6.867 Machine learning and neural networks

Tommi Jaakkola
MIT AI Lab
tommi@ai.mit.edu

Lecture 7: feature selection, combination of methods

Topics

- Feature selection
  - filter methods
  - wrapper methods
- Combination of methods
  - greedy sequential fitting
  - voting methods: bagging, boosting

A bit more general view

- A filtering approach
  - is generic, i.e., not optimized for any specific classifier
  - may sacrifice classification accuracy
  - modular
- A wrapper approach
  - is always tailored to a specific classifier
  - may lead to better accuracy as a result

Example: feature pruning

- The goal here is to remove non-informative features
- Definitions:
  1. $\{\phi_1(\mathbf{x}), \ldots, \phi_m(\mathbf{x})\}$ is the set of possible word detectors,
  2. $\Phi(\mathbf{x}) = [\phi_{i_1}(\mathbf{x}), \ldots, \phi_{i_{m'}}(\mathbf{x})]^T$ is our current feature vector (current set of word detectors),
  3. $\Phi^{-i}(\mathbf{x})$ is the current feature vector without $\phi_i(\mathbf{x})$ component
- We'd like to remove any uninformative word detectors from the current feature vector $\Phi(\mathbf{x})$

  What is "uninformative"?

Feature pruning cont'd

- A word detector $\phi_{i_k}(\mathbf{x})$ is uninformative if it doesn't help predict the label, i.e., if

$$\widehat{P}(y|\Phi^{-i_k}(\mathbf{x})) \approx \widehat{P}(y|\Phi(\mathbf{x}))$$

  for all labels $y = 0, 1$ and documents $\mathbf{x}$.

- If the probabilities here are estimated using a specific classifier such as Naive Bayes, then this is a wrapper approach. Otherwise we are dealing with a filtering method.

Feature pruning with Naive Bayes (wrapper)

- A word detector $\phi_{i_k}(\mathbf{x})$ is uninformative if it doesn't help predict the label, i.e., if

$$P(y|\Phi^{-i_k}(\mathbf{x}), \widehat{\theta}) \approx P(y|\Phi(\mathbf{x}), \widehat{\theta})$$

for all labels $y = 0, 1$ and documents $\mathbf{x}$.

- These probabilities are now computed from the Naive Bayes model:

$$\begin{aligned} P(\Phi(\mathbf{x})|y, \widehat{\theta}) &= \prod_{j=1}^{m'} P(\phi_{i_j}(\mathbf{x})|y, \widehat{\theta}_k) \\ P(y|\Phi(\mathbf{x}), \widehat{\theta}) &= \frac{P(\Phi(\mathbf{x})|y, \widehat{\theta})\widehat{P}(y)}{\sum_{y'=0,1} P(\Phi(\mathbf{x})|y', \widehat{\theta})\widehat{P}(y')} \end{aligned}$$

for each document $\mathbf{x}$.

- Note that the "expert" models $P(\phi_i(\mathbf{x})|y, \widehat{\theta}_k)$ need not be recomputed during the feature search.

Another Wrapper approach

- Let's look at the document classification task again, now with a logistic regression model

  We have m possible binary word detectors $\{\phi_1(\mathbf{x}), \ldots, \phi_m(\mathbf{x})\}$ and

  $$P(y = 1|\mathbf{x}, \mathbf{w}) = g(\,w_0 + w_1\phi_1(\mathbf{x}) + \ldots + w_m\phi_m(\mathbf{x})\,)$$

  when all features are included.

- We'd like to find a small subset of features that lead to good classification

- We can
  1. Greedily add features
  2. Find relevant features using regularization

Greedy selection of features

1. Find k for which

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(\, w_0 + w_k \phi_k(\mathbf{x}) \,)$$

yields the best classifier

2. Find k' for which

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(\, w_0 + w_k \phi_k(\mathbf{x}) + w_{k'} \phi_{k'}(\mathbf{x}) \,)$$

yields the best classifier. w_0, w_k and $w_{k'}$ are all reoptimized in the context of each k' that we try to add

3. ...

- When/how do we stop?

Wrapper example: regularization

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(\, w_0 + w_1\phi_1(\mathbf{x}) + \ldots + w_m\phi_m(\mathbf{x})\,)$$

- We can introduce a regularization penalty that tries to set the weights to zero unless they are "useful"

$$J(\mathbf{w}; C) = \sum_{t=1}^{n} \log P(y_t|\mathbf{x}_t, \mathbf{w}) - C \sum_{i=1}^{m} |w_i|$$

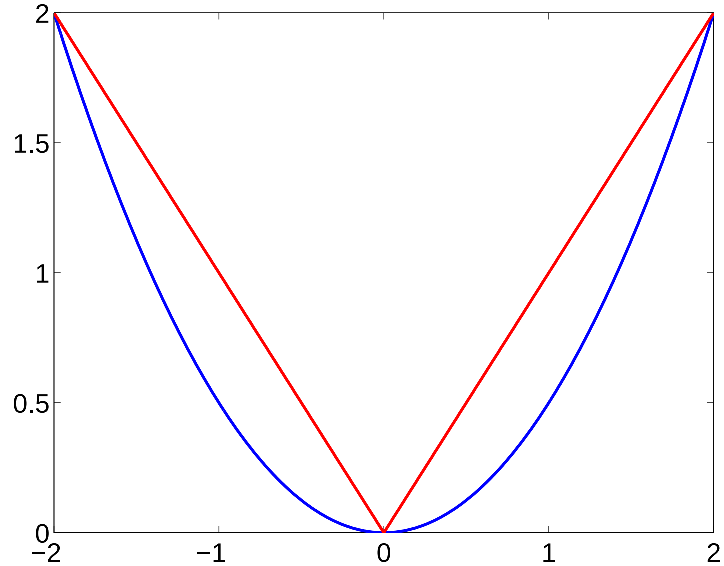
  where $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ is our training set. Note that w_0 is not penalized.

- The selection of non-zero weights here is carried out *jointly*, not individually

- Why should this regularization penalty work at all?

Wrapper example: regularization cont'd

- The effect of the regularization penalty on feature selection depends on its derivative at $w \approx 0$



$w^2/2$ versus $|w|$

$$J(\mathbf{w}; C) = \sum_{t=1}^{n} \log P(y_t|\mathbf{x}_t, \mathbf{w}) - C \sum_{i=1}^{m} |w_i|$$

- How are we dealing with redundant features?

Topics

- Combining multiple methods
  - greedy sequential fitting
  - voting methods: bagging, boosting

Combination of multiple methods

- Why would we want to generate and combine multiple methods rather than use a single method?
  - decompositon into simpler subproblems, modularity
  - multiple "weak" methods can be combined into a single "strong" method
  - robustness
- We have to
  - estimate the component methods in a modular way
  - find an appropriate combination rule
  - worry about generalization

Combination of regression methods

- We want to combine multiple "weak" regression methods into a single "strong" method
- Suppose we are given a training set $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ and a family simple regression methods (components) such as

$$f(\mathbf{x}; \theta) = w\, \phi_k(\mathbf{x})$$

  where $\theta = \{k, w\}$ (the parameters specify a single basis function as well as the associated weight)
- Basic forward fitting idea: sequentially fit new components to the *residuals*

$$\text{Step 1:} \quad \hat{\theta}_1 \leftarrow \arg\min_{\theta} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i; \theta))^2$$

$$\text{Step 2:} \quad \hat{\theta}_2 \leftarrow \arg\min_{\theta} \sum_{i=1}^{n} (\underbrace{y_i - f(\mathbf{x}_i; \hat{\theta}_1)}_{\text{residual}} - f(\mathbf{x}_i; \theta))^2$$

$$\text{Step 3:} \quad \ldots$$

Forward fitting cont'd

Simple family: $f(\mathbf{x};\theta) = w\phi_k(\mathbf{x}),\;\; \theta = \{k, w\}$

$$\text{Step 1:}\qquad \hat{\theta}_1 \leftarrow \arg\min_{\theta} \sum_{i=1}^{n} \left(y_i - f(\mathbf{x}_i;\theta)\right)^2$$

$$\text{Step 2:}\qquad \hat{\theta}_2 \leftarrow \arg\min_{\theta} \sum_{i=1}^{n} (\underbrace{y_i - f(\mathbf{x}_i;\hat{\theta}_1)}_{\text{residual}} - f(\mathbf{x}_i;\theta))^2$$

$$\text{Step 3:}\qquad \ldots$$

- The resulting combined regression method

$$\hat{f}(\mathbf{x}) = f(\mathbf{x};\hat{\theta}_1) + \ldots + f(\mathbf{x};\hat{\theta}_m)$$

  has much lower (training) error.

- How many components? Reuse?

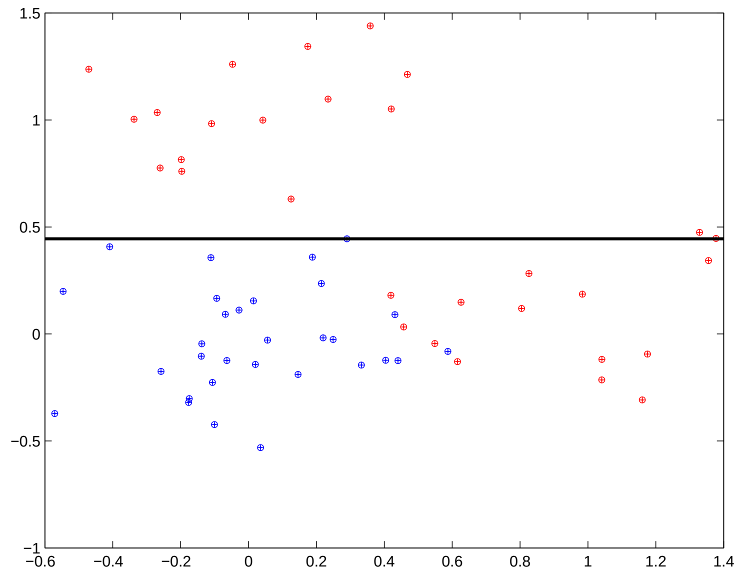
Combination of classifiers

- Suppose we are given a training set $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ of examples and (± 1) labels and a family of component classifiers such as *decision stumps*:

  $$h(\mathbf{x}; \theta) = \text{sign}(\, w_1 \, x_k - w_0 \,)$$

  where $\theta = \{k, w_1, w_0\}$.

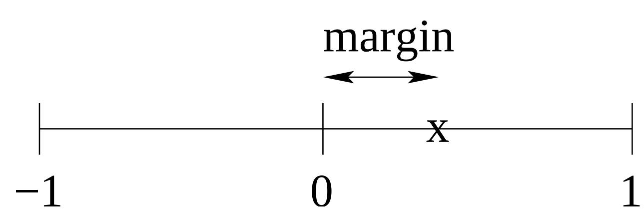
  Each decision stump pays attention to only a single component of the input vector



Bagging

- We can combine classifiers to ensure more *robust* predictions (classifications)
- Given a set of n training examples and labels, repeat
  1. resample (with replacement) a smaller training set of $n' < n$ examples
  2. train a new classifier (decision stump) $h(\mathbf{x};\hat{\theta})$ based on the smaller training set
- The resulting combined classifier is obtained by *voting*

$$\hat{h}(\mathbf{x}) = \text{sign}\left(\frac{1}{m}\sum_{k=1}^{m} h(\mathbf{x};\hat{\theta}_k)\right)$$



Beyond Bagging: reweighting training examples

- The component classifiers should concentrate more on training examples that are difficult to classify correctly
- We can tune the classifiers towards harder examples by reweighting the training examples (small margin $\Rightarrow$ large weight)

  Example: suppose we already have $h(\mathbf{x}; \widehat{\theta}_1), \ldots, h(\mathbf{x}; \widehat{\theta}_m)$. We train the next component classifier $h(\mathbf{x}; \theta_{m+1})$ on a reweighted training set

$$\text{Weight } p(i) \text{ on } (\mathbf{x}_i, y_i)\text{:} \quad p(i) \;\propto\; \exp\Big\{ \overbrace{-\, y_i \sum_{k=1}^{m} h(\mathbf{x}_i; \widehat{\theta}_k)}^{\text{margin}} \Big\}$$

  where examples with small or negative classification margins (difficult examples) will have larger weights

Boosting

- A Boosting algorithm sequentially estimates and combines classifiers by reweighting training sets (concentrating on the harder examples)
  - each component classifiers is presented with a slightly different problem
- AdaBoost preliminaries:
  a) Training set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$ with binary ± 1 labels y_i.
  b) A set of "weak" binary (± 1) classifiers $h(\mathbf{x}; \theta)$ such as *decision stumps*

$$h(\mathbf{x}; \theta) = \text{sign}(\, w_1\, x_k - w_0 \,)$$

  where $\theta = \{k, w_1, w_0\}$.
  c) Initially all weights are equal: $p(i) = 1/n$.