Beyond binary classification

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CMPSCI 689: Machine Learning

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Administrivia

- Mini-project 1 posted
  - One of three
  - Decision trees and perceptrons
  - Theory and programming
  - Due Wednesday, March 04, ~~11:55pm~~ **4:00pm**
    - Turn in a hard copy in the CS office
  - Must be done individually, but feel free to discuss with others
  - Start early …

Today's lecture

- Learning with imbalanced data
- Beyond binary classification
  - Multi-class classification
  - Ranking
  - Collective classification

Learning with imbalanced data

- One class might be rare (E.g., face detection)
- Mistakes on the rare class cost more:
  - cost of misclassifying y=+1 is α (>1)
  - cost of misclassifying y=-1 is 1
- Why? we want is a better f-score (or average precision)

binary classification

$$\mathbb{E}_{(\mathbf{x},y)\sim D}[f(\mathbf{x}) \neq y]$$

α-weighted binary classification

$$\mathbb{E}_{(\mathbf{x},y)\sim D}[\alpha^{y=1} f(\mathbf{x}) \neq y]$$

Suppose we have an algorithm to train a binary classifier, can we use it to train the alpha weighted version?

Training by sub-sampling

- Input: D, α Output: D^α
- While true
  - Sample $(\mathbf{x}, y) \sim D$
  - Sample $t \sim \text{uniform}(0, 1)$
  - If $y > 0 \text{ or } t < 1/\alpha$
    - ➡ return $(\mathbf{x}, y)$

sub-sampling algorithm

We have sub-sampled the negatives by $1/\alpha$

Claim

binary classification	α-weighted binary classification
D^α	D
ϵ	$\alpha\epsilon$

$$\epsilon \longrightarrow \alpha\epsilon$$

Proof of the claim

$$
\begin{aligned}
\text{Error on } \mathcal{D} &= \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[\ell^{\alpha}(\hat{y},y)] \\
&= \sum_{\mathbf{x}} \left(D(\mathbf{x},+1)\alpha[\hat{y}\neq 1] + D(\mathbf{x},-1)[\hat{y}\neq -1]\right) \\
&= \alpha\left(\sum_{\mathbf{x}}\left(D(\mathbf{x},+1)[\hat{y}\neq 1] + \frac{1}{\alpha}D(\mathbf{x},-1)[\hat{y}\neq -1]\right)\right) \\
&= \alpha\left(\sum_{\mathbf{x}}\left(D^{\alpha}(\mathbf{x},+1)[\hat{y}\neq 1] + D^{\alpha}(\mathbf{x},-1)[\hat{y}\neq -1]\right)\right) \\
&= \alpha\epsilon
\end{aligned}
$$

binary classification	α-weighted binary classification
D^{α}	D
ϵ	$\longrightarrow$ $\alpha\epsilon$

Modifying training

- To train simply —
  - Subsample negatives and train a binary classifier.
  - Alternatively, supersample positives and train a binary classifier.
  - Which one is better?
- For some learners we don't need to keep copies of the positives
  - Decision tree
    - Modify accuracy to the weighted version
  - kNN classifier
    - Take weighted votes during prediction
  - Perceptron?

Overview

- Learning with imbalanced data
- Beyond binary classification
  - Multi-class classification
  - Ranking
  - Collective classification

Multi-class classification

- Labels are one of K different ones.
- Some classifiers are inherently multi-class —
  - kNN classifiers: vote among the K labels, pick the one with the highest vote (break ties arbitrarily)
  - Decision trees: use multi-class histograms to determine the best feature to splits. At the leaves predict the most frequent label.
- Question: can we take a binary classifier and turn it into multi-class?

One-vs-all (OVA) classifier

- Train K classifiers, each to distinguish one class from the rest
- Prediction: pick the class with the highest score:

$$i \leftarrow \arg\max f_i(\mathbf{x})$$

score function

- Example
  - Perceptron: $i \leftarrow \arg\max \mathbf{w}_i^T \mathbf{x}$
    - May have to calibrate the weights (e.g., fix the norm to 1) since we are comparing the scores of classifiers
    - In practice, doing this right is tricky when there are a large number of classes

One-vs-one (OVO) classifier

- Train K(K-1)/2 classifiers, each to distinguish one class from another
- Each classifier votes for the winning class in a pair
- The class with most votes wins

$$i \leftarrow \arg\max \left(\sum_j f_{ij}(\mathbf{x}) \right)$$

$$f_{ji} = -f_{ij}$$

- Example
  - Perceptron: $i \leftarrow \arg\max \left(\sum_j \text{sign}\left(\mathbf{w}_{ij}^T \mathbf{x}\right) \right)$ $\quad \mathbf{w}_{ji} = -\mathbf{w}_{ij}$
    - ➡ Calibration is not an issue since we are taking the sign of the score

Directed acyclic graph (DAG) classifier

- DAG SVM [Platt et al., NIPS 2000]
  - Faster testing: O(K) instead of O(K(K-1)/2)
  - Has some theoretical guarantees

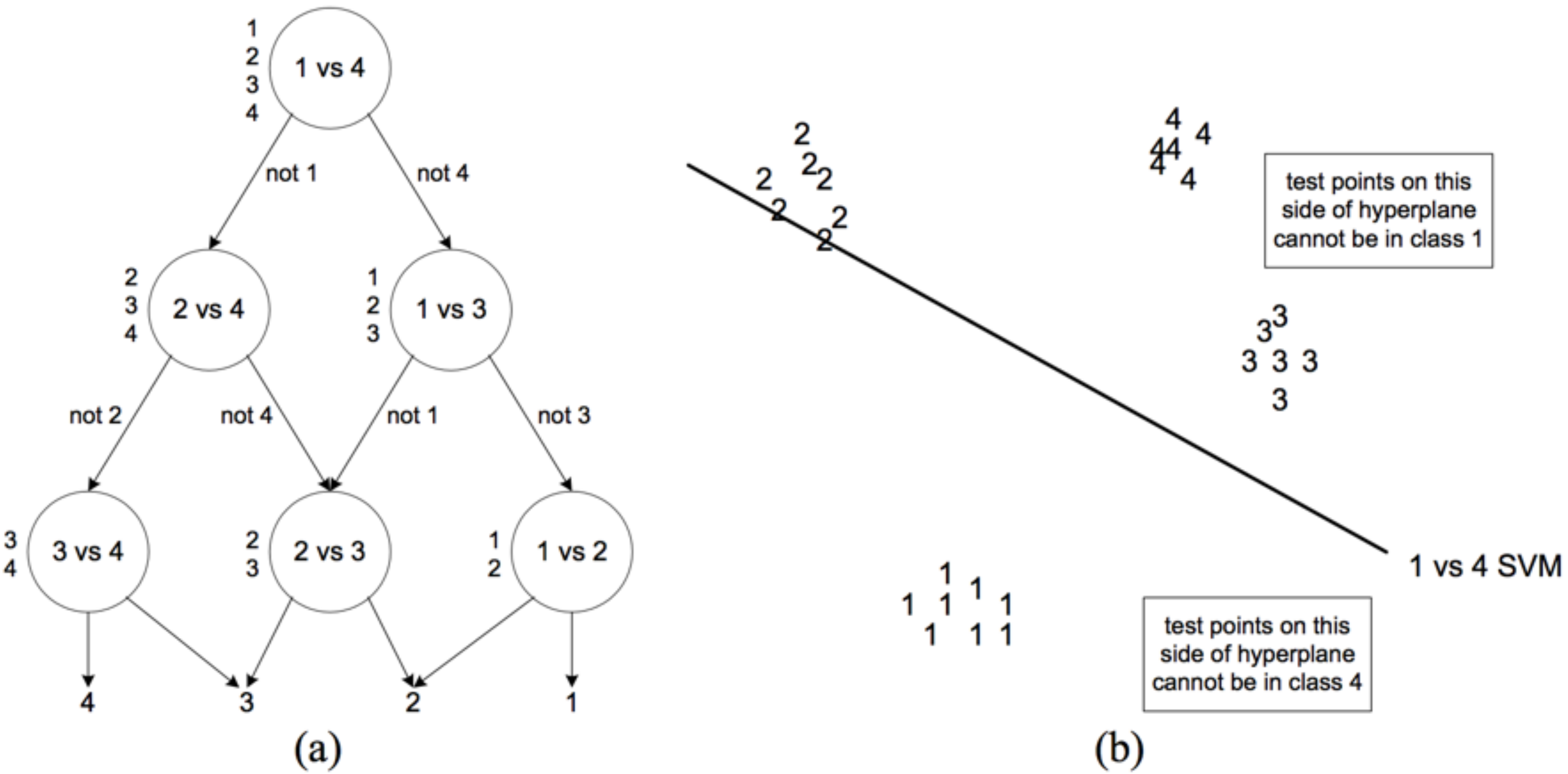

Figure from Platt et al.

Overview

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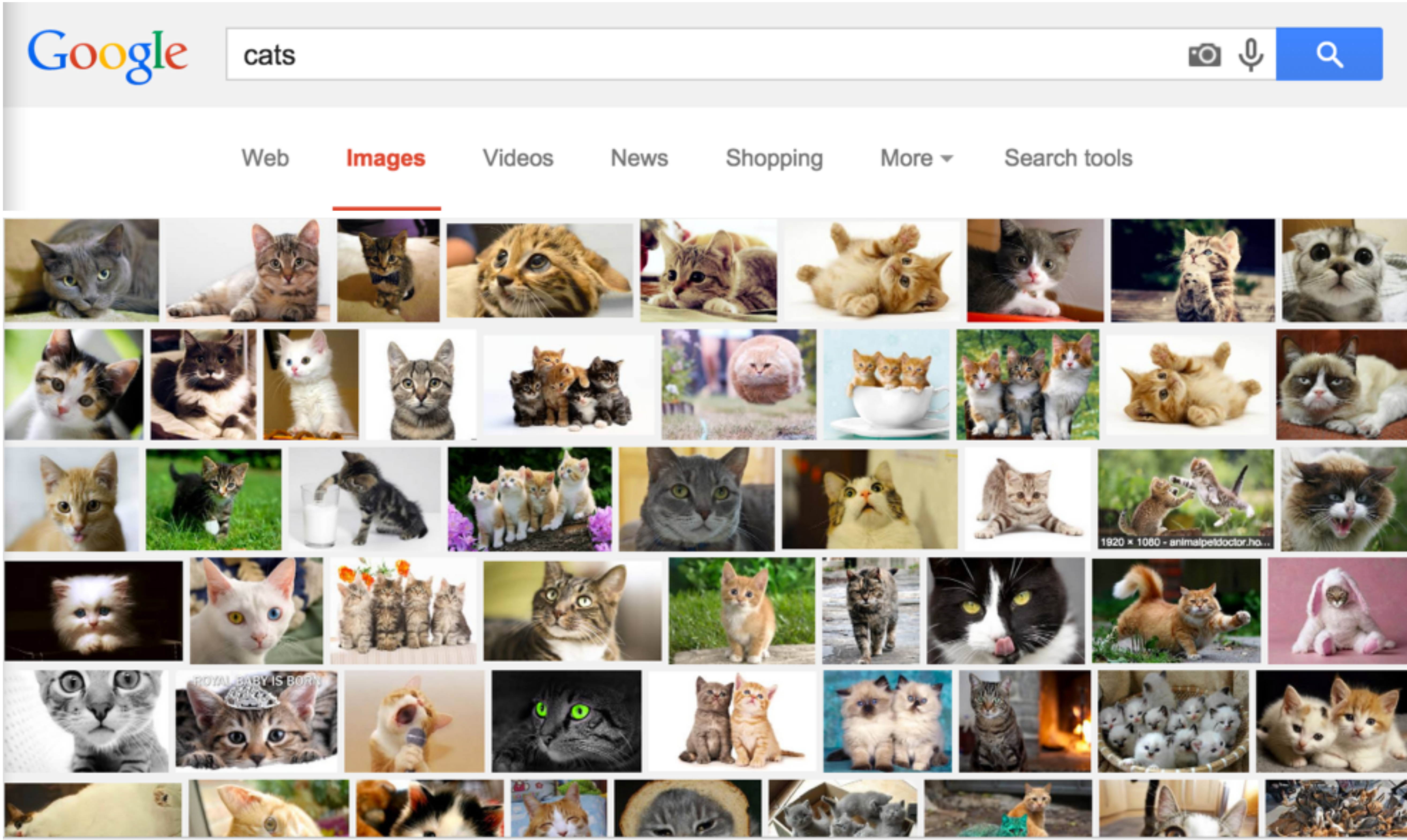
Ranking


Google
cats
Web
Images
Videos
News
Shopping
More
Search tools
1920 × 1080 - animalpetdoctor.ho...
ROYAL BABY IS BORN

Ranking

- Input: query (e.g. “cats”)
- Output: a sorted list of items

- How should we measure performance?
- The loss function is trickier than in the binary classification case
  - Example 1: All items in the first page should be relevant
  - Example 2: All relevant items should be ahead of irrelevant items

Learning to rank

- For simplicity lets assume we are learning to rank for a given query.
- Learning to rank:
  - Input: a list of items
  - Output: a function that takes a set of items and returns a sorted list

- Approaches
  - Pointwise approach:
    - Assumes that each document has a numerical score.
    - Learn a model to predict the score (e.g. linear regression).
  - Pairwise approach:
    - Ranking is approximated by a classification problem.
    - Learn a binary classifier that can tell which item is better given a pair.

Naive rank train

- Create a dataset with binary labels
  - Initialize: $D \leftarrow \phi$
  - For every i and j such that, i ≠ j
    - If item i is ***more*** relevant than j
      - Add a positive point: $D \leftarrow D \cup (\mathbf{x}_{ij}, +1)$
    - If item i is ***less*** relevant than j
      - Add a negative point: $D \leftarrow D \cup (\mathbf{x}_{ij}, -1)$

$\mathbf{x}_{ij} \leftarrow$ features for comparing item i and j

- Learn a binary classifier on D
- Ranking
  - Initialize: $score \leftarrow [0, 0, \ldots, 0]$
  - For every i and j such that, i ≠ j
    - Calculate prediction: $y \leftarrow f(\hat{\mathbf{x}}_{ij})$
    - Update scores: $score_i = score_i + y \quad score_j = score_j - y$

  $ranking \leftarrow \arg \mathtt{sort}(score)$

Problems with naive ranking

- Naive rank train works well for bipartite ranking problems
  - Where the goal is to predict whether an item is relevant or not. There is no notion of an item being *more* relevant than another.
- A better strategy is to account for the positions of the items in the list
- Denote a ranking by: σ
  - If item u appears before item v, we have: $\sigma_u < \sigma_v$
- Let the space of all permutations of M objects be: Σ_M
- A ranking function maps M items to a permutation: $f : \mathcal{X} \rightarrow \Sigma_{\mathcal{M}}$
- A cost function (omega)
  - The cost of placing an item at position i at j: $\omega(i, j)$
- Ranking loss: $\ell(\sigma, \hat{\sigma}) = \sum_{u \neq v} [\sigma_u < \sigma_v][\hat{\sigma}_v < \hat{\sigma}_u]\omega(u, v)$

$$\omega\text{-ranking:} \quad \min_f \mathbb{E}_{(\mathcal{X},\sigma)\sim\mathcal{D}} \left[\ell(\sigma, \hat{\sigma})\right], \text{ where } \hat{\sigma} = f(\mathcal{X})$$

ω-rank loss functions

- To be a valid loss function ω must be:
  - Symmetric: $\omega(i,j) = \omega(j,i)$
  - Monotonic: $\omega(i,j) \leq \omega(i,k)$ if $i < j < k$ or $k < j < i$
  - Satisfy triangle inequality: $\omega(i,j) + \omega(j,k) \geq \omega(i,k)$
- Examples:
  - Kemeny loss:

$$\omega(i,j) = 1, \text{ for } i \neq j$$

  - Top-K loss:

$$\omega(i,j) = \begin{cases} 1 & \text{if } \min(i,j) \leq K, i \neq j \\ 0 & \text{otherwise} \end{cases}$$

ω-rank train

- Create a dataset with binary labels
  - Initialize: $D \leftarrow \phi$
  - For every i and j such that, i ≠ j
    - If $\sigma_i < \sigma_j$ (item i is more relevant)
      - Add a positive point: $D \leftarrow D \cup (\mathbf{x}_{ij}, +1, \omega(i,j))$
    - If $\sigma_i > \sigma_j$ (item j is more relevant)
      - Add a negative point: $D \leftarrow D \cup (\mathbf{x}_{ij}, -1, \omega(i,j))$

$\mathbf{x}_{ij} \leftarrow$ features for comparing item i and j

- Learn a binary classifier on D (each instance has a weight)
- Ranking
  - Initialize: $score \leftarrow [0, 0, \ldots, 0]$
  - For every i and j such that, i ≠ j
    - Calculate prediction: $y \leftarrow f(\hat{\mathbf{x}}_{ij})$
    - Update scores: $score_i = score_i + y \quad score_j = score_j - y$

  $\text{ranking} \leftarrow \arg \mathtt{sort}(score)$

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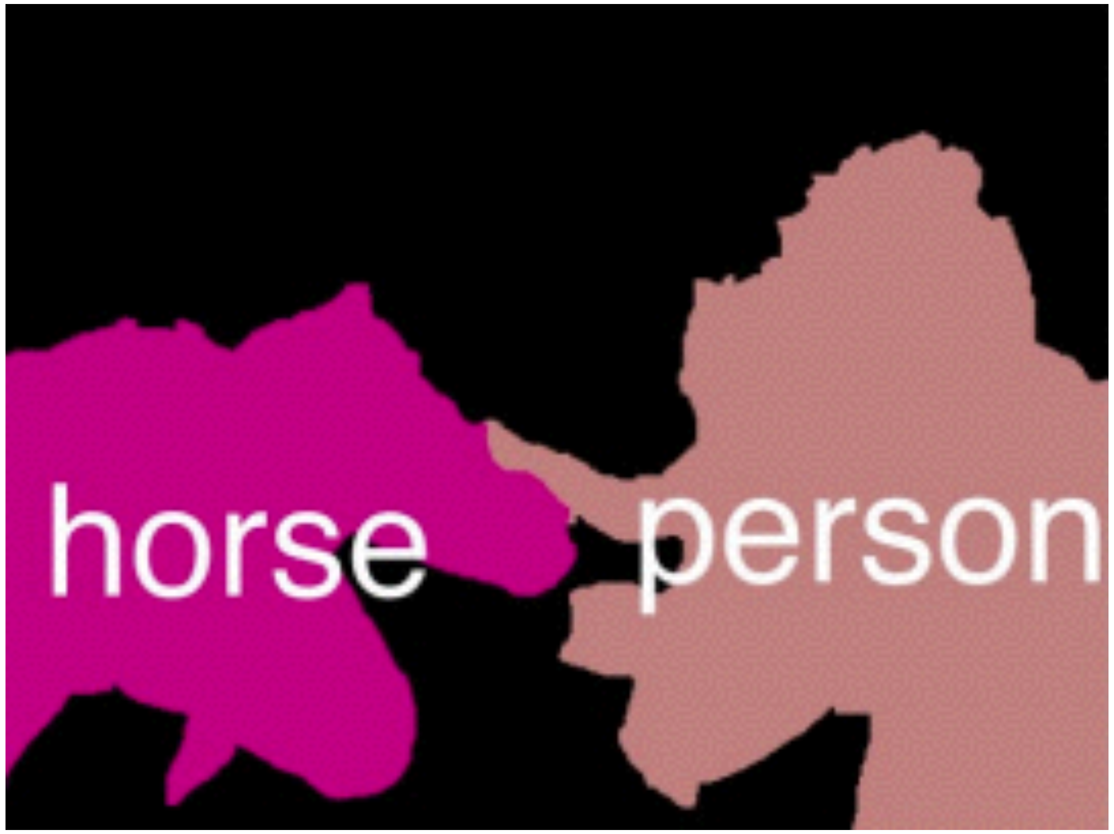
Collective classification

- Predicting multiple correlated variables

input



output

$(\mathbf{x}, k) \in \mathcal{X} \times [K]$

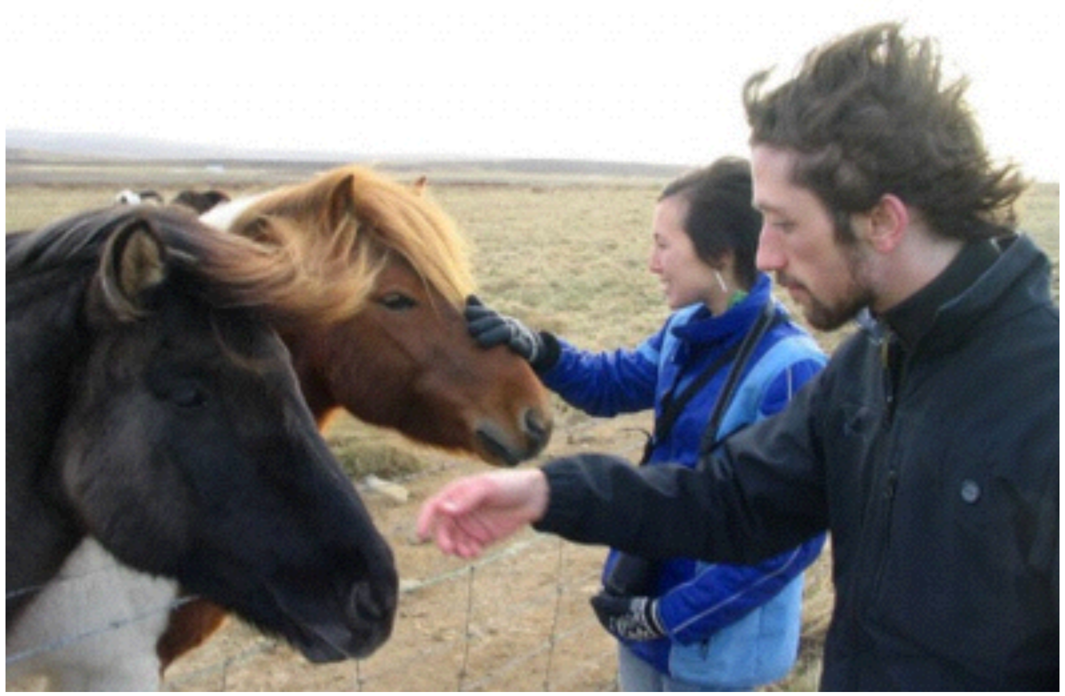
features labels

$\mathcal{G}(\mathcal{X}, k)$ be the set of all graphs

objective $f : \mathcal{G}(\mathcal{X}) \rightarrow \mathcal{G}([K])$ $\mathbb{E}_{(V,E)\sim\mathcal{D}}\left[\Sigma_{v\in V}(\hat{y}_v \neq y_v)\right]$

Collective classification

- Predicting multiple correlated variables



$$\hat{y}_v \leftarrow f(\mathbf{x}_v)$$

independent predictions can be noisy

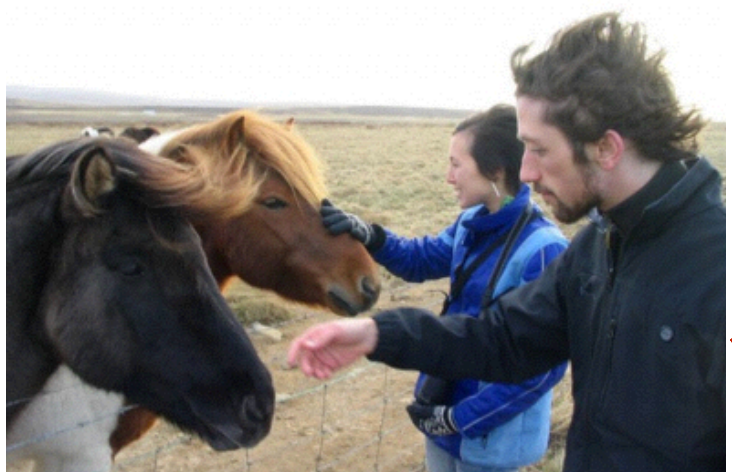
labels of nearby vertices as features

$$\mathbf{x}_v \leftarrow [\mathbf{x}_v, \phi([K], \mathrm{nbhd}(v))]$$

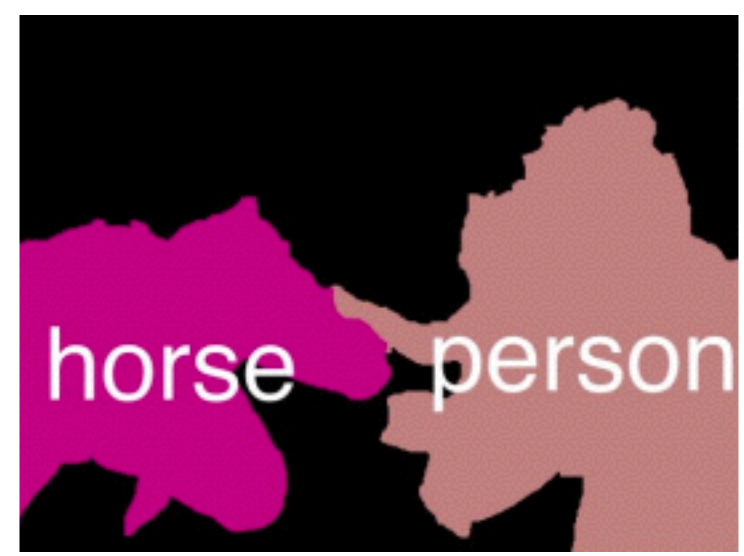
E.g., histogram of labels in a 5x5 neighborhood

Stacking classifiers

- Train a two classifiers
- First one is trained to predict output from the input
- Second is trained on the input and the output of first classifier



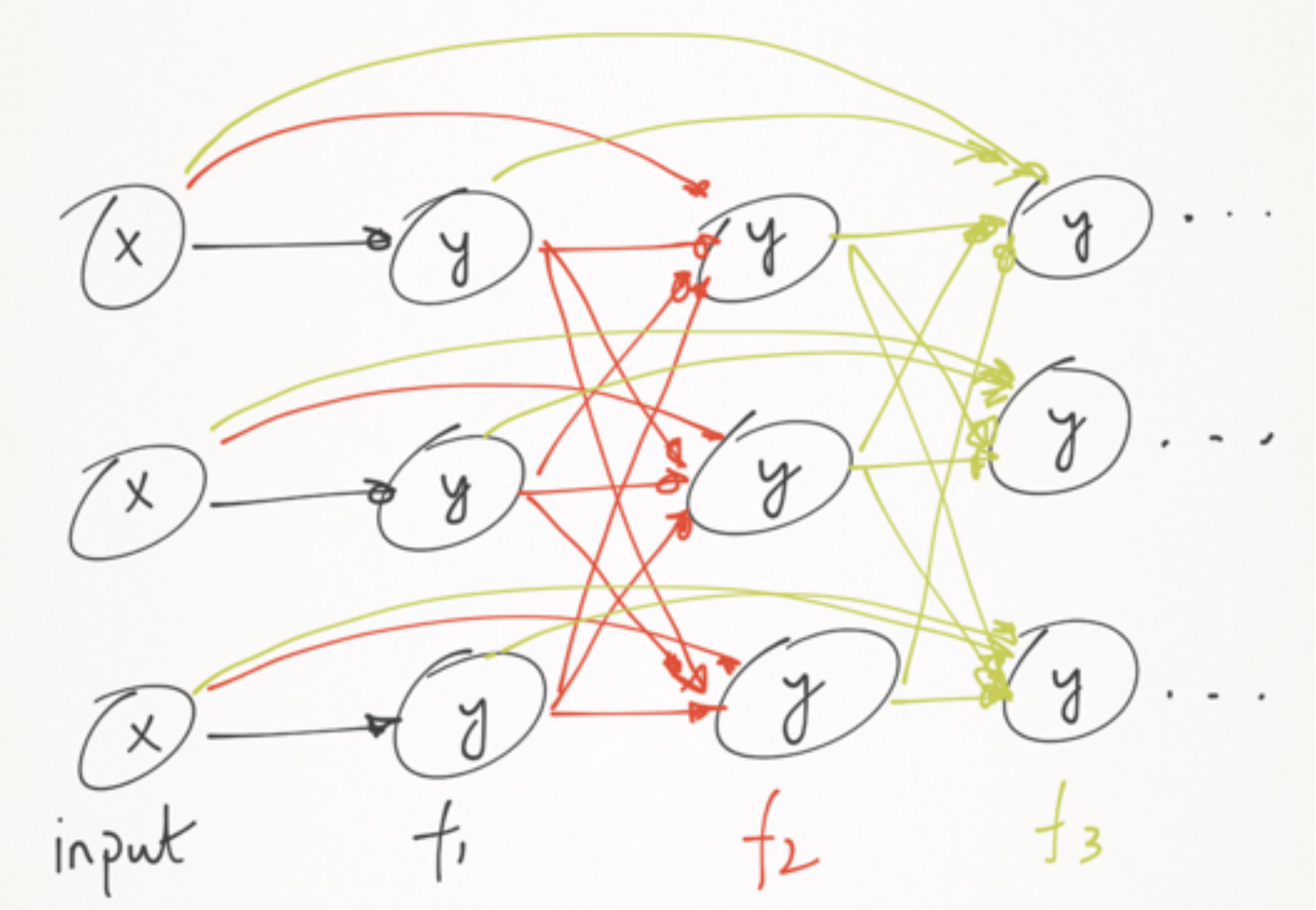
$$\hat{y}_v^{(1)} \leftarrow f_1(\mathbf{x}_v)$$



$$\hat{y}_v^{(2)} \leftarrow f_2\left(\mathbf{x}_v, \phi\left(\hat{y}_v^{(1)}, \mathrm{nbhd}(v)\right)\right)$$

Stacking classifiers

- Train a stack of N classifiers
- i^{th} classifier is trained on the input + output of the previous i-1 classifiers



- Overfitting is an issue: the classifiers are accurate on training data but on not on test data leading to a cascade of overconfident classifiers
- Solution: held-out data

f_1	$f_1 + f_2$	$f_1 + f_2 + f_3$	$\ldots$

Summary

- Learning with imbalanced data
  - Implicit and explicit sampling can be used to train binary classifiers for the weighted loss case
- Beyond binary classification
  - Multi-class classification
    - Some classifiers are inherently multi-class
    - Others can be combined using: one-vs-one, one-vs-all methods
  - Ranking
    - Ranking loss functions to capture distance between permutations
    - Pointwise and pairwise methods
  - Collective classification
    - Stacking classifiers trained with held-out data

Slides credit

- Some slides are adapted from CIML book by Hal Daume
- Images for collective classification are from the PASCAL VOC dataset
  - http://pascallin.ecs.soton.ac.uk/challenges/VOC/
- Some of the discussion is based on Wikipedia
  - http://en.wikipedia.org/wiki/Learning_to_rank