each  $i, y$ .

# Class-Sensitive Loss

- In multiclass, some misclassifications may be worse than others.
- Rather than 0/1 Loss, we may be interested in a more general loss

$$\Delta: \mathcal{Y} \times \mathcal{A} \rightarrow [0, \infty)$$

- We can use this  $\Delta$  as our **target margin** for multiclass SVM.
- Multiclass SVM (Version 2):

$$\min_{w \in \mathbf{R}^d} \frac{1}{2} \|w\|^2 + \frac{c}{n} \sum_{i=1}^n \max_{y \neq y_i} [\max(0, \Delta(y_i, y) - m_{i,y}(w))]$$

- If margin  $m_{i,y}(w)$  meets or exceeds its target  $\Delta(y_i, y) \forall y \neq y_i$ , then no loss on example  $i$ .
- Note: If  $\Delta(y, y) = 0 \forall y \in \mathcal{Y}$ , then we can replace  $\max_{y \neq y_i}$  with  $\max_y$ .

## Interlude: Is This Worth The Hassle Compared to One-vs-All?

## Recap: What Have We Got?

- Problem: Multiclass classification  $\mathcal{Y} = \{1, \dots, k\}$
- Solution 1: One-vs-All
  - Train  $k$  models:  $h_1(x), \dots, h_k(x) : \mathcal{X} \rightarrow \mathbf{R}$ .
  - Predict with  $\arg \max_{y \in \mathcal{Y}} h_y(x)$ .
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass
  - Train one model:  $h(x, y) : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbf{R}$ .
  - 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
    - (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 / score functions
  - multiclass margin
  - target margin
- **Generalizes to situations where  $k$  is very large and one-vs-all is intractable.**
- Key point is that we can generalize across outputs  $y$  by using features of  $y$ .



# Introduction to Structured Prediction

# Part-of-speech (POS) Tagging

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

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

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

- A **structured prediction** problem is a multiclass problem in which  $\mathcal{Y}$  is very large, but has (or we assume it has) a certain structure.
- For POS tagging,  $\mathcal{Y}$  grows exponentially in the length of the sentence.
- Typical **structure** assumption: The POS labels form a Markov chain.
  - i.e.  $y_{n+1} \mid y_n, y_{n-1}, \dots, y_0$  is the same as  $y_{n+1} \mid y_n$ .

# Local Feature Functions: Type 1

- A “type 1” **local feature** only depends on
  - the label at a single position, say  $y_i$  (label of the  $i$ th word) and
  - $x$  at any position
- Example:

$$\phi_1(i, x, y_i) = 1(x_i = \text{runs})1(y_i = \text{Verb})$$

$$\phi_2(i, x, y_i) = 1(x_i = \text{runs})1(y_i = \text{Noun})$$

$$\phi_3(i, x, y_i) = 1(x_{i-1} = \text{He})1(x_i = \text{runs})1(y_i = \text{Verb})$$

## Local Feature Functions: Type 2

- A “type 2” **local feature** only depends on
  - the labels at 2 consecutive positions:  $y_{i-1}$  and  $y_i$
  - $x$  at any position

- Example:

$$\theta_1(i, x, y_{i-1}, y_i) = 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Verb})$$

$$\theta_2(i, x, y_{i-1}, y_i) = 1(y_{i-1} = \text{Pronoun})1(y_i = \text{Noun})$$

## Local Feature Vector and Compatibility Score

- At each position  $i$  in sequence, define the **local feature vector**:

$$\Psi_i(x, y_{i-1}, y_i) = (\phi_1(i, x, y_i), \phi_2(i, x, y_i), \dots, \theta_1(i, x, y_{i-1}, y_i), \theta_2(i, x, y_{i-1}, y_i), \dots)$$

- Local compatibility score** for  $(x, y)$  at position  $i$  is  $\langle w, \Psi_i(x, y_{i-1}, y_i) \rangle$ .

## Sequence Compatibility Score

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

$$\begin{aligned} & \sum_i \langle w, \Psi_i(x, y_{i-1}, y_i) \rangle \\ &= \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i) \right\rangle \\ &= \langle w, \Psi(x, y) \rangle, \end{aligned}$$

where we define the sequence feature vector by

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

- So we see this is a special case of linear multiclass prediction.

# Sequence Target Loss

- How do we assess the loss for prediction sequence  $y'$  for example  $(x, y)$ ?
- **Hamming loss** is common:

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

- Could generalize this as

$$\Delta(y, y') = \frac{1}{|y|} \sum_{i=1}^{|y|} \delta(y_i, y'_i)$$



# What remains to be done?

- To compute predictions, we need to find

$$\arg \max_{y \in \mathcal{Y}} \langle w, \Psi(x, y) \rangle.$$

- This is straightforward for  $|\mathcal{Y}|$  small.
- Now  $|\mathcal{Y}|$  is exponentially large.
- Because  $\Psi$  breaks down into local functions only depending on 2 adjacent labels,
  - we can solve this efficiently using dynamic programming.
  - (Similar to Viterbi decoding.)
- Learning can be done with SGD and a similar dynamic program.