Multiclass and Introduction to Structured Prediction

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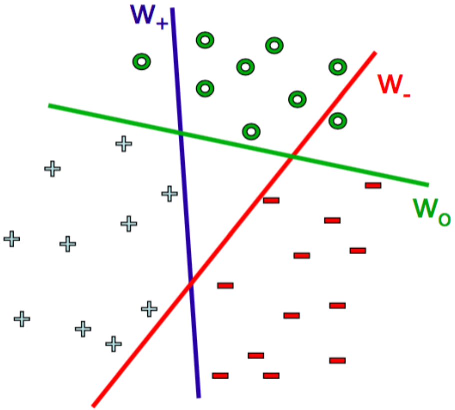
Introduction

Multiclass Setting

- Input space: $\mathcal{X}$
- Ouput space: $\mathcal{Y} = \{1, \ldots, k\}$
- Our approaches to multiclass problems so far:
    - multinomial / softmax logistic regression
    - 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

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 ith classifier to distinguish class i from rest
- Suppose $h_1, \ldots, h_k : \mathcal{X} \to \mathbf{R}$ are our binary classifiers.
  - Can output hard classifications in $\{-1, 1\}$ or scores in $\mathbf{R}$.
- Final prediction is

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

- Ties can be broken arbitrarily.

Linear Classifers: Binary and Multiclass

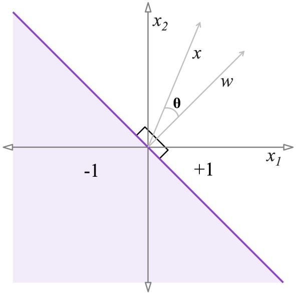
Linear Binary Classifier Review

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

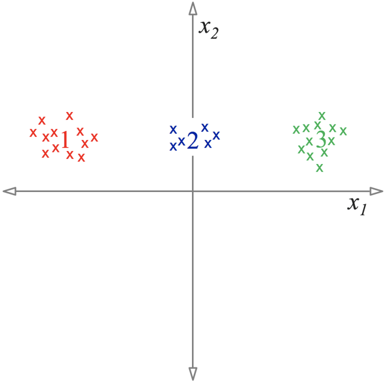
Linear Binary Classifier Review



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

$$
\begin{aligned}
f(x) &= \langle w, x \rangle = \|w\| \|x\| \cos\theta \\
f(x) > 0 &\iff \cos\theta > 0 \iff \theta \in (-90^\circ, 90^\circ) \\
f(x) < 0 &\iff \cos\theta < 0 \iff \theta \notin [-90^\circ, 90^\circ]
\end{aligned}
$$

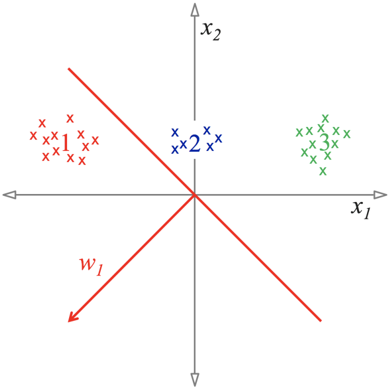
Three Class Example



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

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

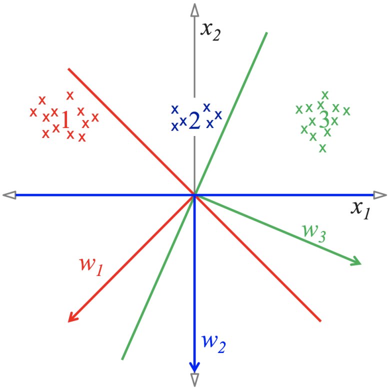
Three Class Example: One-vs-Rest



- Class 1 vs Rest:

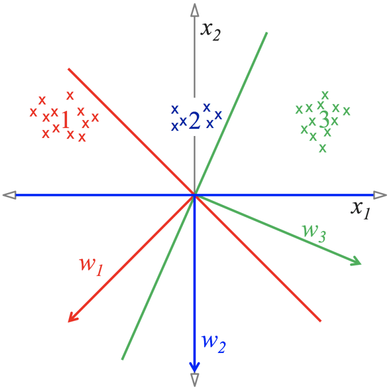
$$f_1(x) = w_1^T x$$

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

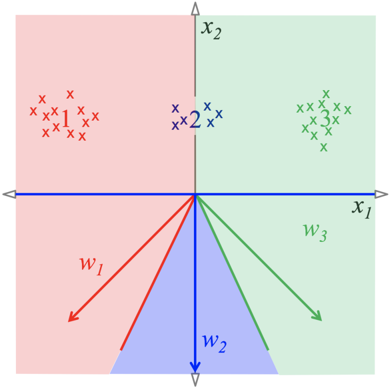
$$f_i(x) = \langle w_i, x \rangle = \|w_i\| \|x\| \cos \theta_i,$$

where θ_i is the angle between x and w_i.

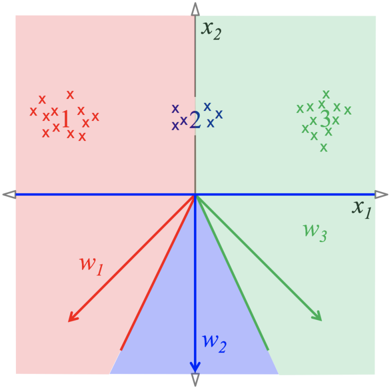
One-vs-Rest: Class Boundaries

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

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



One-vs-Rest: Class Boundaries



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

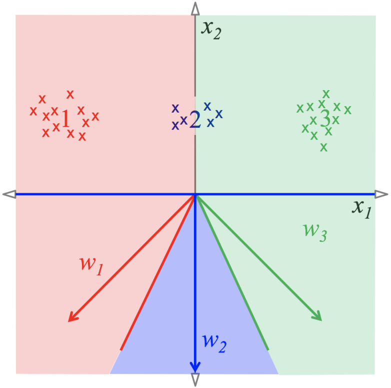
The Linear Multiclass Hypothesis Space

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

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

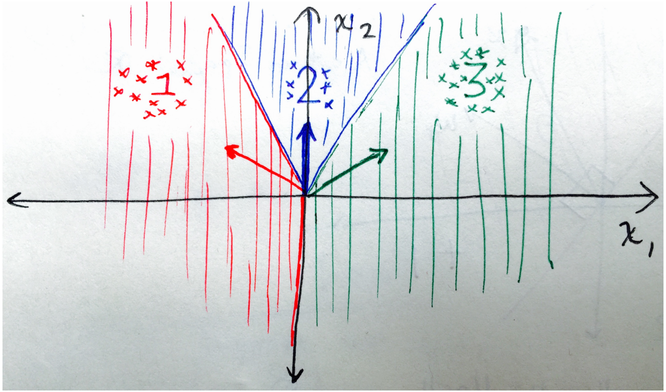
- What's the action space here?

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**: $\mathcal{H} = \{h : \mathcal{X} \to \mathbf{R}\}$ ("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 $\mathcal{Y} = \{1, \ldots, k\}$ 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:

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

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

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

Multiclass Hypothesis Space: Reframed

- **General [Discrete] Output Space:** $\mathcal{Y}$
- **Base Hypothesis Space:** $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}\}$
  - $h(x, y)$ 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 $h \in \mathcal{H}$.

Learning in a Multiclass Hypothesis Space: In Words

- **Base Hypothesis Space:** $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}\}$
- Training data: $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
- 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

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

- 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

- A **linear compatibility score function** is given by

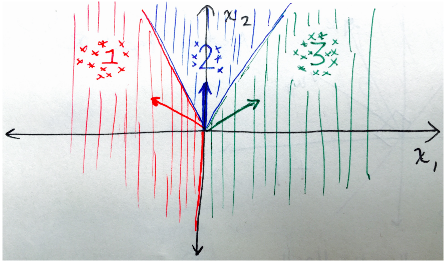
$$h(x,y) = \langle w, \Psi(x,y) \rangle,$$

where $\Psi(x,y) : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}^d$ is a **compatibility feature map**[1].
- $\Psi(x,y)$ 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**

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

[1] Called "class-sensitive" score function and feature map in our SSBD reference.

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:

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

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

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, ...
- $\Psi(x,y) = (\psi_1(x,y), \psi_2(x,y), \psi_3(x,y), \ldots, \psi_d(x,y))$:

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

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

NLP Example: How does it work?

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

$$\begin{aligned} `\psi_1(x,y) &= 1(x = \text{apple AND } y = \text{NOUN}) \\ \psi_2(x,y) &= 1(x = \text{run AND } y = \text{NOUN}) \\ \vdots \quad &\vdots \quad \vdots \end{aligned}$$

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

$$\begin{gathered} \langle w, \Psi(\text{apple}, \text{NOUN}) \rangle \\ \langle w, \Psi(\text{apple}, \text{VERB}) \rangle \\ \langle w, \Psi(\text{apple}, \text{ADVERB}) \rangle \\ \vdots \end{gathered}$$

- 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:

$$\begin{aligned}
\psi_1(x,y) &= 1(x \text{ interested in sports AND } y \text{ relevant to sports}) \\
\psi_2(x,y) &= 1(x \text{ is in target demographic group of } y) \\
\psi_3(x,y) &= 1(x \text{ previously clicked on ad from company sponsoring } y)
\end{aligned}$$

Linear Multiclass SVM

The Margin for Multiclass

- Let $h : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}$ 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 ith 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):

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

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

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

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

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

- 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 $\mathcal{Y} = \{1, \ldots, k\}$
- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathbf{R}$.
  - 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: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathbf{R}$.
  - 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
    - (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	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

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

Structured Prediction

- 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. $y_{n+1} \mid y_n, y_{n-1}, \ldots, y_0$ 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 ith word) and
  - x at any position
- Example:

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

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:

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

Local Feature Vector and Compatibility Score

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

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

- **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 Ψ 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.