

Multiclass and Introduction to Structured Prediction

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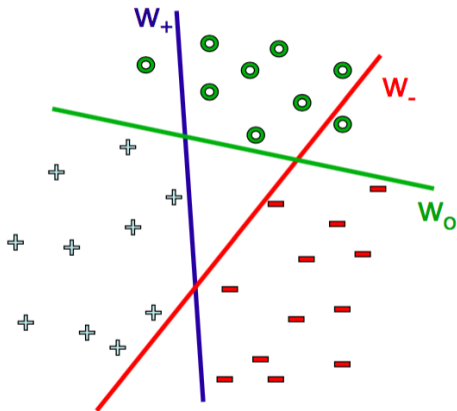
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Introduction

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

- 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

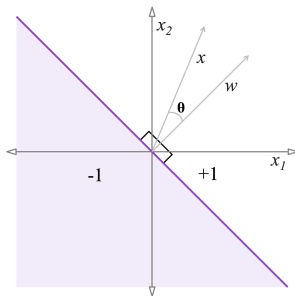
Linear Binary Classifier Review

- 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



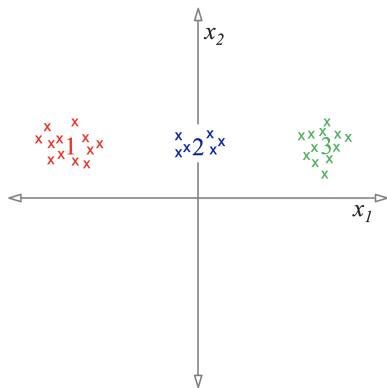
Suppose $\|w\| > 0$ and $\|x\| > 0$:

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

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

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

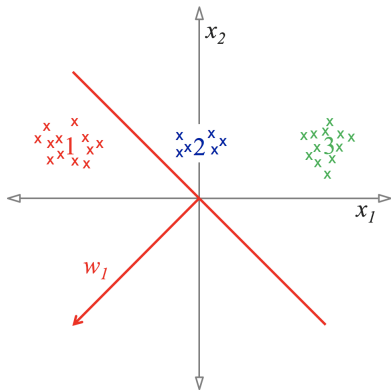
Three Class Example



- 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

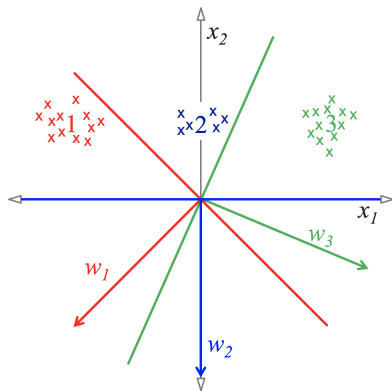
Three Class Example: One-vs-Rest



- Class 1 vs Rest:

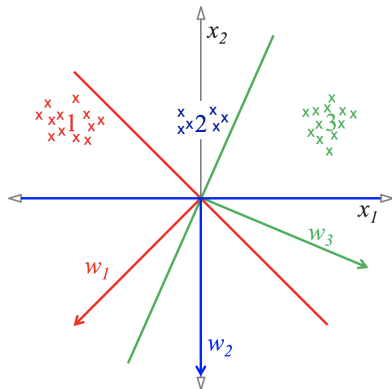
$$f_1(x) = w_1^T x$$

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

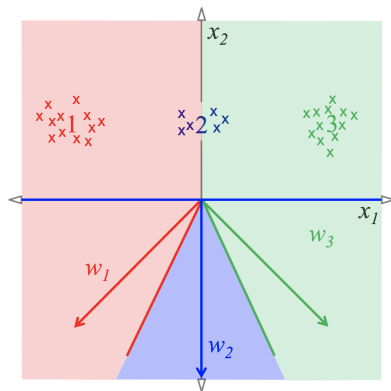
$$f_i(x) = \langle w_i, x \rangle = \|w_i\| \|x\| \cos \theta_i,$$

where θ_i is the angle between x and w_i .

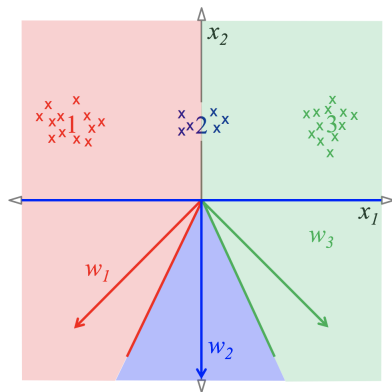
One-vs-Rest: Class Boundaries

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

$\implies x$ 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?

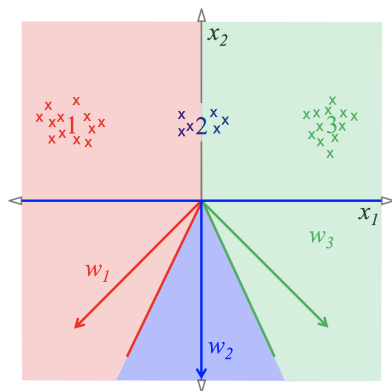
The Linear Multiclass Hypothesis Space

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

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

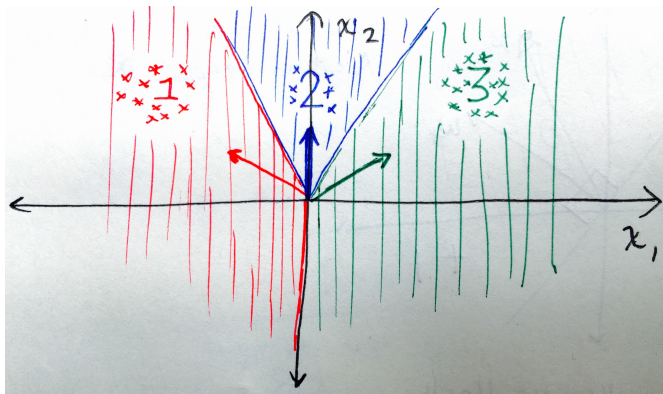
- What's the action space here?

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

Linear Multiclass Prediction Function

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

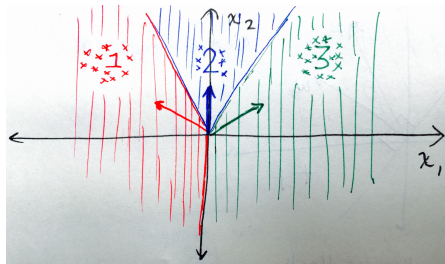
$$h(x, y) = \langle w, \Psi(x, y) \rangle,$$

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 **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

$$\Delta: \mathcal{Y} \times \mathcal{A} \rightarrow \mathbf{R}^{\geq 0}$$

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

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

- We can think of $\Delta(y_i, y)$ as the “target margin” for example i and class y because if each margin $m_{i,y}(w)$ meets or exceeds its corresponding target $\Delta(y_i, y)$, then we don't incur a loss on example i .

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 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.