Model Selection and Feature Selection

Piyush Rai

CS5350/6350: Machine Learning

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(CS5350/6350)

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Note: Usually considered in supervised learning contexts but unsupervised learning too faces this issue (e.g., "how many clusters" when doing clustering)

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 - Held-out data may not be good if there was an unfortunate split
 - Can ameliorate unfortunate splits by repeated random subsampling

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K-fold Cross-Validation

• Create K equal sized partitions of the training data

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- Create K equal sized partitions of the training data
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- Train using K 1 partitions, validate on the remaining partition

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Image: A match a ma

K-fold Cross-Validation

- Create K equal sized partitions of the training data
- Each partition has N/K examples
- Train using K-1 partitions, validate on the remaining partition
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• Finally, choose the model with smallest average validation error

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- Usually K is chosen as 10

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Special case of K-fold CV when K = N (number of training examples)

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- Finally, choose the model with smallest average validation error
- Can be expensive for large N. Typically used when N is small

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Random Subsampling Cross-Validation

• Randomly subsample a fixed fraction αN (0 < α < 1) of examples; call it the validation set

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- Randomly subsample a fixed fraction αN (0 < α < 1) of examples; call it the validation set
- Train using the rest of the examples, measure error on the validate set

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- Randomly subsample a fixed fraction αN (0 < α < 1) of examples; call it the validation set
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- Usually α is chosen as 0.1, K as 10

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- Idea: Sample N elements from this set with replacement
 - An already sampled element could be picked again

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- Training data is *inherently* small \Rightarrow error estimate may be pessimistic

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- Use the following equation to compute the expected model error

$$e = 0.632 \times e_{test-examples} + 0.368 \times e_{training-examples}$$

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• **Note:** the above estimate may still be bad if we overfit and have $e_{training-examples} = 0$. Why?

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• Akaike Information Criteria (AIC)

$$AIC = 2k - 2\log(\mathcal{L})$$

• Bayesian Information Criteria (BIC)

$$BIC = k \log(N) - 2 \log(\mathcal{L})$$

- k: # of model parameters
- \mathcal{L} : maximum value of the model likelihood function

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- Model with the lowest AIC/BIC will be chosen
- Can be used even for model selection in unsupervised learning

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 $MDL = -\log_2 P(z)$

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• Note: it's just the MDL for model's posterior distribution

 $P(\mathbf{w} \mid \mathbf{X}, \mathbf{Y}, M) \propto P(\mathbf{w} \mid M) \times P(\mathbf{Y} \mid \mathbf{X}, \mathbf{w}, M)$

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- $\bullet~\mbox{Complex}$ posterior distribution $\Rightarrow~\mbox{Complex}$ model
- Choose the model with the lowest MDL

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 $Length(M) = -\log P(\mathbf{Y} \mid \mathbf{X}, \mathbf{w}, M) - \log P(\mathbf{w} \mid M)$

• Note: it's just the MDL for model's posterior distribution

 $P(\mathbf{w} \mid \mathbf{X}, \mathbf{Y}, M) \propto P(\mathbf{w} \mid M) \times P(\mathbf{Y} \mid \mathbf{X}, \mathbf{w}, M)$

- $\bullet~\mbox{Complex}$ posterior distribution $\Rightarrow~\mbox{Complex}$ model
- Choose the model with the lowest MDL
- Note: MDL criteria is kind of equivalent to preferring the best regularized model

Selecting a useful subset from all the features

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Selecting a useful subset from all the features Why Feature Selection?

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• Some algorithms scale (computationally) poorly with increased dimension

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- Removal of features can increase (relative) margin (and generalization)
- Reduces data set and resulting model size
- Note: Feature Selection is different from Feature Extraction
 - The latter transforms original features to get a small set of new features
 - $\bullet\,$ More on feature extraction when we cover Dimensionality Reduction

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• Methods agnostic to the learning algorithm

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- Methods agnostic to the learning algorithm
 - Preprocessing based methods
 - E.g., remove a binary feature if it's ON in very few or most examples

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 - Can be computationally expensive
• Uses heuristics but is much faster than wrapper methods

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• Correlation Critera: Rank features in order of their correlation with the labels

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• **Correlation Critera:** Rank features in order of their correlation with the labels

$$R(X_d, Y) = \frac{cov(X_d, Y)}{\sqrt{var(X_d)var(Y)}}$$

Mutual Information Criteria:

$$MI(X_d, Y) = \sum_{X_d \in \{0,1\}} \sum_{Y \in \{-1,+1\}} P(X_d, Y) \frac{\log P(X_d, Y)}{P(X_d)P(Y)}$$

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(CS5350/6350)

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- Note: These probabilities can be easily estimated from the data

(CS5350/6350)

• Two types: Forward Search and Backward Search

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• Two types: Forward Search and Backward Search

• Forward Search

- Start with no features
- Greedily include the most relevant feature
- Stop when selected the desired number of features

Backward Search

- Start with all the features
- Greedily remove the least relevant feature
- Stop when selected the desired number of features
- Inclusion/Removal criteria uses cross-validation

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- Forward Search
 - Let $\mathcal{F} = \{\}$

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Forward Search

- Let $\mathcal{F} = \{\}$
- While not selected desired number of features
- For each unused feature f:

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Forward Search

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- Add f with lowest error to \mathcal{F}

Backward Search

• Let $\mathcal{F} = \{ all \text{ features} \}$

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Backward Search

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Backward Search

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