Machine Learning

Model quality and Ensemble Techniques

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Closed Book Test 1 Announcement

Closed book test 1 will take place on 19.03.2024 12:00 ICT-A1 (usual time and place for the lecture).
As a part of preparation for the Closed Book Test 1 students are required acquire the knowledge about SVD independently. See pages 44-48 in Agarwal's Data Mining book. One have to answer the questions about the meaning and properties of the matrices Q, Σ and P, explain how to apply it on practice and describe the result of its application. Also one should be able to explain similarities and differences to the PCA.

Bias and variance

- Let Y denote the target variable, X vector of inputs and a prediction model $\hat{f}(X)$ that was estimated on the basis of training set D_{train}.
- The loss function is denoted $L(Y, f(\hat{X}))$
- Typical choices of function L are squared error and absolute error.
- Test error or generalization error is the prediction error over the independent test sample.

$$\mathrm{Err}_{D_{\text{train}}} = \mathrm{E}\big[L(Y, f(\hat{X})) \mid D_{\text{train}}\big]$$

- Expected prediction error.

$$\mathrm{Err} = \mathrm{E}\big[L(Y, f(\hat{X}))\big] = \mathrm{E}\big[\mathrm{Err}_{D_{\text{train}}}\big]$$

- Training error

$$\overline{\mathrm{err}} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, f(\hat{x}_i)).$$

Model selection and assessment

- Model selection is the process of estimating the performance of different models in order to chose the most suitable one.
- Model assessment is the process of estimating prediction error of the chosen model on a new data.

The bias-variance decomposition

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$$\begin{aligned}\mathrm{Err} &= \mathrm{E}\big[(Y - \hat{f(x_0)})^2 | X = x_0\big] \\ &= \sigma_\epsilon^2 + \big[\mathrm{E}\hat{f(x_0)} - f(x_0))\big]^2 + \mathrm{E}\big[\hat{f(x_0)} - \mathrm{E}\hat{f(x_0)}\big]^2 \\ &= \sigma_\epsilon^2 + \mathrm{Bias}^2((\hat{f(x_0)}) + \mathrm{Var}(\hat{f(x_0)})\end{aligned}$$

- The first term of the last line is the variance of the target around the mean $f(x_0)$. It can not be avoided. No matter how good is our model.
- The second term is squared bias (the amount by which the average of the estimate differs from the true mean).
- The last term is the variance.
- Typically the more complex the model the lower the bias but the higher the variance.

Structure of the sample

- Does the sample representative?x
- Does it well balanced?
- Is there any other information to take into account?
- Keep in mind the difference between the data mining (data exploration) and targeted machine learning.

Measures of goodness I

- Let us remind: TP- true positive, TN - true negative, FP - false positive, FN - false negative.
- Keep in mind the difference between the cases of information retrieval and true classification.
- Accuracy, recall, precision, $f1$ - score, ROC-AUC score.
- Sensitivity & specificity
  - Sensitivity is the synonym of recall, also may be referred as True Positive Rate (TPR) or simply hit rate.
  - Specificity is the True Negative Rate (TNR) also referred as selectivity is given by

$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}}$$

- Negative predictive value is given by:

$$\mathrm{NPV} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FN}}$$

Measures of goodness II

- False negative rate

$$\mathrm{FNR} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TP}}$$

- False omission rate

$$\mathrm{FOR} = \frac{\mathrm{FN}}{\mathrm{FN} + \mathrm{TN}}$$

- Fall-out or false positive rate

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{TN} + \mathrm{FP}}$$

- You are welcome to continue this list ... .

Let us remind the main idea of Cross Validation

- The method to estimate the expected extra-sample error $\mathcal{E} = E[L(Y, \hat{f}(X))]$ (average generalized error) when the method $\hat{f}(X)$ is applied to and independent test sample from the joint distribution of X an Y (L denots loss function here.)
- Cross-validation estimate of prediction error is given by:

$$\mathcal{E}_{CV} = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{f}^{-k(i)}(x_i)).$$

- Usually 5 or 10 fold cross validation is recommended.

Cross Validation within Machine Learning Work-flow

- Up to a present time we have used synthetic sets of a very small power, treating them as the samples.
- For the real life applications when one have the sample only and not entire population this may lead to serious errors.
- One possible way to fix the problem is to perform feature selection within the cross validation loop. (Point to discuss!!!)

Hastie & Tibshirian view on cross validation

- Consider to study in detail section $7.10.2$
- Classification problem with a large number of predictors.
- What would be the strategy to implement ML work flow?

Example p. 245

- $N = 50$ samples, binary case, two equal sized classes.
- Let the power of feature set be $p = 5000$, each feature normally distributed and independent of class labels.
- True error rate for any classifier is 0.5
- Let us suppose that 100 predictors is chosen.
- 1-nearest neighbour classifier was chosen.
- 50 simulations will result in cross validation error of 0.03, whereas true error rate is 0.5
- Leaving samples out after the feature selection does not mimic correctly the application of the classifier to a previously unseen data.

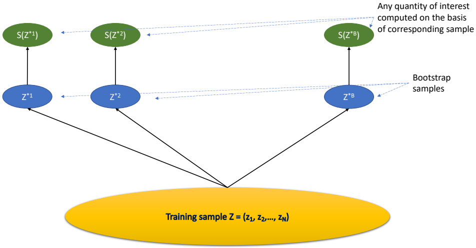
H & T suggest that this is the (correct) way :)̃

- Divide the data set into K cross-validation folds.
- For each fold k perform:
- Use all the folds except the fold k to perform the feature selection and model training.
- Use fold k for model validation.
- Use the results for each k to compute error estimates.

What is the drawback of cross validation?

Bootstrap I

- Let $Z = (z_1, \ldots, z_n)$ is the training set.
- Draw randomly data sets with replacement (the samples are independent) from Z. This will result in B *bootstrap* data sets.
- Fit the model for each of B data sets. Examine behaviour over B replacements.
- This approach allows to estimate any aspect of distribution $S(Z)$.


Any quantity of interest computed on the basis of corresponding sample
S(Z*1)
S(Z*2)
S(Z*B)
Bootstrap samples
Z*1
Z*2
Z*B
Training sample Z = (z1, z2,..., zN)

Bootstrap II

- Let $f^{*b}(x_i)$ be the predicted value at x_i from the model fitted to the b^{th} bootstrap dataset.
- Error estimate is given by:

$$\mathcal{E}_{boot} = \frac{1}{B}\frac{1}{N}\sum_{b=1}^{B}\sum_{i=1}^{N} L\Big(y_i, \hat{f}^{*b}(x_i)\Big).$$

- Better bootstrap estimate may be derived by mimicking cross-validation. For each observation we will keep track of predictions from bootstrap samples not containing this observation. This is referred as leave-one-out bootstrap estimate of prediction error and is defined by the following equation.

$$\mathcal{E}_{boot}^{(1)} = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{C^{-i}}\sum_{b\in C^{-i}} L\Big(y_i, f^{*b}(x_i)\Big).$$

- Notation here may cause a problem. You are welcome to fix it :) .

Bagging

- Induced from the bootstrap technique (which is used to assess accuracy of estimate).
- Draw B samples with replacements and train the model on each sample.
- The bagging estimate then is defined by:

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^{*b}(x).$$

Random Forests

The idea is to build large collection of de-correlated trees, and then average them.

- For $b = 1$ to B:
  - Draw a bootstrap sample Z^* of size N from the available training data.
  - Grow tree T_b. Repeat recursively for each terminal node until minimum node size is reached.
    - Select m variables from p.
    - Pick the best variable among m.
    - Split the node.
- Output the ensemble of trees $\{T_b\}_1^B$.
- Prediction:
  - Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.
  - Classification: $\hat{C}_{\text{rf}}^B(x) = \text{mode}\{\hat{C}_b(x)\}_1^B$.

Committee learning

- Some times referred as ensemble learning.
- The idea is to combine a number of weak (accuracy is slightly larger than of random guessing) classifiers into a powerful committee.
- Motivation is to improve estimate by reducing variance and sometimes bias.

Boosting

- The final prediction is given by:

$$G(x) = \operatorname{sign}\Big(\sum_{m=1}^{M} \alpha_m G_m(x)\Big).$$

  which is weighted majority vote of classifiers $G_m(x)$. Here α_m are weights describing contribution of each classifier.
- While on the first view result is very similar to the bagging, there are some major differences.
- Two class problem where output variable coded as $Y \in \{-1, 1\}$.
- For the classifier $G(X)$ error rate is given by:

$$\overline{\mathrm{err}} = \frac{1}{N}\sum_{i=1}^{N} I(y_i \neq G(x_i)),$$

  where N is the power of training data set.

Ada Boost

AdaBoost.M1. by Freund and Shcapire (1997).

- Initialize observation weights $w_i = 1/N$, $i = 1, \dots, N$.
- For $m = 1$ to M:
  - Fit weak classifier G_m that minimizes the weighted sum error for misclassified points.

$$\epsilon_m = \frac{\sum_{i=1}^{N} w_i I(G_m(x_i) \neq y_i)}{\sum_{i=1}^{N} w_i}$$

  - Compute $\alpha_m = \log((1 - \epsilon_m)/\epsilon_m)$.
  - Update weights w_i as

$$w_i = w_i * \exp(\alpha_m * I(y_i \neq G_m(x_i))), \quad i = 1, \dots, N.$$

- Output classifier:

$$G(x) = \operatorname{sign}\Big(\sum_{m=1}^{M} \alpha_m G_m(x)\Big).$$