CS-E4710 Machine Learning: Supervised Methods

Lecture 10: Multi-class Classification

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Multi-class classification

- Given a training data set $\{(\mathbf{x}_i, y_i)\}_{i=1}^m, (\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}$
- Outputs belongs to a set of possible classes or labels: $y_i \in \mathcal{Y} = \{1, 2, \ldots, k\}$
- In **multi-class classification**, one of the labels is considered to be the correct label, the other ones incorrect[1]
- In **multi-label classification**, several of the labels can be correct for a given input x_i, the output space will be $\mathcal{Y} = \{-1, +1\}^k$, each output $\mathbf{y}_i$ is a k-dimensional vector (next Lectures)
- In both cases, we aim learning a function

$$f : X \mapsto \mathcal{Y},$$

for predicting the outputs

[1] Mohri et al. book calls this case **mono-label** multi-class classification, but that is not standard vocabulary

Multi-class classification

Two basic strategies to solve the problem:

1. Aggregated methods using multiple binary classifiers:
   - One-versus-all approach : Separate each class from all the others
   - One-versus-one or all-pairs approach: Separate each class pair from each other
   - Error-correcting output code approach: Represent each class with a binary code vector and predict the bits of the vector
2. Standalone models: learning to predict multiple classes directly
   - Multiclass SVM
   - Multiclass Boosting

One-versus-All Classification

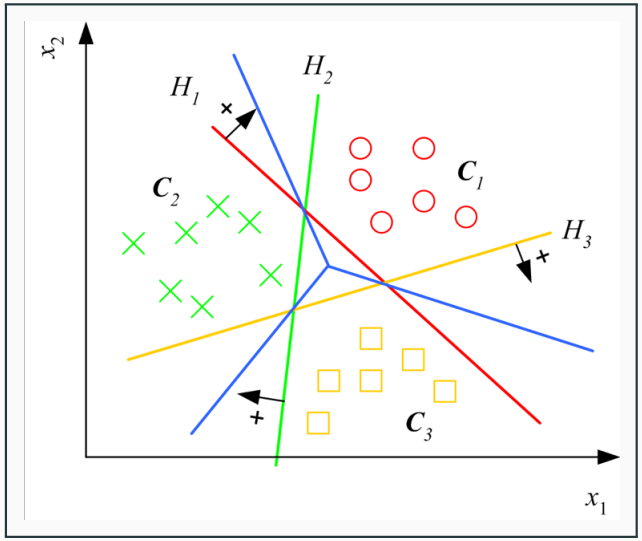
One-versus-All Classification

- Given a training data set $\{(\mathbf{x}_i, y_i)\}_{i=1}^m, (\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}$
- If we have $k > 2$ classes we will train k binary hypotheses $h_1, \ldots, h_k$, $h_\ell : X \mapsto \{+1, -1\}$
- For training the ℓth hypothesis, new binary labels, called the **surrogate labels** are computed $\tilde{y}_i^{(\ell)} = \begin{cases} +1, & \text{if } y_i = \ell, \\ -1, & \text{if } y_i \neq \ell \end{cases}$
- A binary classifier is trained to predict the surrogate labels
- The hypothesis class for the binary classifiers is not restricted: we can use any that is deemed suitable

Geometry of the linear OVA model: separable case

n example with three classes in two-dimensional space (green crosses, red circles and yellow boxes)

- Linear classifiers $\mathbf{w}_\ell^T \mathbf{x} + w_{\ell 0}$ are used as the predictors (Note that the bias terms $w_{\ell 0}$ are written out excplicitly)
- In the linearly separable case, there is a hyperplane $H_\ell : \mathbf{w}_\ell^T \mathbf{x} + w_{\ell 0} = 0$ so that all $\mathbf{x} \in C_i$ lie in the positive halfspace and all other points lie in the negative halfspace
- $h_\ell(\mathbf{x}) = \text{sgn}\left(\mathbf{w}_\ell^T \mathbf{x} + w_{\ell 0}\right) = +1$ for a single class ℓ



OVA prediction

- In general, there may be more than one class ℓ for which $h_\ell(\mathbf{x}) = +1$
- Some arbitrary tie-breaking could be used, e.g. predict the class with the smallest index ℓ
- Better results can be obtained if the hypotheses also provide some real-valued score $f_\ell(\mathbf{x}) \in \mathbb{R}$ (confidence, margin, etc.) for the label to be ℓ.
- In that case, we can choose the label with the highest score

$$h(\mathbf{x}) = \operatorname{argmax}_\ell f_\ell(\mathbf{x})$$

- With linear models $h_\ell(\mathbf{x}) = \operatorname{sgn}\left(\mathbf{w}_\ell^T \mathbf{x}\right)$ using the margin of the example is a natural choice $f_\ell(\mathbf{x}) = \mathbf{w}_\ell^T \mathbf{x}$

OVA training pseudo-code

Input: Dataset $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^m, \mathbf{x}_i \in X,\ y_i \in \mathcal{Y} = \{1, \ldots, k\}$

Output: Multiclass hypothesis $h : X \mapsto \mathcal{Y}$

for $\ell \in \{1, \ldots, k\}$ **do**

Generate training dataset with surrogate labels: $\{(\mathbf{x}_i, \tilde{y}_i^{(\ell)})\}_{i=1}^m$

Train a binary hypothesis $h_\ell : X \mapsto \{-1, +1\}$

Let $f_\ell(\mathbf{x})$ be the score for $\mathbf{x}$ given by the model h_ℓ

end for

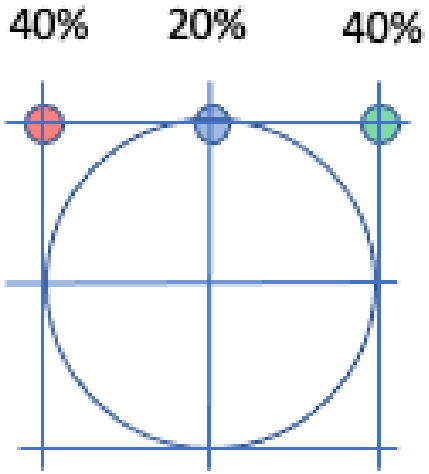
$h(\mathbf{x}) = \operatorname{argmax}_\ell f_\ell(\mathbf{x})$

Pros and cons of the OVA approach

- OVA classification is simple to implement and therefore popular
- Training is relatively efficient with $O(kt)$ time where t is the time to train a single binary classifier, if k is not too large
- The method may suffer from the **class imbalance** of the training sets for a given class ℓ: there may be a low number of positive examples and a high number of negative examples per class
- In general OVA approach suffers from a **calibration problem**: the scores $f_\ell(\mathbf{x})$ returned by the individual classifiers may not be comparable
- It does not always produce the optimal empirical error rate for the dataset (example below)

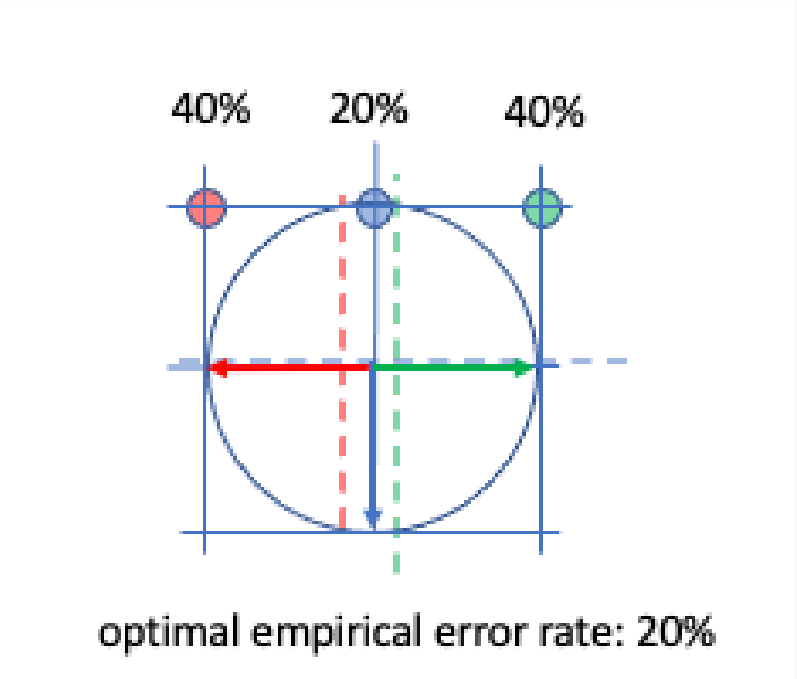
Example: sub-optimality of OVA classification

- Consider a dataset with 3 classes (red, blue, green), with class frequencies 40%, 20%, 40%, respectively
- The classes are concentrated in distinct clusters centered at $(-1, 1), (0, 1)$, and $1, 1)$, respectively



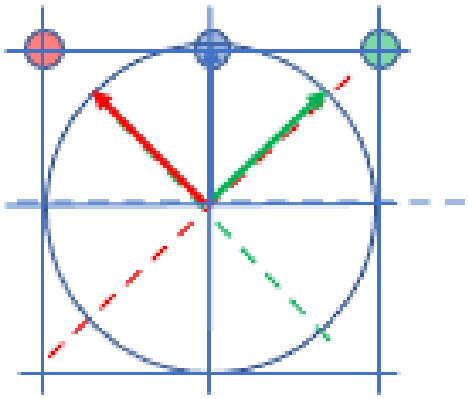
Example: sub-optimality of OVA classification

- Optimal linear classifies can separate red and green classes from the other two
- However, the optimal linear classifier for the blue class classifies all data as negative
- Combination of the three classifiers will predict (incorrectly) blue cluster to be either red or green, depending on tie breaking
- Empirical error rate is 20%



Example: sub-optimality of OVA classification

- However, the three classes are separable by three hyperplanes $f_\ell(\mathbf{x}) = \mathbf{w}_\ell^T \mathbf{x}$, $\mathbf{w}_{red} = (-1\sqrt{2}, 1\sqrt{2}), \mathbf{w}_{blue} = (0, 1)$ and $\mathbf{w}_{green} = (1/\sqrt{2}, 1/\sqrt{2})$ using the rule $h(\mathbf{x}) = \text{argmax}_\ell f_\ell(\mathbf{x})$
- Note that the hyperplane $\mathbf{w}_{blue}$ is not a good classifier as a independent model, its empirical error rate is 80%!



optimal empirical error rate: 0%

  - Thus we see that independent training of the binary hypotheses loses information and may result in sub-optimal error rates.

One-versus-One Classification

One-versus-one approach

- An alternative is one-versus-one (OVO) or all-pairs approach
- In OVO classification, we divide a multiclass problem into a set of $k(k-1)/2$ binary classification problems, one for each pair of classes $(\ell, \ell'), 1 \leq \ell < \ell' \leq k$
- This entails generating a new training set consisting of examples of the pair of classes (ℓ, ℓ') and generating a surrogate label

$$\tilde{y}^{\ell,\ell'} = \begin{cases} +1 & \text{if } y = \ell \\ -1 & \text{if } y = \ell' \end{cases}$$

- For each class pair, a binary hypothesis $h_{\ell,\ell'}(\mathbf{x}) : X \mapsto \{-1, +1\}$ is trained using the generated training set

OVO prediction

- In predicting, for each class ℓ we have $k-1$ pairwise hypotheses, one for each class containing ℓ ($h_{\ell,\ell'}$ and $h_{\ell',\ell}$, for all $\ell' \neq \ell$)
- In the ideal case, all of the $k-1$ hypotheses involving class ℓ would predict class ℓ
- In practice this may not happen, we might have for some classes ℓ', ℓ''
  - $h_{\ell,\ell'}(\mathbf{x}) = +1$ - predicting class ℓ for $\mathbf{x}$
  - $h_{\ell,\ell''}(\mathbf{x}) = -1$ - predicting class ℓ'' for $\mathbf{x}$
- We need to resolve these discrepancies

OVO prediction

A voting approach can be used:

- We count for each input $\mathbf{x}$, how many pairwise hypotheses predict class ℓ (the votes)

$$h(\mathbf{x}) = \operatorname{argmax}_{\ell} \sum_{\ell < \ell'} \mathbf{1}_{\{h_{\ell\ell'}(\mathbf{x})=+1\}} + \sum_{\ell > \ell'} \mathbf{1}_{\{h_{\ell'\ell}(\mathbf{x})=-1\}}$$

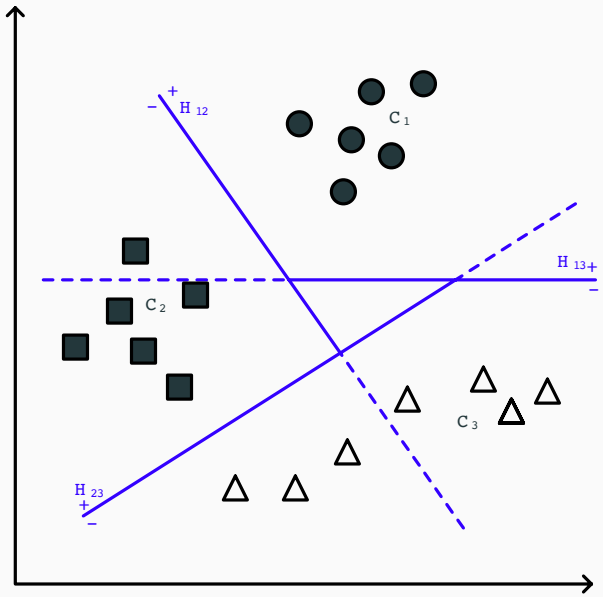
- Ties can occur with several classes receiving the same number of votes, we can break them arbitrarily (e.g. predicting the smallest index ℓ)

Geometry of linear OVO classifier

An example with three classes and linear predictors ${\mathbf{w}_{\ell'\ell}}^T\mathbf{x} + b_{\ell\ell'}$ for each class pair (Again the bias terms $b_{\ell\ell'}$ written out explicitly)

- A class ℓ is predicted within a region of the feature space where the number of votes for the class equal the maximum
- Geometrically, the region is defined by intersection of half-spaces

$$H_{\ell,\ell'} = \{\mathbf{x} | {\mathbf{w}_{\ell\ell'}}^T\mathbf{x} + b_{\ell\ell'} > 0\}, \text{ for all } \ell < \ell'$$
$$H_{\ell',\ell} = \{\mathbf{x} | {\mathbf{w}_{\ell'\ell}}^T\mathbf{x} + b_{\ell'\ell} < 0\}, \text{ for all } \ell > \ell'$$



- The triangle in the middle represents the region where all classes have one vote

Pros an cons of the OVO model

- Compared to OVA, we are training many more binary classifiers: $O(k^2)$ compared to $O(k)$
- However, the training sets are smaller since they only contain examples of two classes at a time:
  - Faster to train
  - Increased chance of overfitting
- The OVA training sets are less likely to be imbalanced than in OVA
- Better theoretical justification through the voting approach

Generalization performance of OVO models

- OVO model has some theoretical justification through viewing it as a kind of **majority voting ensemble**
- Assume that the pairwise hypotheses have generalization error of at most r
- Now if an example $\mathbf{x}$ with true class ℓ' is miclassified by the OVO model, there must be at least one pairwise hypothesis $h_{\ell\ell'}$ or $h_{\ell'\ell}$ that makes an error on $\mathbf{x}$
- The probability of this event is at most

$$\sum_{\ell<\ell'} P(\text{"}h_{\ell\ell'} \text{ makes an error"}) + \sum_{\ell'<\ell} P(\text{"}h_{\ell'\ell}\text{" makes an error"}) \leq r(k-1)$$

- Thus if the pairwise classifiers are accurate enough, the risk of the multiclass classifier can kept relatively low

Error-correcting codes

Error-correcting codes (ECOC)

- Error-correcting output codes (ECOC) is a general methods for reducing multi-class problems to binary classification
- In the ECOC approach, each class ℓ is allocated a codeword m_ℓ of length $c > 1$
- In the simplest case a binary vector can be used $m_\ell \in \{-1, +1\}^c$
- The code words of all k classes together form a matrix $M \in \{-1, +1\}^{k \times c}$

codes

classes	1	2	3	4	5	6
1	-1	-1	-1	+1	-1	-1
2	+1	-1	-1	-1	-1	-1
3	-1	+1	+1	-1	+1	-1
4	+1	+1	-1	-1	-1	-1
5	+1	+1	-1	-1	+1	-1
6	-1	-1	+1	+1	-1	+1
7	-1	-1	+1	-1	-1	-1
8	-1	+1	-1	+1	-1	-1

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
-1	+1	+1	-1	+1	+1

new example x

Error-correcting codes

- Given the codeword matrix, a binary classifier $f_j : X \mapsto \{-1, +1\}$ is learned for each column $j = 1, \ldots, c$ of the codeword matrix
- The training data for the classifier of column j is relabeled with surrogate labels $\tilde{y}_i^{(j)} = \begin{cases} m_{\ell j} & \text{if } y_i = \ell \\ -m_{\ell j} & \text{if } y_i \neq \ell \end{cases}$
- The prediction of the ECOC model is taken as the class ℓ with the fewest wrongly predicted columns of the keyword:

$$h(\mathbf{x}) = \operatorname{argmin}_{\ell=1}^{k} \sum_{j=1}^{c} \mathbf{1}_{f_j(\mathbf{x}) \neq m_{\ell j}}$$

codes

classes	1	2	3	4	5	6
1	-1	-1	-1	+1	-1	-1
2	+1	-1	-1	-1	-1	-1
3	-1	+1	+1	-1	+1	-1
4	+1	+1	-1	-1	-1	-1
5	+1	+1	-1	-1	+1	-1
6	-1	-1	+1	+1	-1	+1
7	-1	-1	+1	-1	-1	-1
8	-1	+1	-1	+1	-1	-1

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
-1	+1	+1	-1	+1	+1

new example x

How to generate the codewords?

How to generate the codewords

- Deterministic code: decide on the length c and choose binary vectors for each class so that the between class Hamming distance is as large as possible
- Random code: draw code words randomly
- Use domain knowledge: each column could be a feature describing the class

codes

classes	1	2	3	4	5	6
1	-1	-1	-1	+1	-1	-1
2	+1	-1	-1	-1	-1	-1
3	-1	+1	+1	-1	+1	-1
4	+1	+1	-1	-1	-1	-1
5	+1	+1	-1	-1	+1	-1
6	-1	-1	+1	+1	-1	+1
7	-1	-1	+1	-1	-1	-1
8	-1	+1	-1	+1	-1	-1

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
-1	+1	+1	-1	+1	+1

new example x

Why does ECOC work?

- The prediction of the ECOC model can be seen as correcting incorrectly predicted bits of the codeword
- The corrected codeword is then the one in the codebook (matrix M) that has the smallest Hamming distance to the predicted codeword
- If the between class Hamming distance of the codewords is at least d, the upto $\lfloor \frac{d-1}{2} \rfloor$ one bit errors can be corrected
- Another explanation comes from ensemble learning: model averaging between diverse classifiers f_j happens by minimizing the Hamming distance between codewords

codes

classes	1	2	3	4	5	6
1	-1	-1	-1	+1	-1	-1
2	+1	-1	-1	-1	-1	-1
3	-1	+1	+1	-1	+1	-1
4	+1	+1	-1	-1	-1	-1
5	+1	+1	-1	-1	+1	-1
6	-1	-1	+1	+1	-1	+1
7	-1	-1	+1	-1	-1	-1
8	-1	+1	-1	+1	-1	-1

$f_1(x)$	$f_2(x)$	$f_3(x)$	$f_4(x)$	$f_5(x)$	$f_6(x)$
-1	+1	+1	-1	+1	+1

new example x

Standalone multi-class classifiers

Standalone models

- Models that directly aim to minimize a multi-class loss function may give better predictive performance than the approaches based on aggregating binary classifiers
- Defining a combined model may be more efficient to train
- Multiclass models
  - Multiclass SVM
  - Multiclass boosting

Multi-class SVM

Multi-class SVM

- Multi-class SVM learns k hyperplanes $f_\ell(\mathbf{x}) = \mathbf{w}_\ell^T \mathbf{x} = 0$ simultaneously
- The predicted class is the class with the highest score

$$h(\mathbf{x}) = \text{argmax}_\ell f_\ell(\mathbf{x})$$

- The ideal objective would be to minimize the zero-one loss

$$L(h(\mathbf{x}), y_i) = \frac{1}{m} \sum_{i=1}^{m} \mathbf{1}_{h(\mathbf{x}) \neq y_i}$$

but like in binary classification, this is non-convex and NP-hard to optimize

Multi-class SVM

- Instead, multi-class SVM focuses on the score differences between pairs of classes

$$f_\ell(\mathbf{x}) - f_{\ell'}(\mathbf{x}) = \mathbf{w}_\ell^T \mathbf{x}_i - \mathbf{w}_{\ell'}^T \mathbf{x}_i$$

- In particular, the margins between the correct class y_i and all the incorrect classes $\ell \neq y_i$ are optimized
- We aim the score of the correct class to be higher than all the other classes by a margin (of 1)

$$\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_\ell^T \mathbf{x}_i \geq 1 - \xi_i, \text{ for all } \ell \neq y_i$$

- Above, slack $\xi_i \geq 0$ in used in the analogous way to binary SVMs to allow some examples to not to have the required margin

Multi-class SVM

- Multi-class SVM has k weight vectors $\mathbf{w}_1, \ldots, \mathbf{w}_k$ to control
- This is achieved by a regularizer that computes the sum of norms: $\sum_{\ell=1}^{k} \|\mathbf{w}_\ell\|_2^2$
- The regularizer is motivated by controlling the empirical Rademacher complexity $\hat{\mathcal{R}}(H)$ of the hypothesis class H of multi-class SVMs:

$$\hat{\mathcal{R}}(H) \leq \sqrt{\frac{r^2 \Lambda^2}{m}},$$

  where $\sum_{\ell=1}^{k} \|\mathbf{w}_\ell\|_2^2 \leq \Lambda^2$ and $\|\mathbf{x}_i\|_2^2 \leq r^2$ for all $i = 1, \ldots, m$
- Thus, minimizing the sum of norms aids achieving good generalization

Multi-class SVM

The Multi-class SVM optimization problem can be written as follows:

$$\begin{aligned}
\min_{\mathbf{W},\boldsymbol{\xi}} \ & \frac{1}{2}\sum_{\ell=1}^{k}\|\mathbf{w}_\ell\|^2 + C\sum_{i=1}^{m}\xi_i \\
\text{s.t. } & \mathbf{w}_{y_i}{}^T\mathbf{x}_i - \mathbf{w}_\ell{}^T\mathbf{x}_i \geq 1 - \xi_i, \\
& \text{for all } \ell \neq y_i \\
& \text{and for all } i = 1, \ldots, m \\
& \xi_i \geq 0, i = 1, \ldots, m
\end{aligned}$$

- Above, we have denoted by $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_k]$ a matrix that contains the weight vectors as columns
- The problem has quadratic objective and linear constraints
- Thus with small to medium sized data, it can be solver by Quadratic Programming (QP) solvers
- For large data, gradient approaches are more suitable

Multi-class Hinge loss

- Rewrite the constraint

$$\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_\ell^T \mathbf{x}_i \geq 1 - \xi_i, \text{ for all } \ell \neq y_i, \xi_i \geq 0 \Leftrightarrow$$
$$\mathbf{w}_{y_i}^T \mathbf{x}_i - \max_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i \geq 1 - \xi_i, \xi_i \geq 0 \Leftrightarrow$$
$$\xi_i \geq 1 - [\mathbf{w}_{y_i}^T \mathbf{x}_i - \max_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i], \xi_i \geq 0$$

- Minimizing ξ_i corresponds to minimizing the **multi-class Hinge loss**

$$L_{MCHinge}(\mathbf{W}\mathbf{x}_i, y_i) = \max\{0, 1 - [\mathbf{w}_{y_i}^T \mathbf{x}_i - \max_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i]\}$$

- Intuitively, it measures by how much the score difference between the correct class y_i and all the other classes ℓ fails to have the desired margin 1 (margin violation)

Multi-class SVM as a regularized loss minimization problem

- We can write the Multi-class SVM as regularized loss minimization problem:

$$\min_{\mathbf{W},\boldsymbol{\xi}} \frac{\lambda}{2} \sum_{\ell=1}^{k} \|\mathbf{w}_\ell\|_2^2 + \sum_{i=1}^{m} \max\{0, 1 - [\mathbf{w}_{y_i}^T \mathbf{x}_i - \max_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i]\}$$

- This problem corresponds to the QP formulation by setting $\lambda = 1/C$
- The problem is convex but but the loss is piecewise linear, thus not differentiable everywhere

Gradients of the Multi-class Hinge loss

- We need to differentiate the pieces of the loss function separately
- The pieces are defined by the class $\bar{\ell} \neq y_i$ which has the largest margin violation:

$$L_{MCHinge}(\mathbf{W}\mathbf{x}_i, y_i) = \max\{0, 1 - [\mathbf{w}_{y_i}^T \mathbf{x}_i - \max_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i]\}$$

  equals $1 - [\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_{\bar{\ell}}^T \mathbf{x}_i]$ when $\bar{\ell} = \operatorname{argmax}_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i$ and when $\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_{\bar{\ell}}^T \mathbf{x}_i < 1$ and its zero otherwise
- The gradients with respect to the weight vectors $\mathbf{w}_\ell$ will therefore satisfy

$$\frac{\partial}{\partial \mathbf{w}_{y_i}} L_{MCHinge}(\mathbf{W}\mathbf{x}_i, y_i) = -\mathbf{x}_i$$

$$\frac{\partial}{\partial \mathbf{w}_{\bar{\ell}}} L_{MCHinge}(\mathbf{W}\mathbf{x}_i, y_i) = \mathbf{x}_i$$

$$\frac{\partial}{\partial \mathbf{w}_{\ell}} L_{MCHinge}(\mathbf{W}\mathbf{x}_i, y_i) = 0 \text{ for } \ell \neq \bar{\ell}, \ell \neq y_i$$

SGD update

- The gradients of the regularizer are given by

$$\frac{\partial}{\partial \mathbf{w}_\ell} \frac{\lambda}{2} \sum_{\ell=1}^{k} \|\mathbf{w}_\ell\|_2^2 = \lambda \mathbf{w}_\ell$$

- Putting everything together we get an update direction towards the negative gradient
- If $\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_{\bar{\ell}}^T \mathbf{x}_i < 1$:

$$\mathbf{w}_{y_i} = \mathbf{w}_{y_i} - \eta(-\mathbf{x}_i + \lambda \mathbf{w}_{y_i})$$
$$\mathbf{w}_{\bar{\ell}} = \mathbf{w}_{\bar{\ell}} - \eta(\mathbf{x}_i + \lambda \mathbf{w}_{\bar{\ell}})$$
$$\mathbf{w}_\ell = \mathbf{w}_\ell - \eta(\lambda \mathbf{w}_\ell), \text{ for } \ell \neq \bar{\ell}, \ell \neq y_i$$

- Otherwise:

$$\mathbf{w}_\ell = \mathbf{w}_\ell - \eta(\lambda \mathbf{w}_\ell), \text{ for } \ell = 1, \ldots, k$$

where $\eta > 0$ is a step-size

SGD pseudo-code for Multi-class SVM

Initialize $\mathbf{w}_\ell = 0, \ell = 1, \ldots, k$

repeat

Draw a training example (x_i, y_i) uniformly at random

Find the worst margin violator: $\bar{\ell} = \mathrm{argmax}_{\ell \neq y_i} \mathbf{w}_\ell^T \mathbf{x}_i$

Determine a stepsize η (e.g. diminishing stepsize)

Compute the update direction corresponding to the training example:

if $\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_{\bar{\ell}}^T \mathbf{x}_i < 1$ **then**

$\mathbf{w}_{y_i} = \mathbf{w}_{y_i} + \eta \mathbf{x}_i$

$\mathbf{w}_{\bar{\ell}} = \mathbf{w}_{\bar{\ell}} - \eta \mathbf{x}_i$

end if

Add regularization by shrinking the weight vectors:

$\mathbf{w}_\ell = \mathbf{w}_\ell - \eta \lambda \mathbf{w}_\ell, \ell = 1, \ldots, k$

until stopping criterion satisfied (e.g. relative improvement of objective)

Output $\mathbf{W} = [\mathbf{w}_1, \ldots, \mathbf{w}_k]$

Multi-class SVM with kernels

- We can perform non-linear multi-class classification by using a kernel $\kappa(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$ over the data
- The kernelized version of the multi-class SVM optimizes dual variables $\alpha = (\alpha_{i,\ell}), i = 1 \ldots, m, \ell = 1, \ldots, k$ (one dual variable for each training example i and possible class ℓ)
- The optimization problem is given by

$$\max \sum_{i=1}^{m} \alpha_{i,y_i} - \frac{1}{2} \sum_{\ell=1}^{k} \sum_{i,i'=1}^{m} \alpha_{i,\ell} \alpha_{i',\ell} \kappa(\mathbf{x}_i, \mathbf{x}_{i'})$$

$$\text{s.t.} \sum_{\ell} \alpha_{i,\ell} = 0$$

$$\alpha_{i,\ell} \leq 0, \text{ for } \ell \neq y_i, 0 \leq \alpha_{i,y_i} \leq C,$$

- Model's prediction in dual form:

$$\hat{y}(\mathbf{x}) = \text{argmax}_{\ell=1,\ldots,k} \sum_{i=1}^{m} \alpha_{i,\ell} \kappa(\mathbf{x}_i, \mathbf{x})$$

Multi-class boosting

Adaboost for multi-class problems

- AdaBoost.MH is a variant of AdaBoost designed for multi-class problems
- Like Adaboost, it learns a linear combination of base classifiers $f_N(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j h_j(\mathbf{x})$
- The labels are represented as vectors $\mathbf{y}_i = (y_{i1}, \ldots, y_{ik})^T \in \{-1, +1\}^k$, where $y_{i\ell} = +1$ for the correct class and $y_{i\ell'} = -1$ for all incorrect classes ℓ'
- The base classifiers also return vectors $h_j(\mathbf{x}) \in \{-1, +1\}^k$, $h_j(\mathbf{x}, \ell) \in \{-1, +1\}$
- Prediction by taking the sign component-wise: $h(\mathbf{x}) = \text{sgn}\left(f_N(\mathbf{x})\right)$

Adaboost for multi-class problems

- A distribution over the training examples and the possible classes is maintained: $D_t(i, \ell)$ is the weight of example $\mathbf{x}_i$ and class ℓ at iteration t
- The updates to the example weights is given by the formula:

$$D_{j+1}(i, \ell) = \frac{D_j(i, \ell) exp(-\alpha y_{i\ell} h_j(\mathbf{x}_i, \ell))}{Z_j}, \ell = 1, \ldots, k$$

- Z_j is a normalization factor
- All weights $D_j(i, \ell)$ where $y_{i\ell} \neq h_j(\mathbf{x}_i, \ell)$ are exponentially upweighted
- AdaBoost.MH can be seen to minimize an exponential loss which upper bounds zero-one loss in a multi-class setting

$$\sum_{i=1}^{m} \sum_{\ell=1}^{k} \mathbf{1}_{y_{i\ell} \neq h(\mathbf{x}_i, \ell)} \leq \sum_{i=1}^{m} \sum_{\ell=1}^{k} \exp(-y_{i\ell} h(\mathbf{x}_i, \ell))$$

Adaboost.MH pseudo-code

ADABOOST.MH$(S = ((x_1, y_1), \ldots, (x_m, y_m)))$

1 **for** $i \leftarrow 1$ **to** m **do**
2 **for** $l \leftarrow 1$ **to** k **do**
3 $\mathcal{D}_1(i,l) \leftarrow \frac{1}{mk}$
4 **for** $j \leftarrow 1$ **to** N **do**
5 $h_j \leftarrow$ base classifier in $\mathcal{H}$ with small error $\epsilon_j = \mathbb{P}_{(i,l)\sim\mathcal{D}_j}[h_j(x_i,l) \neq y_i[l]]$
6 $\bar{\alpha}_j \leftarrow \frac{1}{2}\log\frac{1-\epsilon_j}{\epsilon_j}$
7 $Z_t \leftarrow 2[\epsilon_j(1-\epsilon_j)]^{\frac{1}{2}}$ ▷ normalization factor
8 **for** $i \leftarrow 1$ **to** m **do**
9 **for** $l \leftarrow 1$ **to** k **do**
10 $\mathcal{D}_{j+1}(i,l) \leftarrow \frac{\mathcal{D}_j(i,l)\exp(-\bar{\alpha}_j y_i[l] h_j(x_i,l))}{Z_j}$
11 $f_N \leftarrow \sum_{j=1}^{N} \bar{\alpha}_j h_j$
12 **return** $h = \mathrm{sgn}(f_N)$

Summary

- Multi-class classification can be approached as an aggregation of binary classification problems
  - One-versus-All, One-versus-One, and Error-correcting codes
- Standalone models aim to directly minimize a multiclass loss function
  - SVM and Boosting models
- Also other models exist: Multi-class neural networks, Decision trees