Bayesian Methods & Multiclass

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(Slides credit to David Rosenberg, He He, et al.)

NYU

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Slides

Announcement

- Project proposal due Oct 31 noon.
- Schedule your project consultation soon (they are on the week after the proposal).
- Use the provided template! (if your final report fails to use template then there will be marks off)
- Homework 3 will be released soon and due Nov 12 11:59AM.

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters

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

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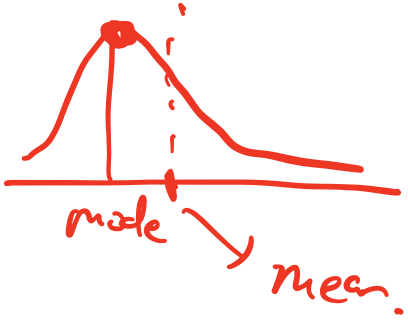
- Common options:
  - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
  - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg\max_{\theta} p(\theta \mid \mathcal{D})$
    - Note: this is the **mode** of the posterior distribution



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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**

Bayesian Decision Theory

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$. → choosing one θ from posterior.
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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 : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ 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

p(θ | D)
distribution

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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

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- **Input space** $\mathcal{X}$
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  - where $p(y \mid x, \theta)$ is a density on **outcome space** $\mathcal{Y}$ for each x in **input space** $\mathcal{X}$, and
  - θ is a **parameter** in a [finite dimensional] **parameter space** Θ.

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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

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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

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- The corresponding prediction function is

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

Bayesian Conditional Probability Models

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- Posterior represents the **rationally updated beliefs** after seeing $\mathcal{D}$.
- Each θ corresponds to a prediction function,
  - i.e. the conditional distribution function $p(y \mid x, \theta)$.

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- 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.

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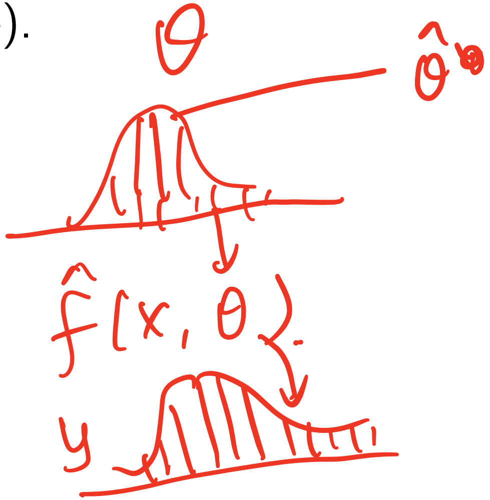
  - and a prior distribution $p(\theta)$ on this set.
- Having set our Bayesian model, how do we predict a distribution on y for input x?
- We don't need to make a discrete selection from the hypothesis space: we **maintain uncertainty**.



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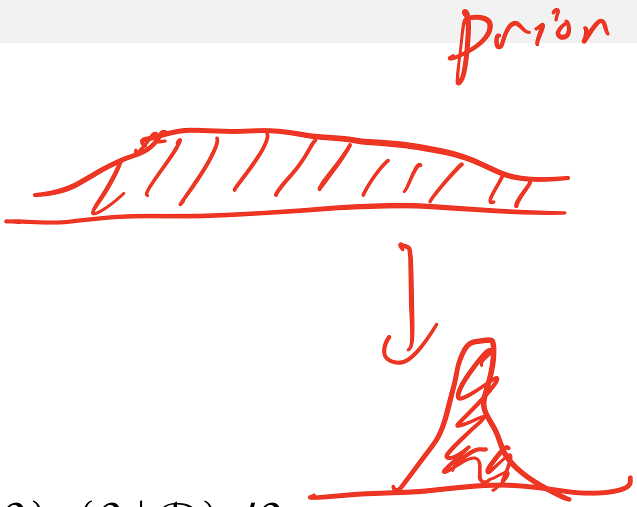

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- In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta \mid \mathcal{D})$ and predict with

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- 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 $\mathcal{Y} = \mathbf{R}$
- Given x, the world generates y as

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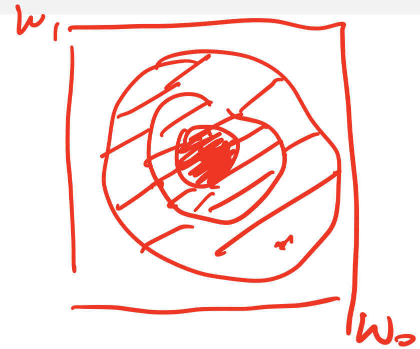

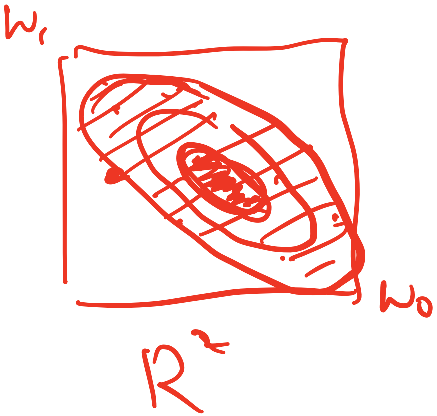

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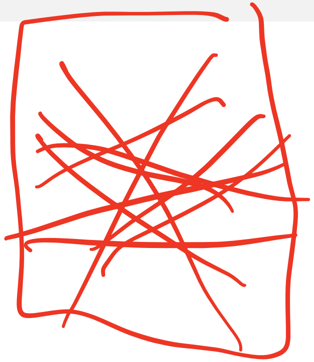
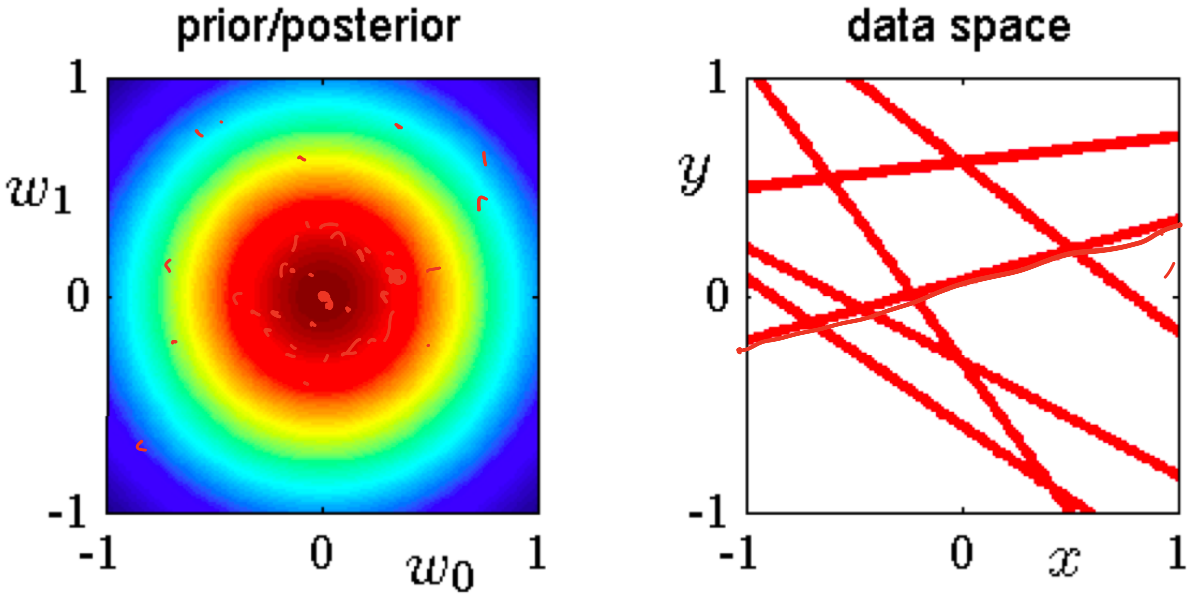
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)

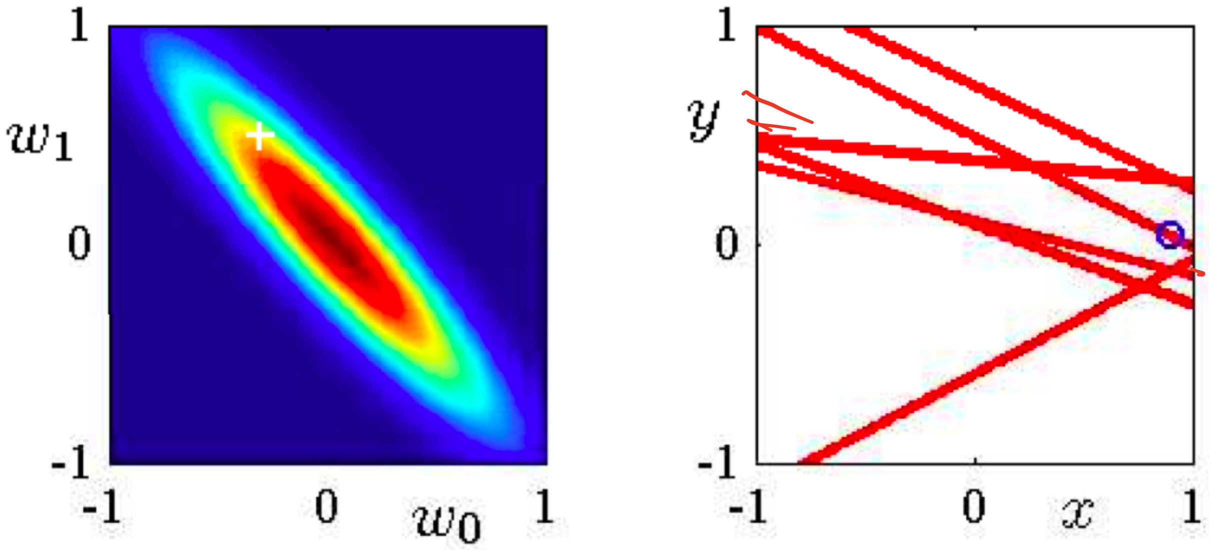




- On right, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}\left(0, \frac{1}{2}I\right)$.

Bishop's PRML Fig 3.7

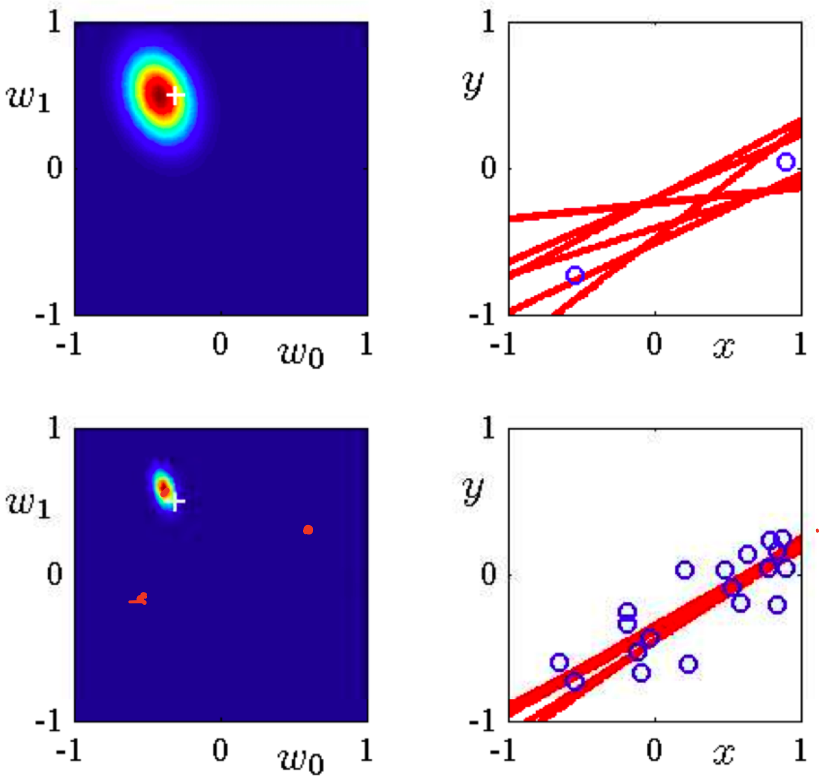
Example in 1-Dimension: 1 Observation



- 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



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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 $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

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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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posterior for theta

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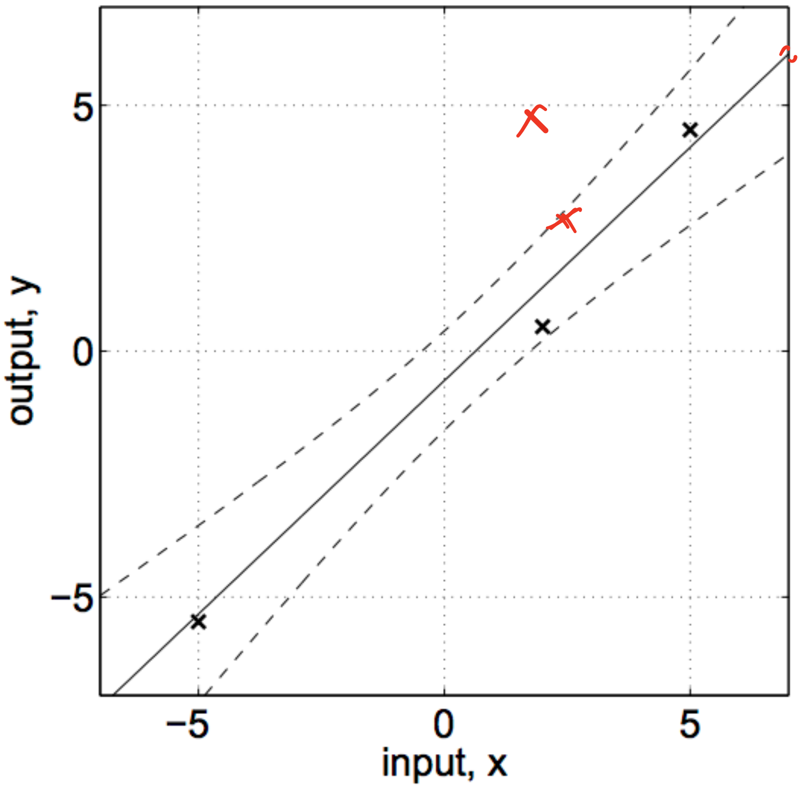
Bayesian Regression Provides Uncertainty Estimates

- 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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- Many real-world problems have more than two classes.
- What are some potential issues when we have a large number of classes?

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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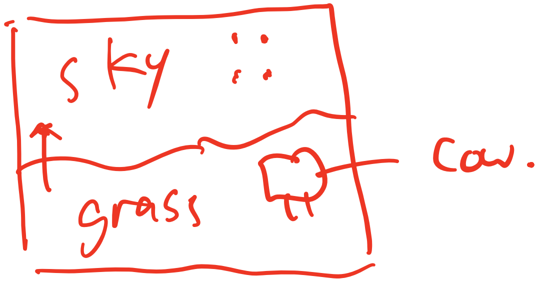
  - We also need to think about the loss function.
- Example of very large output space: structured prediction.
  - Multi-class: Mutually exclusive class structure.
  - Text: Temporal relational structure.



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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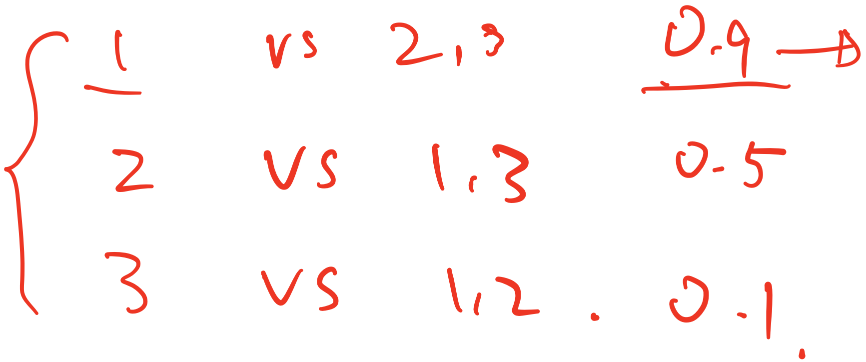

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Prediction

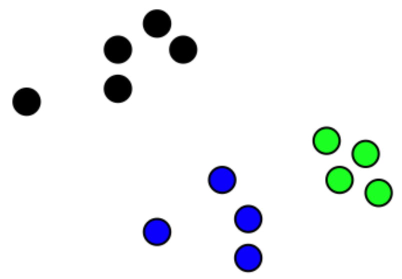
- Majority vote:

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

- Ties can be broken arbitrarily.

OvA: 3-class example (linear classifier)

Consider a dataset with three classes:



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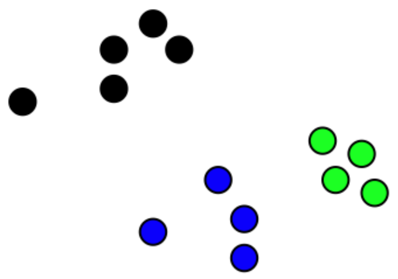

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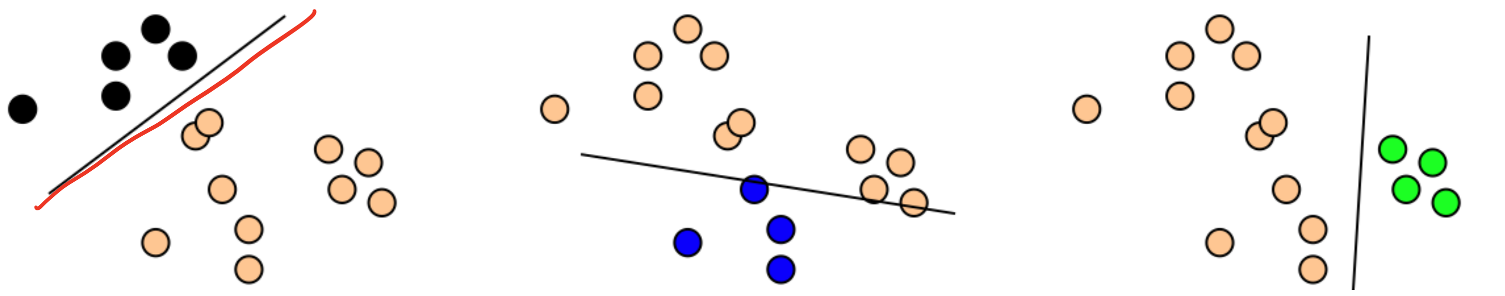

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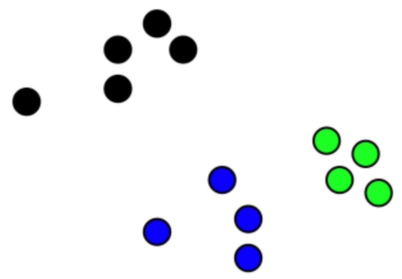
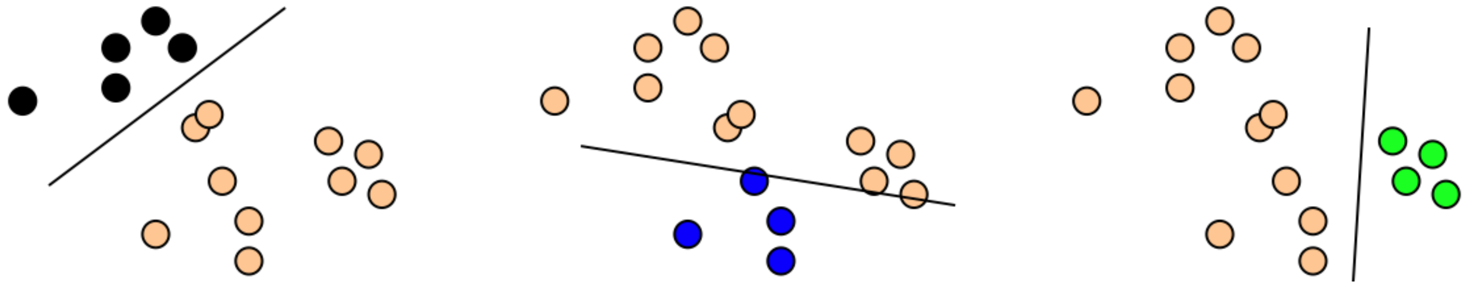


Assumption: each class is linearly separable from the rest.

Ideal case: only target class has positive score.

Train OvA classifiers:



OvA: 4-class non linearly separable example

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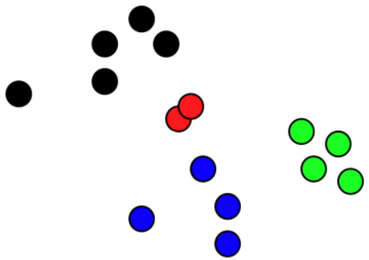

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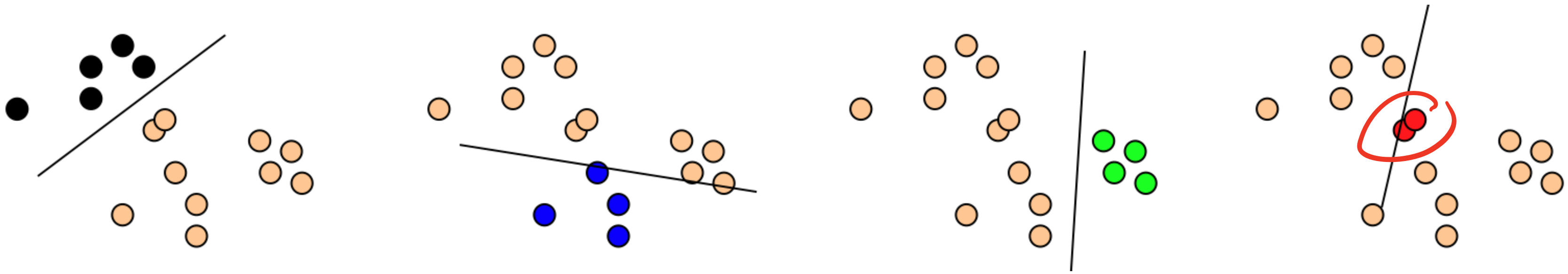

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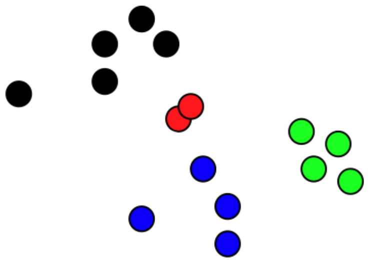
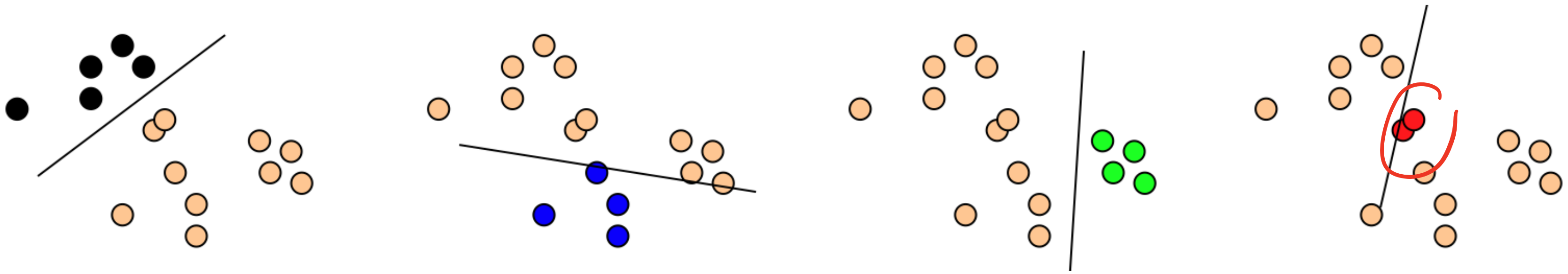


Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

Setting

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- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \rightarrow \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
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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

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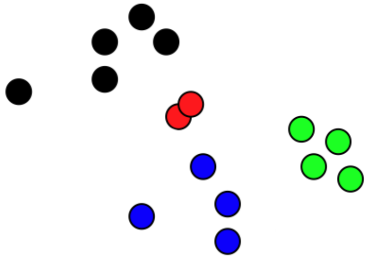
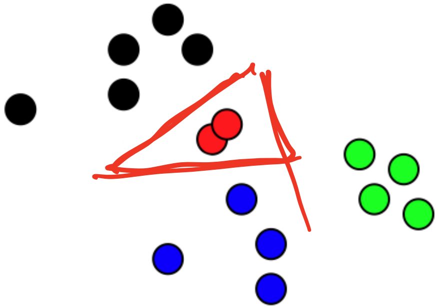


What's the decision region for the red class?



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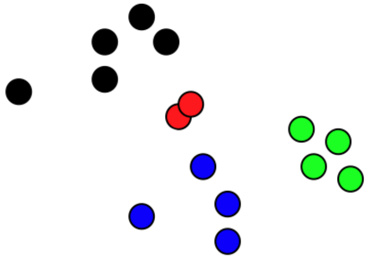
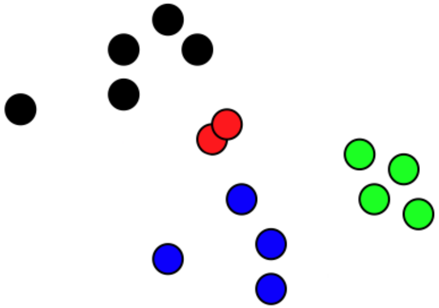


Assumption: each pair of classes are linearly separable.
More expressive than OvA.

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

OvA vs AvA

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

1000 10.

ex. 10 vs. 9990

10 vs. 10

$1000^2 = 1M$

Review

Reduction-based approaches:

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

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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).

$$f(x) = sigmoid(z) = \frac{1}{1 + \exp(-z)} = \frac{1}{1 + \exp(-w^\top x - b)}. \quad (1)$$

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class 1

- The other class is represented in $1 - f(x)$: — class 0

$$1 - f(x) = \frac{\exp(-w^\top x - b)}{1+\exp(-w^\top x - b)} = \frac{1}{1+\exp(w^\top x + b)} = sigmoid(-z) \quad (2)$$

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- Another way to view: one class has $(+w, +b)$ and the other class has $(-w, -b)$.

Multi-class Logistic Regression

Binary case

+ class: $+w$, $+b$
− class: $-w$, $-b$.
] tied.

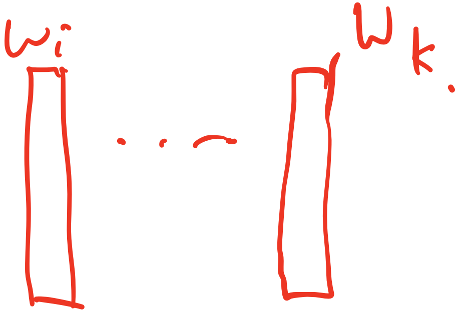
Multi-class.

class i: w_i, b_i.

- Now what if we have one w_c for each class c?

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?
- Also called "softmax" in neural networks.



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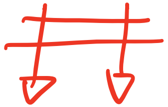
- Loss function: $-\log \text{softmax}(y)$.
- Gradient: $\frac{\partial L}{\partial z} = f - y$. Recall: MSE loss.



Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (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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- Intuitively, $h_i(x)$ 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.

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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

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{3}$$

Multiclass Perceptron

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

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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
  end
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?

$$w_i^T x = w^T \psi(x, i) \quad (4)$$

$$h_i(x) = h(x, i) \quad (5)$$

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

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

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

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

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feature.

vector.

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

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

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How to construct the feature vector?

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

$$\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \ldots, \psi_d(x, y)) \tag{6}$$

  - Size can be bounded by d.

Features

Sample training data:

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

Features

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```
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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?
- 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).
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- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

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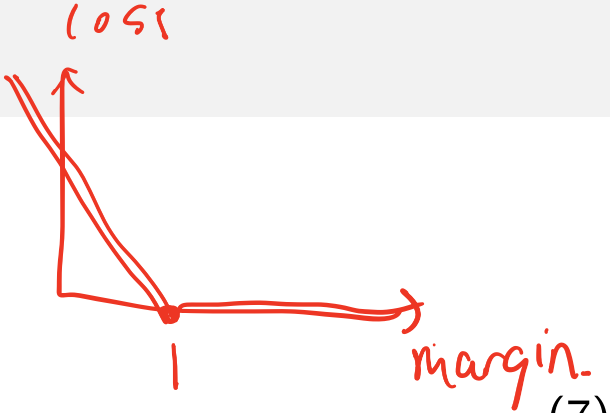
Next,

- How to generalize SVM to the multiclass setting.
- Concept check: Why might one prefer SVM / perceptron?

Margin for Multiclass



Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{7}$$

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

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{8}$$

- 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 Recall binary formulation.

Multiclass SVM: separable case

Binary Recall binary formulation.

$$\min_w \frac{1}{2}\|w\|^2$$

$$\text{s.t. } \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}} \geq 1 \quad \forall x^{(n)}, y^{(n)}.$$

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

$$m_{n,y}(w) \stackrel{\text{def}}{=} \underbrace{\langle w, \Psi(x^{(n)}, y^{(n)}) \rangle}_{\text{target}} - \underbrace{\langle w, \Psi(x^{(n)}, y) \rangle}_{\text{pred. score}}$$

$$\min_w \frac{1}{2}\|w\|^2$$

$$\text{s.t. } m_{n,y} \geq \text{target margin.}$$

Multiclass SVM: separable case

Binary Recall binary formulation.

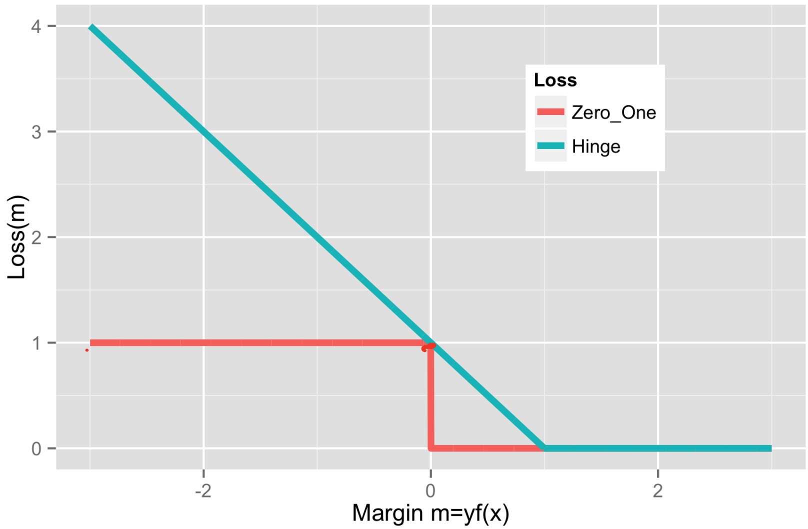
Multiclass As in the binary case, take 1 as our target margin.

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

$$\ell_{\text{hinge}}(y, \hat{y}) = \max(0, 1 - yh(x)) \tag{9}$$



Generalized hinge loss

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

$$ \tag{10}$$

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Generalized hinge loss

$\max(0, 1 - yh)$ — binary hinge

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

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

$\Delta(y, y') \leq \Delta(y, y') - \langle \text{target score} - \text{pred. score} \rangle$ (negative)

- Generalized hinge loss:

$\ell(y, x, w) = \max_{y'} \left(\Delta(y, y') - \langle w, (\Psi(x, y) - \Psi(x, y')) \rangle \right)$ (y: target)

Multiclass SVM with Hinge Loss

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

Multiclass SVM with Hinge Loss

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

$$\min_{w} \frac{1}{2}\|w\|^2 + C\sum_{n=1}^{N} \max\left(0,\ 1 - y^{(n)} w^T x^{(n)}\right).$$

- The multiclass objective:

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

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