Bayesian Methods & Multiclass

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Announcement

- Schedule your project consultation soon.
- Use the provided template! (if your final report fails to use template then there will be marks off)
- Homework 3 is released and due Nov 14 11:59AM.

Recap

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- Conjugate prior: Having the same form of distribution as the posterior.

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- Common options:
    - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
    - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg\max_{\theta} p(\theta \mid \mathcal{D})$
        - Note: this is the **mode** of the posterior distribution

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- Select a point estimate using **Bayesian decision theory**:
    - Choose a loss function.
    - Find action **minimizing expected risk w.r.t. posterior**

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  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
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- A **Bayes action** a^* is an action that minimizes posterior risk:

$$
r(a^*) = \min_{a \in \mathcal{A}} r(a)
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Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2$ $\Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}]$ $\Rightarrow$ posterior mode
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- Example: I have a card drawing from a deck of 2,3,3,4,4,5,5,5, and you guess the value of my card.
- mean: 3.875; mode: 5; median: 4

Bayesian Point Estimation: Square Loss

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- The **Bayes action** for **square loss** is the posterior mean.

Interim summary

Recap and Interpretation

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  - For decision making, we need a **loss function**.

Recap: Conditional Probability Models

Conditional Probability Modeling

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$$\{p(y \mid x, \theta) : \theta \in \Theta\},$$

  - where $p(y \mid x, \theta)$ is a density on **outcome space** $\mathcal{Y}$ for each x in **input space** $\mathcal{X}$, and
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  - θ is a **parameter** in a [finite dimensional] **parameter space** Θ.
- This is the common starting point for either classical or Bayesian regression.

Classical treatment: Likelihood Function

- **Data:** $\mathcal{D} = (y_1, \ldots, y_n)$
- The probability density for our data $\mathcal{D}$ is

$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) \quad = \quad \prod_{i=1}^{n} p(y_i \mid x_i, \theta).$$

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- For fixed $\mathcal{D}$, the function $\theta \mapsto p(\mathcal{D} \mid x, \theta)$ is the **likelihood function**:

$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid x, \theta),$$

where $x = (x_1, \ldots, x_n)$.

Maximum Likelihood Estimator

- The **maximum likelihood estimator (MLE)** for θ in the family $\{p(y \mid x, \theta) \mid \theta \in \Theta\}$ is

$$\hat{\theta}_{\mathsf{MLE}} \;=\; \underset{\theta \in \Theta}{\arg\max}\, L_{\mathcal{D}}(\theta).$$

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- The corresponding prediction function is

$$\hat{f}(x) = p(y \mid x, \hat{\theta}_{\mathsf{MLE}}).$$

Bayesian Conditional Probability Models

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    - A **prior distribution** $p(\theta)$ on $\theta \in \Theta$.

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- Each θ corresponds to a prediction function,
    - i.e. the conditional distribution function $p(y \mid x, \theta)$.

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- We can use **Bayesian decision theory** to derive point estimates.
- We may want to use
    - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
    - $\hat{\theta} = \text{median}[\theta \mid \mathcal{D}, x]$
    - $\hat{\theta} = \arg\max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$

Back to the basic question - Bayesian Prediction Function

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  - and a prior distribution $p(\theta)$ on this set.
- Having set our Bayesian model, how do we predict a distribution on y for input x?
- We don't need to make a discrete selection from the hypothesis space: we **maintain uncertainty**.

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- This is an average of all conditional densities in our family, weighted by the prior.

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$$x \mapsto p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D}) \, d\theta.$$

- This is an average of all conditional densities in our family, weighted by the posterior.

Comparison to Frequentist Approach

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- In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta \mid \mathcal{D})$ and predict with

$$p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D}) \, d\theta$$

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- $x \mapsto \arg\max_{y \in \mathcal{Y}} p(y \mid x, \mathcal{D})$, to minimize expected 0/1 loss
- Each of these can be derived from $p(y \mid x, \mathcal{D})$.

Gaussian Regression Example

Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathbb{R}$
- Given x, the world generates y as

$$y \;=\; w_0 + w_1 x + \varepsilon,$$

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- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$

Example in 1-Dimension: Prior Situation

- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)

prior/posterior   data space
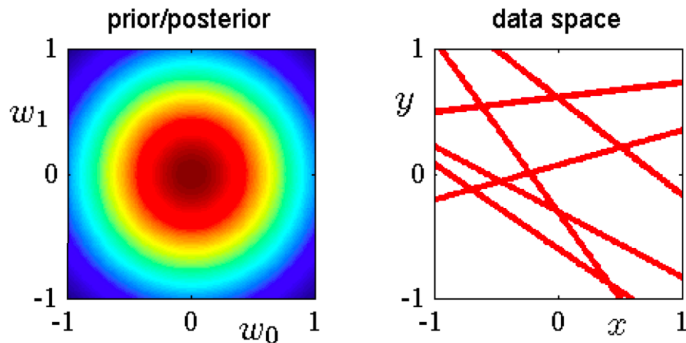
- On right, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}\left(0, \frac{1}{2}I\right)$.

Bishop's PRML Fig 3.7

Example in 1-Dimension: 1 Observation
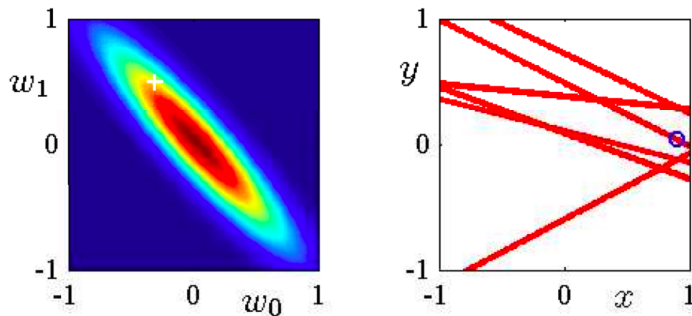
- On left: posterior distribution; white cross indicates true parameters
- On right:
  - blue circle indicates the training observation
  - red lines, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w|\mathcal{D})$ (posterior)

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations

Bishop's PRML Fig 3.7
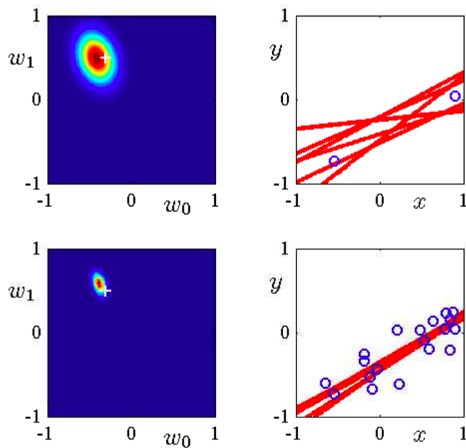
Gaussian Regression: Closed form

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- **Posterior Variance Σ_P gives us a natural uncertainty measure.**

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which is of course the ridge regression solution.

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\text{prior}}\underbrace{\prod_{i=1}^{n}\exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\text{likelihood}}$$

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- Which is the ridge regression objective.

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- For Gaussian regression, predictive distribution has closed form.

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Bayesian Regression Provides Uncertainty Estimates

- With predictive distributions, we can give mean prediction with error bands:

Rasmussen and Williams' *Gaussian Processes for Machine Learning*, Fig.2.1(b)

Multi-class Overview

Motivation

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    - 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)

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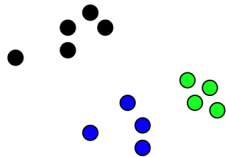
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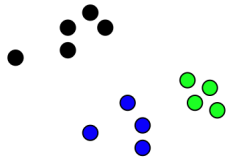
Train OvA classifiers:
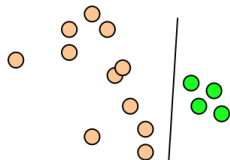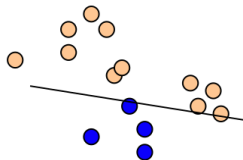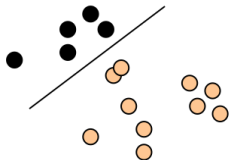
OvA: 3-class example (linear classifier)

Consider a dataset with three classes:
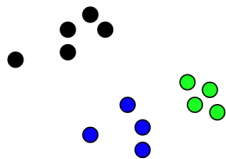
Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.
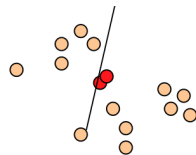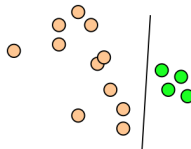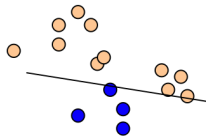
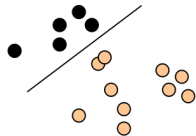Train OvA classifiers:
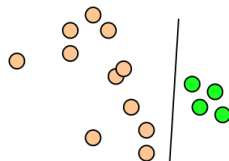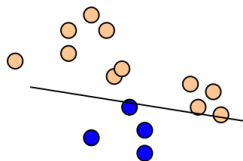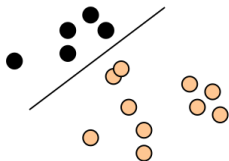
OvA: 4-class non linearly separable example
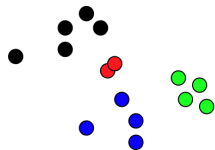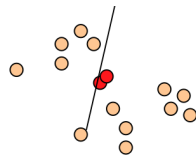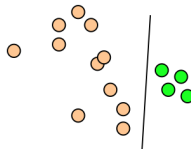
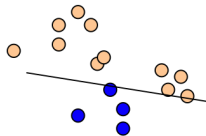Consider a dataset with four classes:

Train OvA classifiers:

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

Train OvA classifiers:
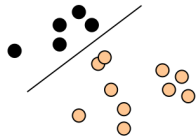
All vs All / One vs One / All pairs

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

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- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathsf{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

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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

Consider a dataset with four classes:
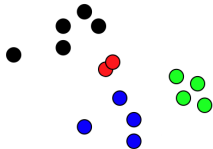
What's the decision region for the red class?
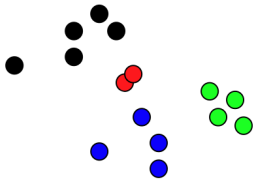
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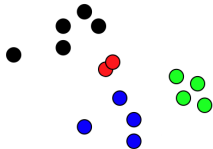
Assumption: each pair of classes are linearly separable. More expressive than OvA.

What's the decision region for the red class?
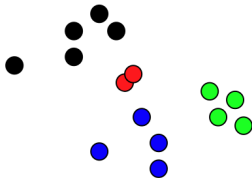
OvA vs AvA

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

OvA vs AvA

		OvA	AvA
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challenges

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
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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).

Code word for labels

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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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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.
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- 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).

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design "natural" binary classification problems without large computation cost.

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- 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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- 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**: $\mathcal{H} = \{h : \mathcal{X} \to \mathbb{R}\}$ (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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- 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

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

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  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

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  end

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?

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- How to rewrite the equation such that we have one w instead of k?

$$w_i^T x = w^T \psi(x, i) \tag{5}$$
$$h_i(x) = h(x, i) \tag{6}$$

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

The Multivector Construction

How to construct the feature map ψ?

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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: $\Psi : R^2 \times \{1, 2, 3\} \to R^6$ defined by

$$\begin{aligned} \Psi(x, 1) &:= (x_1, x_2, 0, 0, 0, 0) \\ \Psi(x, 2) &:= (0, 0, x_1, x_2, 0, 0) \\ \Psi(x, 3) &:= (0, 0, 0, 0, x_1, x_2) \end{aligned}$$

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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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Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

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- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,}\dots\}$.

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How to construct the feature vector?

- Multivector construction: $w \in \mathsf{R}^{d \times k}$—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., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$

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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?

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$\psi_1(x, y) = \mathbb{1}[x = \text{apple AND } y = \text{NOUN}]$$
$$\psi_2(x, y) = \mathbb{1}[x = \text{run AND } y = \text{NOUN}]$$
$$\psi_3(x, y) = \mathbb{1}[x = \text{run AND } y = \text{VERB}]$$
$$\psi_4(x, y) = \mathbb{1}[x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}]$$
$$\cdots$$

- 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 $\implies$ 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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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

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

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

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

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

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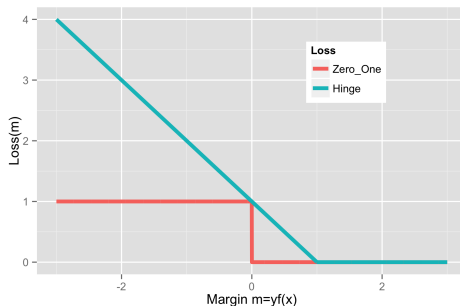
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Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

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

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

Generalized hinge loss

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

$$(16)$$

Generalized hinge loss

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

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

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- Generalized hinge loss:

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

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:

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

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

- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$

Recap: What Have We Got?

- Problem: Multiclass classification $\mathcal{Y} = \{1, \ldots, k\}$

- Solution 1: One-vs-All
  - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathbb{R}$.
  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
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- Solution 2: Multiclass loss
  - Train one model: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathsf{R}$.
  - 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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  - target margin / multiclass loss

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- 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

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

x	[START]	He	eats	apples
	x_0	x_1	x_2	x_3
y	[START]	Pronoun	Verb	Noun
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- $\mathcal{V} = \{\text{all English words}\} \cup \{[\text{START}], "."\}$
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- $\mathcal{P} = \{\text{START}, \text{Pronoun}, \text{Verb}, \text{Noun}, \text{Adjective}\}$
- $\mathcal{Y} = \mathcal{P}^n$, $n = 1, 2, 3, \ldots$ [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)
  - Size depends on input x

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- 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:

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

Markov features

- A **markov feature** only depends on
  - two adjacent labels, y_{i-1} and y_i, and x
- Example:

$$\theta_1(x, y_{i-1}, y_i) = \mathbb{1}[y_{i-1} = \mathsf{Pronoun}]\,\mathbb{1}[y_i = \mathsf{Verb}]$$
$$\theta_2(x, y_{i-1}, y_i) = \mathbb{1}[y_{i-1} = \mathsf{Pronoun}]\,\mathbb{1}[y_i = \mathsf{Noun}]$$

- 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):

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

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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:

$$\sum_i \langle w, \Psi_i(x, y_{i-1}, y_i) \rangle = \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i) \right\rangle = \langle w, \Psi(x, y) \rangle, \qquad (23)$$

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
    end
end

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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:

$$\Delta(y, y') = \frac{1}{L} \sum_{i=1}^{L} \mathbb{1}[y_i \neq y_i']$$

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.

The argmax problem for sequences

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

The argmax problem for sequences

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Solution Dynamic programming (similar to the Viterbi algorithm)
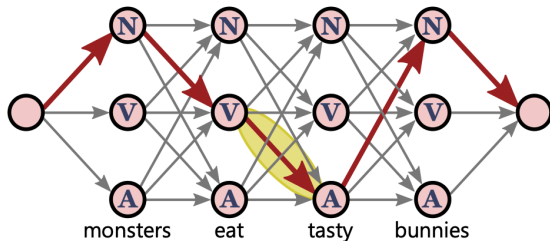
What's the running time?

Conditional random field (CRF)

- Recall that we can write logistic regression in a general form:

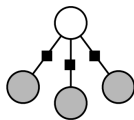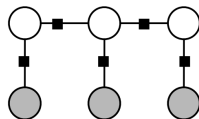$$p(y|x) = \frac{1}{Z(x)} \exp(w^\top \psi(x, y)).$$

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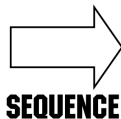
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- Z is normalization constant: $Z(x) = \sum_{y \in Y} \exp(w^\top \psi(x, y))$.
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$

Logistic Regression   SEQUENCE   Linear-chain CRFs

Conditional random field (CRF)

- Compared to Structured SVM, CRF has a probabilistic interpretation.
- We can draw samples in the output space.

Conditional random field (CRF)

- Compared to Structured SVM, CRF has a probabilistic interpretation.
- We can draw samples in the output space.
- How do we learn w? Maximum log likelihood, and regularization term: $\lambda \|w\|^2$
- Loss function:

$$
\begin{aligned}
l(w) &= -\frac{1}{N} \sum_{i=1}^{N} \log p(y^{(i)} | x^{(i)}) + \frac{1}{2} \lambda \|w\|^2 \\
&= -\frac{1}{N} \sum_i \sum_t \sum_k w_k \psi_k(y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N} \sum_i \log Z(x^{(i)}) + \frac{1}{2} \sum_k \lambda w_k^2
\end{aligned}
$$

Conditional random field (CRF)

- Loss function:

$$l(w) = -\frac{1}{N}\sum_i \sum_t \sum_k w_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_i \log Z(x^{(i)}) + \frac{1}{2}\sum_k \lambda w_k^2$$

- Gradient:

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

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

- What is $\frac{1}{N} \sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})$?

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})$?
- 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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- What is $\frac{1}{N} \sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y_t', y_{t-1}'))$?

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$$= \frac{1}{N}\sum_i \left[\sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_t, y'_{t-1})) \right]^{-1} \tag{28}$$

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$$= \frac{1}{N}\sum_i \sum_t \sum_{y' \in Y} p(y'_t, y'_{t-1}|x) \psi_k(x^{(i)}, y'_t, y'_{t-1}) \tag{30}$$

Conditional random field (CRF)

- What is $\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'}\psi_{k'}(x^{(i)}, y'_t, y'_{t-1}))$?

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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.

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