Linear Multiclass Predictors

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Slides based on Lecture 09 from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

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OvA revisit

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

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

- $h_i(x)$ 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, for (x, i) we only need

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{1}$$

Multiclass perceptron

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

- 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

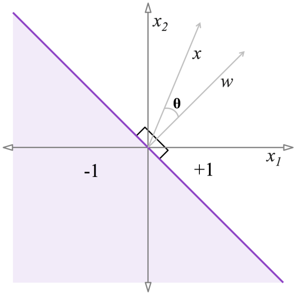
Side note: Linear Binary Classifier Review

- 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 $\operatorname{sign}(f(x)) = -1$?

Side note: Linear Binary Classifier Review



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

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

Rewrite the scoring function

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

$$w_i^T x = w^T \psi(x, i) \tag{2}$$

$$h_i(x) = h(x, i) \tag{3}$$

  - 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., $x \in \mathbf{R}^2, \mathcal{Y} = \{1,2,3\}$)

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

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

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

$$\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \ldots, \psi_d(x, y)) \tag{4}$$

  - 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 $\Longrightarrow$ 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 $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{5}$$

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

Multiclass

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

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{6}$$

- 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

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{7}$$

$$\text{s.t.} \quad \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}} \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D} \tag{8}$$

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

$$m_{n,y}(w) \stackrel{\text{def}}{=} \underbrace{\left\langle w, \Psi(x^{(n)}, y^{(n)}) \right\rangle}_{\text{score of correct class}} - \underbrace{\left\langle w, \Psi(x^{(n)}, y) \right\rangle}_{\text{score of other class}} \tag{9}$$

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

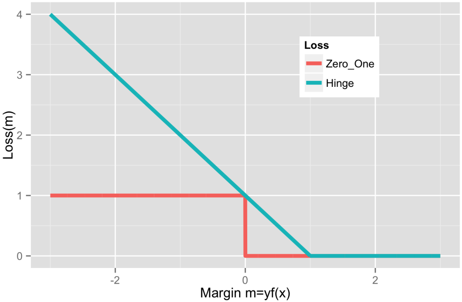
$$\text{s.t.} \quad m_{n,y}(w) \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D}, y \neq y^{(n)} \tag{11}$$

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

$$\ell_{\text{hinge}}(y, \hat{y}) = \max(0, 1 - yh(x)) \tag{12}$$



[discussion]Generalized hinge loss

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

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{13}$$

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

$$\hat{y} \overset{\text{def}}{=} \underset{y' \in \mathcal{Y}}{\arg\max} \langle w, \Psi(x, y') \rangle \tag{14}$$

$$\Longrightarrow \langle w, \Psi(x, y) \rangle \leqslant \langle w, \Psi(x, \hat{y}) \rangle \tag{15}$$

$$\Longrightarrow \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, (\Psi(x, y) - \Psi(x, \hat{y})) \rangle \qquad \text{When are they equal?} \tag{16}$$

- Generalized hinge loss:

$$\ell_{\text{hinge}}(y, x, w) \overset{\text{def}}{=} \max_{y' \in \mathcal{Y}} \left(\Delta(y, y') - \left\langle w, \left(\Psi(x, y) - \Psi(x, y') \right) \right\rangle \right) \tag{17}$$

Multiclass SVM with Hinge Loss

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

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

- The multiclass objective:

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

  - $\Delta(y, y')$ 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: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathbf{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass 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
        - (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.