Practical introduction to machine learning

Part 4 : Validation and interpretation

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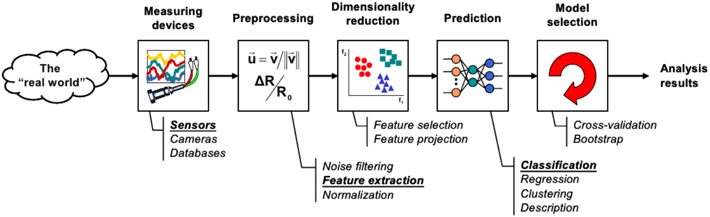
Overview of MAP654I

1. **Data and Machine Learning problems**
   - Data properties and visualization
   - Pre-processing
   - Finding your Machine Learning problem
2. **Unsupervised learning**
   - Clustering
   - Density estimation and generative modeling
   - Dictionary learning and collaborative filtering
   - Dimensionality reduction and manifold learning
3. **Supervised learning**
   - Bayesian decision and Nearest neighbors
   - Linear models nonlinear methods for regression and classification
   - Trees, forest and ensemble methods
4. **Validation and interpretation**
   - Performance measures
   - Models and parameter selection (validation)
   - Interpretation of the methods

Overview for the current part

Machine Learning in practice



Selecting the model

- For a given ML problem several kinds of method can be applied.
- Even for a given method several parameters can greatly change its performance.
- Selecting the "best" method/parameters is called **model selection** or **validation**.
- An important question is which **performance measure** to use.

Understanding the model

- Interpret the perfomance, identifying bad predictions, detect bias in the predictor/data.
- Most important variables for the model.
- Explaining a given prediction (what lead to this prediction).
- Robustness to noise, to adversarial attacks.

Section

Performance measure

Unsupervised learning

- Clustering
  - Supervised (actual clusters ar known, `perf_measure(y_true,y_pred)`).
  - Unsupervised (actual clusters unknown, `perf_measure(X,y_pred)`)).
- Dimensionality reduction performance is often the objective of the optimization problem (same as regression performance for invertible methods).

Supervised learning

- Classification (default is accuracy/0-1 loss).
  - How accurate is the class prediction.
  - How separable are the classes in the score function space.
- Regression (prediction error)
  - Average prediction error.
  - Correlation (focus on the dynamic).

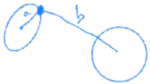
Performance measures

- Performance measures provided below are functions of `sklearn.metrics`.
- Measures with $\uparrow$ are better with large values and $\downarrow$ with low or negative values.

Warning

Always evaluate performance on data that was not used to train the model for supervised learning (also sometimes on unsupervised).

Clustering performance



Silhouette score ↑, `silhouette_score` [Rousseeuw, 1987]

No labels

- Score is the average of $(b-a)/max(a,b)$ when a is the distance to the cluster and b the distance to the closest other cluster.
- Non-supervised measure between -1 (worst) and 1 (best).

Rand Index ↑, `rand_score` [Rand, 1971] Kind of Accuracy

- Ratio of samples belonging in the same clusters in the predicted and true clustering (similar to accuracy but invariant to class permutation).
- Supervised measure between 0 (worst) and 1 (perfect).
- Adjusted Rand Index `ajusted_rand_score` has score 0 when random prediction.

Mutual Information ↑, `mutual_info_score` [Vinh et al., 2010]

- Measure of the mutual information between the true and predicted clustering.
- Supervised measure ≥ 0 (where 0 is worst).
- Adjusted Mutual Information `adjusted_mutual_info_score` has score 0 when random prediction and 1 when perfect.

Regression performances

Mean Square Error (MSE) ↓, `mean_squared_error`

label

- $MSE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{n}\sum_i (y_i - \hat{y}_i)^2$, classical convex and smooth loss in regression, can be used as performance measure on new data.
- Can be normalized by the mean square of the true labels (which computes the Signal to Noise Ratio, SNR).

Pearson Correlation Coefficient ↑, `np.corrcoef`

1 means $\hat{y}$ goes up y goes up but don't tell how fast. linear correlat

- $r = cov(\mathbf{y}, \hat{\mathbf{y}})/\sqrt{cov(\mathbf{y}, \mathbf{y})cov(\hat{\mathbf{y}}, \hat{\mathbf{y}})}$, between -1 and 1 (random pred. is 0).
- Measure of linearity between the true and predicted labels (invariant to scaling).

R^2 coefficient of determination ↑, `r2_score`

= maximize

→ normalized MSE

- $R^2 = 1 - MSE(\mathbf{y}, \hat{\mathbf{y}})/MSE(\mathbf{y}, \bar{\mathbf{y}})$ where $\bar{\mathbf{y}}$ contains the mean of $\mathbf{y}$.
- 1 when perfect prediction, 0 when random prediction (can be negative).

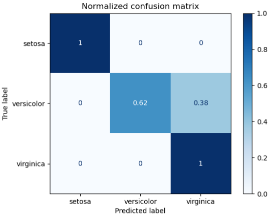
Mean/Median absolute error ↓, `mean_absolute_error`,`median_absolute_error`

- $MeanAE(\mathbf{y}, \hat{\mathbf{y}}) = \frac{1}{n}\sum_i |y_i - \hat{y}_i|$
- More robust to outliers in the data but non-smooth (harder to optimize).

Classification performances

Confusion matrix, `confusion_matrix`

- Matrix $\mathbf{C}$ that counts for $C_{i,j}$ the number of samples that are from the true class i and are predicted as class j.
- For binary classification we have
  - $C_{0,0}$ True Negative (TN) and $C_{1,1}$ True Positive (TP).
  - $C_{1,0}$ False Negative (FN) and $C_{0,1}$ False Positive (FP).
- Used for many performance measures.



Accuracy ↑, `accuracy_score`

Sum of diagonal of cm / all of the matrix

- Ratio of correctly classified samples $\frac{TP+TN}{n} = \frac{1}{n}\sum_k C_{k,k}$.
- Balanced accuracy $\frac{1}{p}\sum_k \frac{C_{k,k}}{\sum_l C_{l,k}}$ better when unbalanced classes.

Area Under the Receiver Operating Curve (ROC) curve ↑, `roc_auc_score`

- Compute the Area under the curve plotting $TPR = \frac{TP}{TP+FN}$ as a function of $FPR = \frac{FP}{FP+TN}$ when varying the threshold on the score function.
- Estimates for binary classification the probability for a positive sample to have a larger score than a negative sample (measure of separability in the score space).

Interpreting the performance

⚠ Look at several Perf measure.
on regarde un score en 1D
un leve fct à la base très compliqué. faire attention à ça.

Performance measure

- A performance measure even when computed on test data is a 1D (partial) measure of the quality of a model.
- Know the side effect of the performance measure (e.g. MSE is very sensitive to outliers, Pearson-s correlation coeff is invariant to scaling).
- Always compute other performance measures and compare them on a given model/data.

Interpreting the prediction

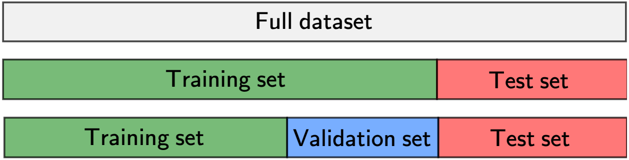
- Visualize the predictions (confusion matrix, scatterplot for regression).
- Search for bias in the predictions (some groups always badly predicted?).
- Look at mispredicted samples (bad label or systematic error).

Warning

Always be careful what you wish for (in terms of performances). Optimizing a given criterion can/will have unintended effect.

Section

Splitting the data



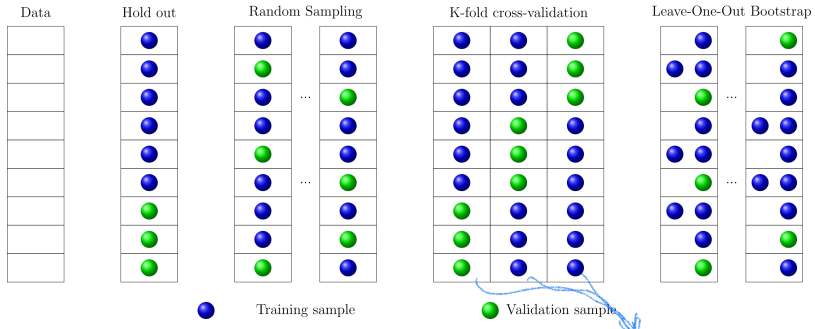
Principle of Hold-Out cross-validation

- Split the training data in a training and validation sets (non overlapping).
- Train different models (different methods and/or parameters) on the train data.
- Evaluate performance on the validation data and select the method/parameters with best performance.

Final estimator

- The validation is a method of selection for the method/parameters not the estimator.
- After selecting the optimal parameters, one should retrain the estimator on the whole training dataset using the optimal method/parameters.
- For methods that can have a large variability (neural network) the best classifier on validation set is often kept (also used for early stopping).

Different ways to split the data

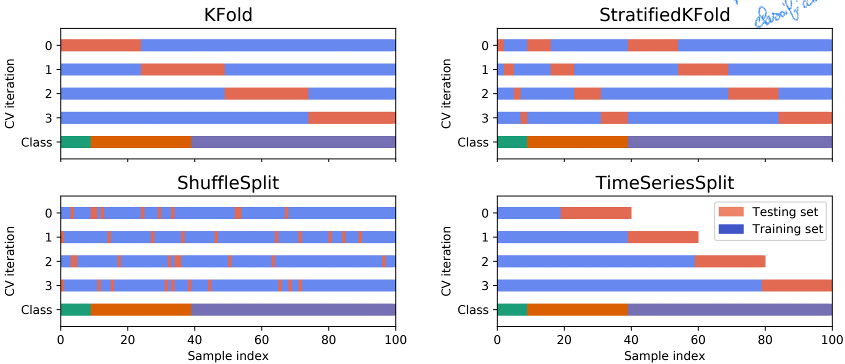


Data splitting for cross-validation [Arlot and Celisse, 2010]

- The training data is split in non-overlapping training/validation sets.
- **Hold-Out** uses a unique split and computes the performance on the validation set.
- More robust cross-validation approaches actually investigate several splits of the data and compute the average performance:
  - **K-fold** (split in K sets and use one split as test for all k)
  - Random sampling (aka **Shuffle split**) draws several random splittings.
  - Leave one out bootstrap draws training samples with replacement.
- Scikit-learn implementation : `sklearn.model_selection.cross_validate`

Data splitting with Scikit-learn

nice for classification

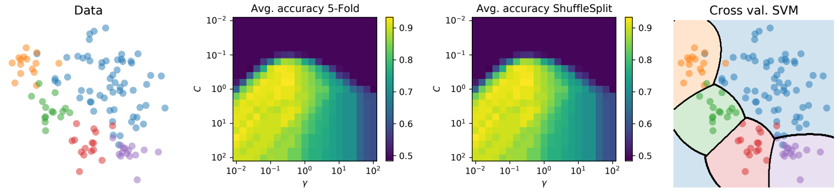


- Scikit-learn implements iterator classes for data split in `sklearn.model_selection`.
- KFold is the classical K-fold cross-validation.
- StratifiedKFold ensures a data split that preserves the proportion of classes.
- ShuffleSplit randomly selects a proportion of the samples for train/validation.
- TimeSeriesSplit preserves the temporal sequences and ensures that the validation data is in the future (see practical session 2).

Source :

`https://scikit-learn.org/stable/auto_examples/model_selection/plot_cv_indices.html`

Validation with Scikit-learn



Principle

- GridSearchCV takes a model and a grid of parameters as input and performs cross-validation.
- Both the best estimator (retrained on the whole data) and the best parameters can be recovered.
- Number of splits and type of data splitting can be chosen.
- For large number of parameters complexity is exponential, RandomizedSearchCV can be more efficient.

Python code

```
from sklearn.svm import SVC
from sklearn.model_selection import
      GridSearchCV

ngrid=21
clf = SVC()
param_grid={'C':np.logspace(-2,2,ngrid),
         'gamma':np.logspace(-2,2,ngrid),}

cv = GridSearchCV(clf,param_grid)

cv.fit(xn,y)

# recover best parameters and estimators
clf_opt = cv.best_estimator_
params_opt = cv.best_params_
```

Section

Interpretation of the model and data

ML interpretation and model explainability [Molnar, 2020]

- Important question of understanding the model and the data.
- Interpretation: how does the model work?
- Explainability: why did it predict this?
- GDPR brought the "right to explanation" in European countries.

Linear models

- Linear models are the simplest models and the importance of each variable is provided in the weights.
- Remember to standardize the data before interpretation because the weights depend on the scaling of the variables.
- Example in Scikit-learn documentation : `https://scikit-learn.org/stable/auto_examples/inspection/plot_linear_model_coefficient_interpretation.html`

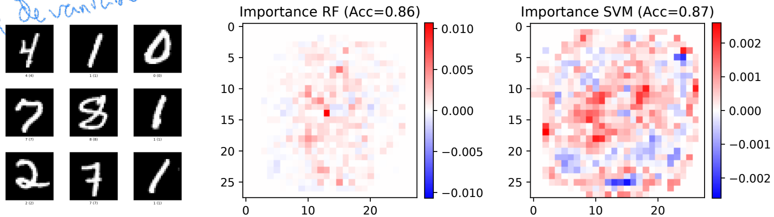
Feature selection [Guyon and Elisseeff, 2003]

- Can be seen as both pre-processing and promotion of interpretability.
- Can be done simultaneously with model estimation with linear models (Lasso).
- Wrapper methods perform a validation over the subset of variables (forward/backward methods add/remove variables one by one).

Feature permutation importance

très long si beaucoup de variables

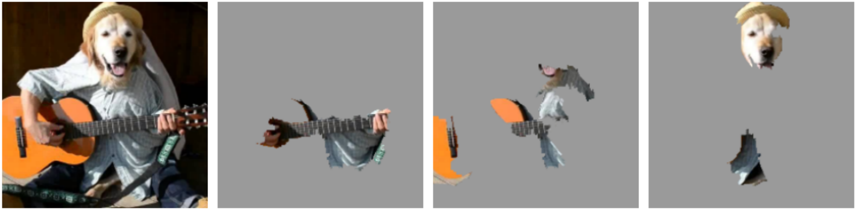
areas in red are the one importants



Principle [Breiman, 2001]

- Computed by doing a random permutation for one feature (permute one column).
- The loss/gain of performance is computed on a held-out data and is a measure of the importance of this variable.
- Mean Decrease in Impurity (MDI) is an alternative for random forests.
- Correlated features will all be "important" even when non necessary.
- Computational complexity is high on high dimensional data.
- Scikit-learn : `sklearn.inspection.permutation_importance`

Local Interpretable Model-agnostic Explanations (LIME)

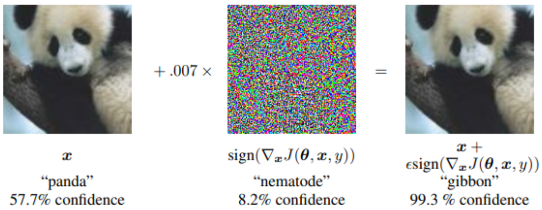


(a) Original Image (b) Explaining *Electric guitar* (c) Explaining *Acoustic guitar* (d) Explaining *Labrador*

Principle [Ribeiro et al., 2016]

- The image to interpret is segmented in homogeneous super-pixels.
- Generate perturbed samples where only some super-pixels contain the image information the other being replaced by their average value.
- Estimate weights for the perturbed samples with a kernel.
- Perform Ridge regression trying to predict the output of model f on the perturbed samples from the binary activation of the super-pixels: the weights give the importance of the superpixels in the decision.
- When LS is used instead of Ridge we recover SHAP [Lundberg and Lee, 2017].
- Python implementation in ELI5: https://eli5.readthedocs.io/

Adversarial attacks



Principle [Goodfellow et al., 2014]

- A model that generalizes should be robust to small perturbation of the samples.
- Adversarial attacks search for samples $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{p}$ close to the true sample $\mathbf{x}$ of label y that maximize the change in the prediction of the model f :

$$\max_{\tilde{\mathbf{x}}, \|\mathbf{x}-\tilde{\mathbf{x}}\| \leq \epsilon} L(y, f(\tilde{\mathbf{x}})), \quad \text{or,} \quad \max_{\tilde{\mathbf{x}}, \|\mathbf{x}-\tilde{\mathbf{x}}\| \leq \epsilon} L(f(\mathbf{x}), f(\tilde{\mathbf{x}})) \tag{1}$$

- Virtual Adversary (right) does not require the true label [Miyato et al., 2018].
- Adversarial examples can be used for manipulating the output of a model [Brown et al., 2017], for evaluating its robustness and for regularization.
- Python implementation : https://adversarial-robustness-toolbox.readthedocs.io/

Interpretability and explainability

Main approaches

- Linear models and sparsity (Lasso)
- Global agnostic models
  - Partial Dependence Plot [Goldstein et al., 2015]
  - Feature permutation importance [Breiman, 2001]
- Local approximation (smooth)
  - Linear local approximation [Erhan et al., 2009, Shrikumar et al., 2017].
  - Integrated gradients [Sundararajan et al., 2017]
- Local model agnostic methods
  - Game theory: Shapley [Strumbelj and Kononenko, 2014], SHAP [Lundberg and Lee, 2017]
  - LIME [Ribeiro et al., 2016]
- By design of the model (attention mechanism [Vaswani et al., 2017])

References

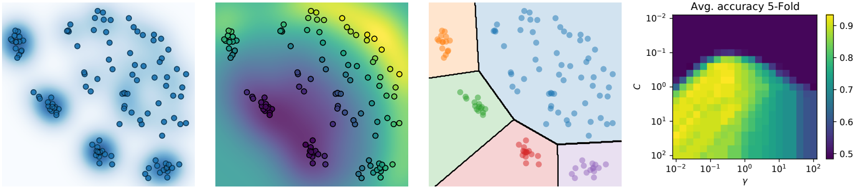
- Free book [Molnar, 2020]: https://christophm.github.io/interpretable-ml-book/
- Recent tutorial: https://explainml-tutorial.github.io/

Python toolboxes

- Interpretability: https://eli5.readthedocs.io/
- Adversarial robustness: https://adversarial-robustness-toolbox.readthedocs.io/

Section

Conclusion



Last words

- Know the data (visualize it, talk with experts, pre-process it).
- Know the problem (unsupervised, supervised, final goal).
- Know the methods (linear/nonlinear, trees, neural networks).
- Validate the methods and parameters (performance measure, cross-validation).
- Be critical with the model (interpretation, explainability, adversaries).

References

- Elements of statistical learning (free PDF online) [Friedman et al., 2001].
- Pattern recognition and machine learning [Bishop Christopher et al., 2006].
- Machine learning: a probabilistic perspective [Murphy, 2012].

Go practice !

M2 DS : Data Camp (required course)

- Application of ML methods and data analysis on a real challenge.
- Part 1 : Data Challenge.
- Part 2 : Building a workflow.
- Jupyter notebooks and leaderboard : https://www.ramp.studio/.

MAP670T : Data Challenge NLP for Finance

- Objective : Predicting variation in stock value using textual data.
- Data : BCE statements and other sources of financial data.
- Dates : From February 19, 2022 to March 31, 2022 (3 full days meetings).
- Competition + 5 pages reports (2.5 ECTS).
- Sponsored by Chaire BAFB in collaboration with Natixis.

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