Introduction to Machine Learning

Tutorial VI

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Disclaimer

The slides may vary slightly from what has been discussed during the tutorial to incorporate some of the student's questions as well as some aspects discussed on the black-board only. The new slides have the title background colored in grey.

Outline

1. Class imbalance
   a. Problem setting
   b. Simple solutions
   c. Cost-sensitive algorithms
2. Evaluation
   a. Evaluation metrics in standard case
   b. Evaluation metrics in case of imbalanced classes
3. Multi-class SVM
   a. Naive approaches
   b. Multi-class Hinge loss
   c. Evaluation
4. Outlook: cross-entropy loss

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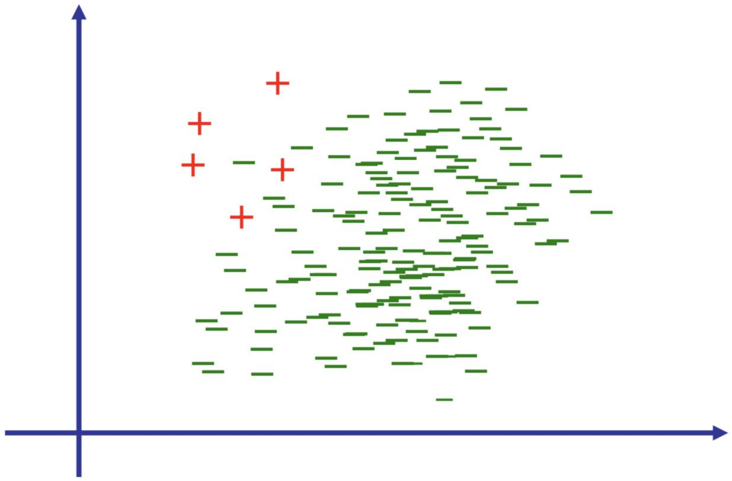
Class imbalance: problem setting

- Binary classification: one class substantially outnumbers the other class (wlog. positive class is rare)
- Examples
  - Diagnosis of rare diseases
  - Spam detection
  - Image detection: identification of rare fish population
- Why problematic?
  - Minority class contributes little to the empirical risk
  - Algorithms tend to predict negative class only
  - Evaluation of algorithm’s performance is deceiving



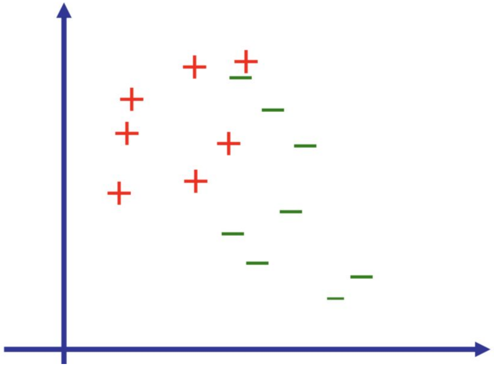
Class imbalance: simple approaches

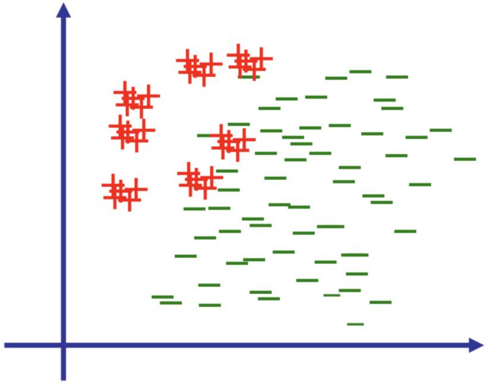
- Undersampling of the majority class
  - faster (+)
  - waste of available data (-)
  - loss of information about majority class (-)

- Upsampling of the minority class
  - uses all data (+)
  - risk of overfitting the minority class (-)
  - arbitrarily chosen data perturbation (-)

- => Naive solutions, but still used in practice

- Many extensions including generation of synthetic data exist, see Elrahman and Abraham (2013) A Review of Class Imbalance Problem, *JNIC* 1: 332-340





Class imbalance: cost-sensitive algorithms

- Idea: modify the loss function to account for class imbalance

- E.g. cost-sensitive Hinge-loss

$$\ell_{CS-H}(\mathbf{w};\mathbf{x},y) = c_y \max(0, 1 - y\mathbf{w}^T\mathbf{x})$$

- How does introduction of cost-sensitivity influence the loss function?
  - It changes the slope of the loss function

- How does introduction of cost-sensitivity influence the gradient?
  - It scales the gradient

Class imbalance: cost-sensitive algorithms (2)

Clarification:

- Wlog. the positive class in the minority class
- To avoid redundancy, instead of using two cost-parameters, it is sufficient to combine them in a ratio $c = \frac{c_+}{c_i}$ (see lecture slides p.12). Then the resulting cost-sensitive loss function can be decomposed as

$$l_c(\mathbf{w}; \mathbf{x}_i, y_i, c) = \begin{cases} 0 & \text{if } \mathbf{w}^T\mathbf{x}_i y_i \geq 0 \text{ (correctly classified)} \\ -c y_i \mathbf{w}^T\mathbf{x}_i & \text{if } \mathbf{w}^T\mathbf{x}_i y_i < 0 \wedge y_i = 1 \quad \text{(false negatives)} \\ -y_i \mathbf{w}^T\mathbf{x}_i & \text{if } \mathbf{w}^T\mathbf{x}_i y_i < 0 \wedge y_i = -1 \quad \text{(false positives)} \end{cases}$$

- Now, the slope of the loss changes only for the minority class after reparametrization (see lecture slides p.10, green corresponds to the minority-class loss and black to the majority-class loss)

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Evaluation: standard case

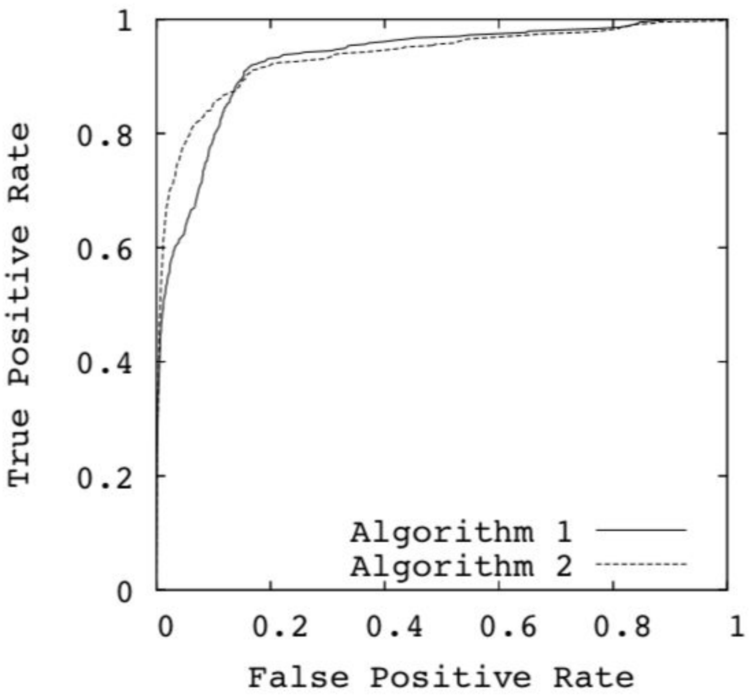
True labels

Predicted labels

	Positive	Negative
Positive	TP	FP
Negative	FN	TN

- Accuracy: (TP + TN)/n
- TPR: TP/(TP+FN)
- FPR: FP/(FP+TN)

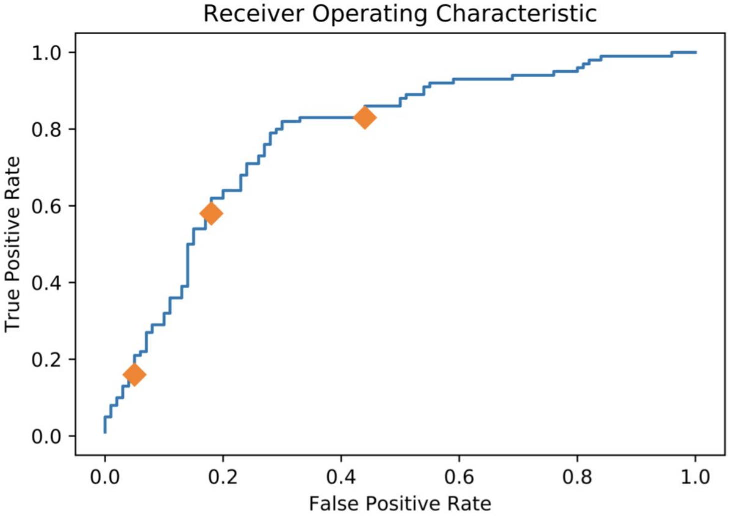
Evaluation: ROC curve



Davis and Goadrich
(ICML 2006)

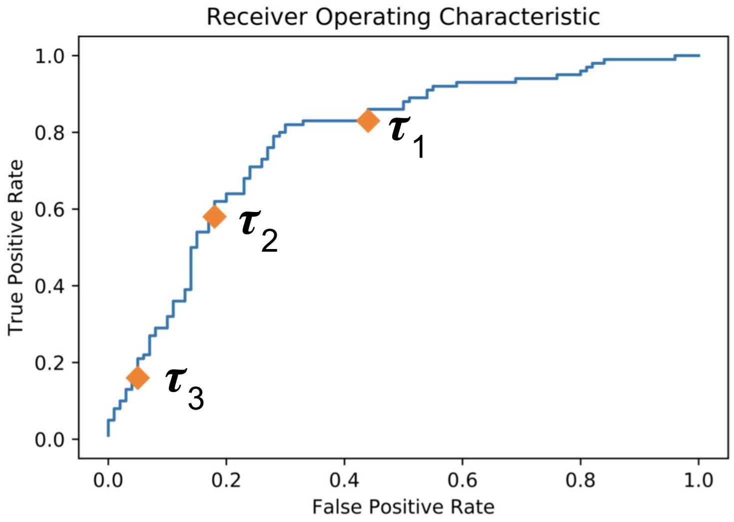
Evaluation: ROC curve (2)

- Imagine that your classifier's output is h(x) and that we use a decision threshold τ (i.e. $\hat{y}_i = +$ if $h(x_i) \geq \tau$)
- Now, place the decision thresholds $\tau_1 < \tau_2 < \tau_3$ on the diamonds: (exam2017 question)



Evaluation: ROC curve (3)

- Correct solution



- Both the TPR and FPR have a constant denominator (#true positive labels and #true negative labels, respectively); if τ decreases sufficiently, more instances will be classified as + and hence, the TP as well as FP will raise

Evaluation: class imbalance case

		True labels	
		Positive	Negative
Predicted labels	Positive	TP	FP
	Negative	FN	TN

- ~~Accuracy: (TP + TN)/n~~
- Recall: TP/(TP+FN)
- Precision: TP/(TP+FP)

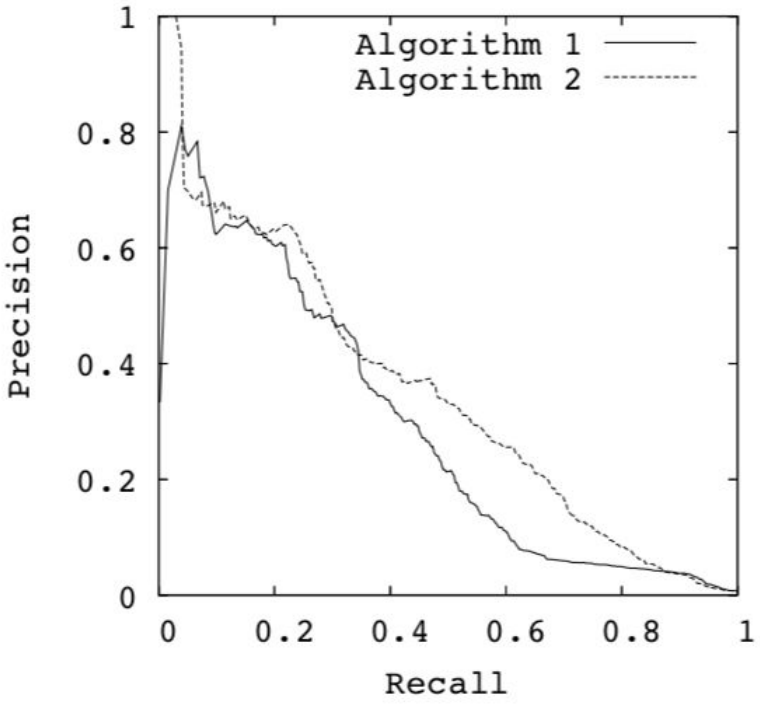
Evaluation: precision-recall trade-off

- Hypothetical situation: we use an algorithm that outputs probabilities (e.g. logistic regression later in the course), with decision threshold τ

- What happens to precision and recall if we raise the decision threshold?
  - Precision will probably, but not necessarily, increase (higher τ leads to lower FP)
  - Recall will decrease or stay the same

- Precision-recall trade-off depends on the situation
  - FN worse, e.g. in disease diagnostics
  - FP worse, e.g. in spam detection (we miss an important email)

Evaluation: precision-recall curve



Davis and Goadrich
(ICML 2006)

Evaluation: precision-recall trade-off (2)

- Hypothetical situation: alg1 has higher precision, alg2 higher recall
- Would averaging precision and recall be a good solution to determine which algorithm works better?
  - No! => Use F-score
- F-score: 2TP/(2TP + FP + FN) $= \frac{2}{precision^{-1} + recall^{-1}} = 2\frac{precision * recall}{precision + recall}$
  - Harmonic mean of precision and recall
  - Equal weights on precision and recall
  - Comment: Hand and Christen (2017). A note on using the F-measure for evaluating record linkage algorithms. *Statistics and Computing*. 10.1007/s11222-017-9746-6.
  - More emphasis on recall (β-times):

F_{β} -score = $(1+\beta^2)\frac{precision * recall}{\beta^2 precision + recall}$

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Multi-class SVM: simple approaches

- Idea: use binary classification in the multi-class (c) case => reduction
- One-versus-all (OVA)/ all-versus-rest (AVR)
  - c binary classifiers: one class vs. all other classes at a time
  - Predict

$$\hat{y} = argmax_i \; f^{(i)}(\mathbf{x}) = argmax_i \; \mathbf{w}^{(i)T}\mathbf{x}$$

  - (+) simple, fast
  - (-) requires comparable scaling, class imbalance issue, problematic if one class not linearly separable from all other
- One-versus-one (OVO)/ all-versus-all (AVA)
  - c(c-1)/2 binary classifiers
  - (+) simple, doesn’t use confidence
  - (-) slow, ties
- Both used in practice, see e.g. Rifkin and Klautau (2004).In Defense of One-Vs-All Classification.*JMLR* 5: 101-141

Multi-class SVM: Hinge-loss

- Idea: use C weight vectors, one per class and optimize jointly
- Given each data point (**x**, y) we want to achieve that

$$\mathbf{w}^{(y)T}\mathbf{x} \geq max_{i \neq y}\, \mathbf{w}^{(i)T}\mathbf{x} + 1 \qquad (*)$$

- Multi-class Hinge-loss

$$l_{MC-H}(\mathbf{w}^{(1)}, \ldots, \mathbf{w}^{(c)}; \mathbf{x}, y) = max(0, 1 + max_{j \in \{1,\ldots,y-1,y+1,\ldots,c\}} \mathbf{w}^{(j)T}\mathbf{x} - \mathbf{w}^{(y)T}\mathbf{x})$$

- $\nabla_{\mathbf{w}^{(i)}}\, l_{MC-H}(\mathbf{w}^{(1:c)}; \mathbf{x}, y)$?

Multi-class classification: tutorial highlights

- During the tutorial we discussed the pros and cons of the reduction approaches as well as possible solutions to the shortcomings

- During the tutorial we worked through an example of image classification (3 labels, 3 training examples) and analyzed what happens with the multi-class Hinge loss

- During the tutorial we discussed in more details the gradient of the multi-class Hinge loss (see lecture slides p.39)

Multi-class SVM: evaluation

- Based on the extended confusion matrix
- Micro- and macro-averaged metrics
- E.g. Extensions of the F-score
  - Macro-averaged F-score

$$\frac{1}{c}\sum_{i=1}^{c} F(i)$$

  - Micro-averaged F-score: F-score on pooled counts from each class contingency table
  - More information: K.Murphy (2012). Machine Learning A Probabilistic Approach. p. 183
- Class imbalance case
  - Weight metric towards largest classes => use micro-averaging
  - Weight metric towards smallest classes => use macro-averaging

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Outlook: cross-entropy and KL-divergence

Definition 1 (KL-divergence). *Let p and q be a valid probability distributions over the same probability space Ω s.t. $q(x) > 0 \forall x \in \Omega$, then KL-divergence between two distributions is defined as*

$$D_{KL} = \mathbb{E}_p \left[\log \left(\frac{p(x)}{q(x)} \right) \right]. \tag{1}$$

Definition 2 (Cross-entropy). *Let p and q be a valid probability distributions over the same probability space Ω s.t. $q(x) > 0 \forall x \in \Omega$, then cross-entropy is defined as follows,*

$$\mathrm{CE}(p, q) = \mathbb{E}_p[-\log(q(x)))] \tag{2}$$

which is equivalent to $\mathrm{CE}(p, q) = H(p) + D_{KL}(p, q)$, where H is the entropy.

Ian Goodfellow, Yoshua Bengio, Aaron Courville, *Deep learning*, vol.1 MIT press Cambridge 2016

Outlook: cross-entropy interpretation

- Information theory view:
  "Cross-entropy is the average number of bits needed to encode data coming from a source with distribution *p* when we use model *q* to define our codebook" [Murphy (2012). Machine Learning A Probabilistic Perspective. p.57-58]

- Probabilistic view:
  minimizing the cross-entropy corresponds to minimizing the negative log-likelihood of the correct class (see the upcoming lectures)

Outlook: cross-entropy loss

- Used for classification algorithms with probability ($\in [0,1]$) as the output
- E.g. a softmax classifier (generalization of logistic regression to multi-class case; more in the upcoming lectures)
- Cross-entropy loss

$$l_{MC-CE}(\mathbf{w}^{(1)}, \ldots, \mathbf{w}^{(c)}; \mathbf{x}, y) = -\,log\left(\frac{e^{\mathbf{w}^{(y)T}\mathbf{x}}}{\sum_{j=1}^{c} e^{\mathbf{w}^{(j)T}\mathbf{x}}}\right)$$

- The scores for each class are normalized by applying the softmax function

$$f_j(\mathbf{z}) = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}$$

=> the real-valued scores (in **z**) are normalized, i.e. $\in [0,1]$) and sum to 1

Outlook: cross-entropy loss (tutorial highlights)

- During the tutorial we discussed and saw on an example the differences between SVM and softmax classifier with emphasis on the scores
  - SVM outputs uncalibrated, unscaled scores that are possibly difficult to interpret
  - Softmax (due to applying the softmax function to the scores) allows for interpretation as normalized class probabilities
- During the tutorial we looked at the shape of the cross-entropy loss (for binary positive class) and saw that the penalization is not linear and that it changes (decreases) depending on how close to 1 the resulting probability is;
- The SVM “cares” only about the confidence in the true class to be higher by some margin than the confidences in all the other classes; Softmax classifier “cares” about the details, i.e. the true class probability could always be higher;

Questions

- Question regarding the project => Piazza
- Other questions to: joanna.ficek@inf.ethz.ch