Tree models with Scikit-Learn

Great learners with little assumptions

Material: https://github.com/glouppe/talk-pydata2015

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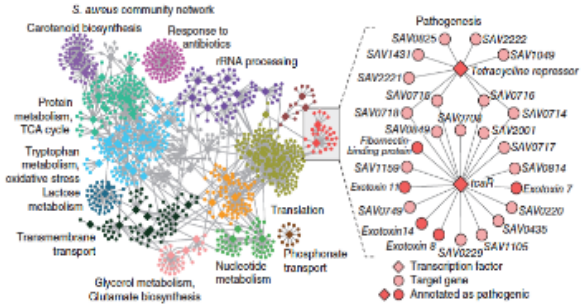
CERN

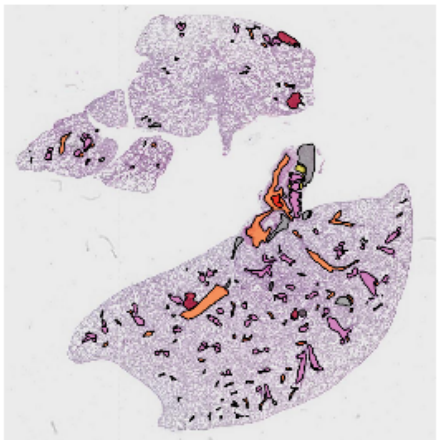
PyData, April 3, 2015

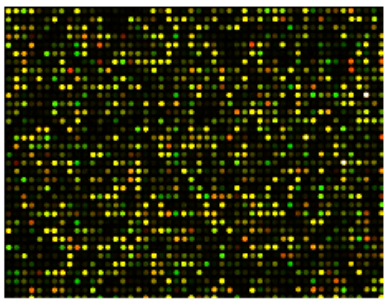
Outline

Motivation

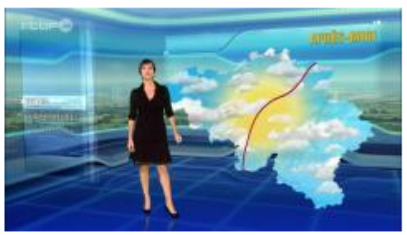

CERN


S. aureus community network
Carotenoid biosynthesis
Response to antibiotics
rRNA processing
Protein metabolism, TCA cycle
Tryptophan metabolism, oxidative stress
Lactose metabolism
Translation
Transmembrane transport
Nucleotide metabolism
Phosphonate transport
Glycerol metabolism, Glutamate biosynthesis
Pathogenesis
SAV1625
SAV2222
SAV1431
SAV1049
SAV2221
Tetracycline repressor
SAV0716
SAV0714
SAV0718
SAV2001
SAV0717
SAV0814
SAV1159
Exotoxin 7
SAV0220
SAV0435
Exotoxin 14
SAV1105
Exotoxin 8
SAV0229
Transcription factor
Target gene
Annotated as pathogenic






XBOX 360




Google
Google Search
I'm Feeling Lucky

Running example

From **physicochemical properties** (alcohol, acidity, sulphates, ...),

learn a **model**

to predict **wine taste preferences**.

Outline

Supervised learning

- Data comes as a finite learning set $\mathcal{L} = (\mathtt{X}, \mathtt{y})$ where
  - Input samples are given as an array of shape `(n_samples, n_features)`

    E.g., feature values for wine physicochemical properties:

    ```
    # fixed acidity, volatile acidity, ...
    X = [[  7.4    0.      ...   0.56   9.4    0.  ]
         [  7.8    0.      ...   0.68   9.8    0.  ]
                           ...
         [  7.8    0.04    ...   0.65   9.8    0.  ]]
    ```

  - Output values are given as an array of shape `(n_samples,)`

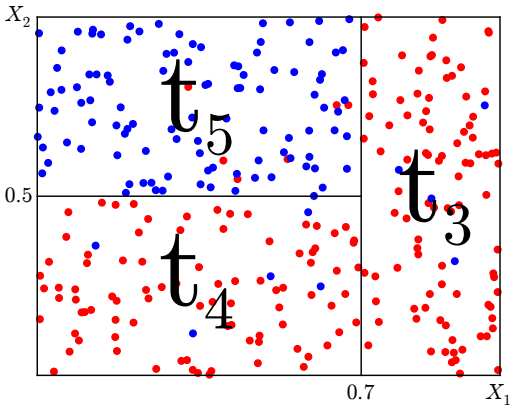
    E.g., wine taste preferences (from 0 to 10):

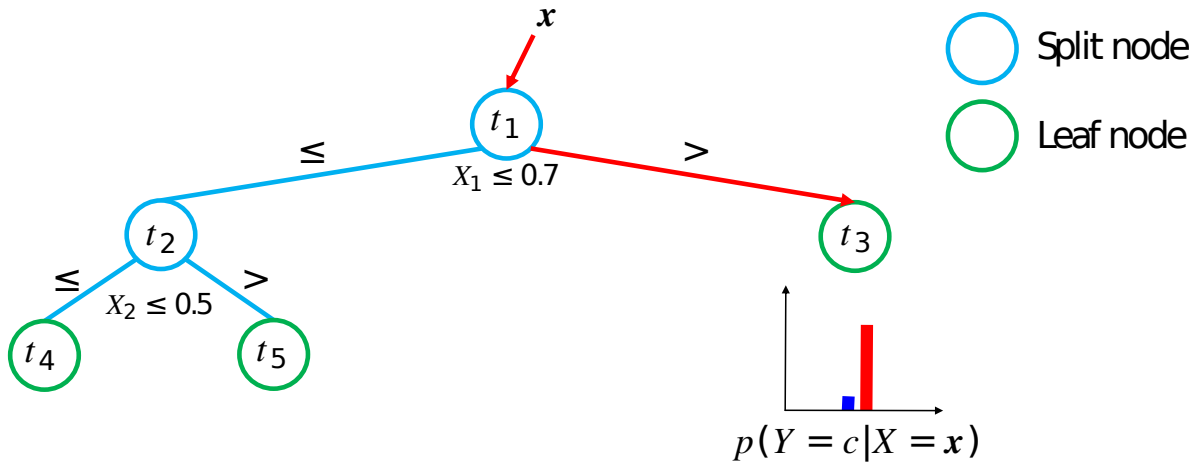
    ```
    y = [5 5 5 ... 6 7 6]
    ```

- The goal is to build an estimator $\varphi_{\mathcal{L}} : \mathcal{X} \mapsto \mathcal{y}$ minimizing

$$Err(\varphi_{\mathcal{L}}) = \mathbb{E}_{X,Y}\{L(Y, \varphi_{\mathcal{L}}.\mathtt{predict}(X))\}.$$

Decision trees (Breiman et al., 1984)





function BUILDDECISIONTREE($\mathcal{L}$)
    Create node t
    if the stopping criterion is met for t **then**
        Assign a model to $\widehat{y}_t$
    else
        Find the split on $\mathcal{L}$ that maximizes impurity decrease

$$s^* = \arg\max_s i(t) - p_L i(t_L^s) - p_R i(t_R^s)$$

        Partition $\mathcal{L}$ into $\mathcal{L}_{t_L} \cup \mathcal{L}_{t_R}$ according to s^*
        $t_L =$ BUILDDECISIONTREE($\mathcal{L}_{t_L}$)
        $t_R =$ BUILDDECISIONTREE($\mathcal{L}_{t_R}$)
    end if
    return t
end function

Composability of decision trees

Decision trees can be used to solve several machine learning tasks by swapping the impurity and leaf model functions:

0-1 loss (classification)

$\widehat{y}_t = \arg\max_{c \in \mathcal{Y}} p(c|t)$, $i(t) = \text{entropy}(t)$ or $i(t) = \text{gini}(t)$

Mean squared error (regression)

$\widehat{y}_t = \text{mean}(y|t)$, $i(t) = \frac{1}{N_t} \sum_{\mathbf{x}, y \in \mathcal{L}_t} (y - \widehat{y}_t)^2$

Least absolute deviance (regression)

$\widehat{y}_t = \text{median}(y|t)$, $i(t) = \frac{1}{N_t} \sum_{\mathbf{x}, y \in \mathcal{L}_t} |y - \widehat{y}_t|$

Density estimation

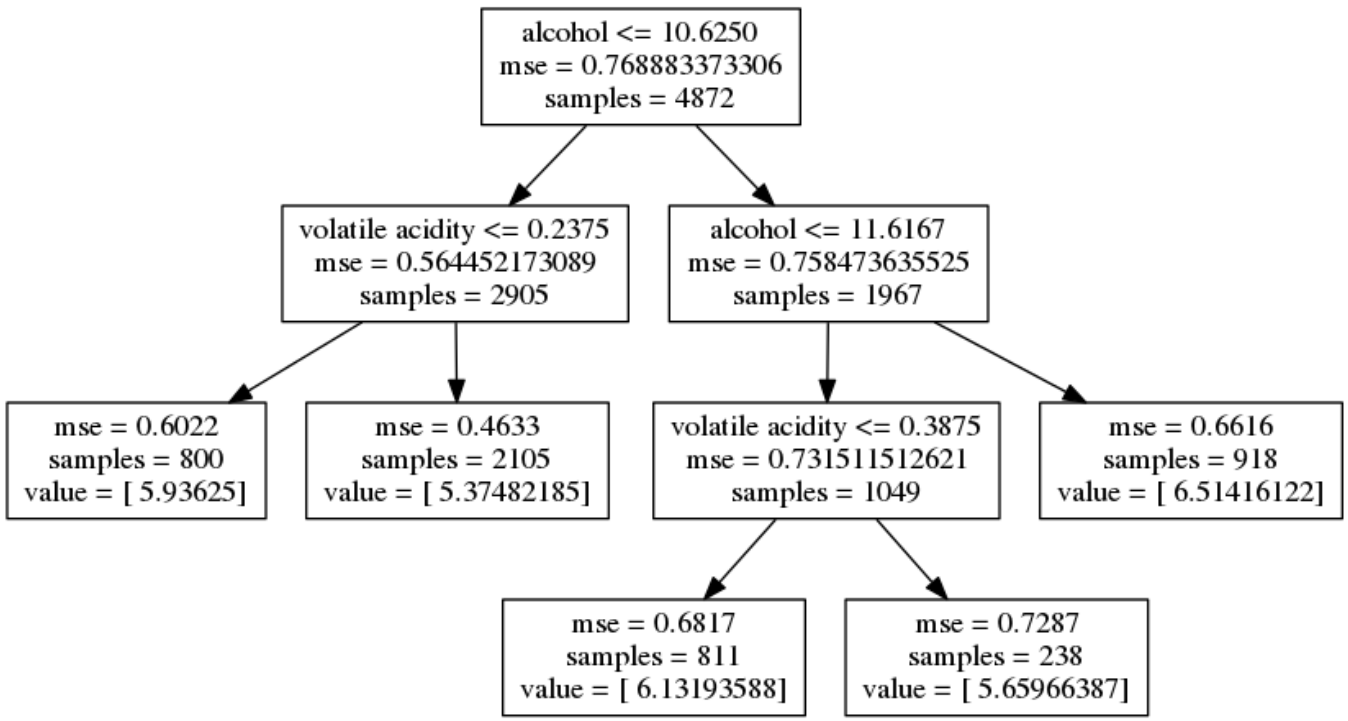
$\widehat{y}_t = \mathcal{N}(\mu_t, \Sigma_t)$, $i(t) = \text{differential entropy}(t)$

sklearn.tree

```
# Fit a decision tree
from sklearn.tree import DecisionTreeRegressor
estimator = DecisionTreeRegressor(criterion="mse",    # Set i(t) function
                                  max_leaf_nodes=5)   # Tune model complexity
                                                      # with max_leaf_nodes,
                                                      # max_depth or
                                                      # min_samples_split

estimator.fit(X_train, y_train)

# Predict target values
y_pred = estimator.predict(X_test)

# MSE on test data
from sklearn.metrics import mean_squared_error
score = mean_squared_error(y_test, y_pred)
>>> 0.572049826453
```

Visualize and interpret

```
# Display tree
from sklearn.tree import export_graphviz
export_graphviz(estimator, out_file="tree.dot",
                feature_names=feature_names)
```

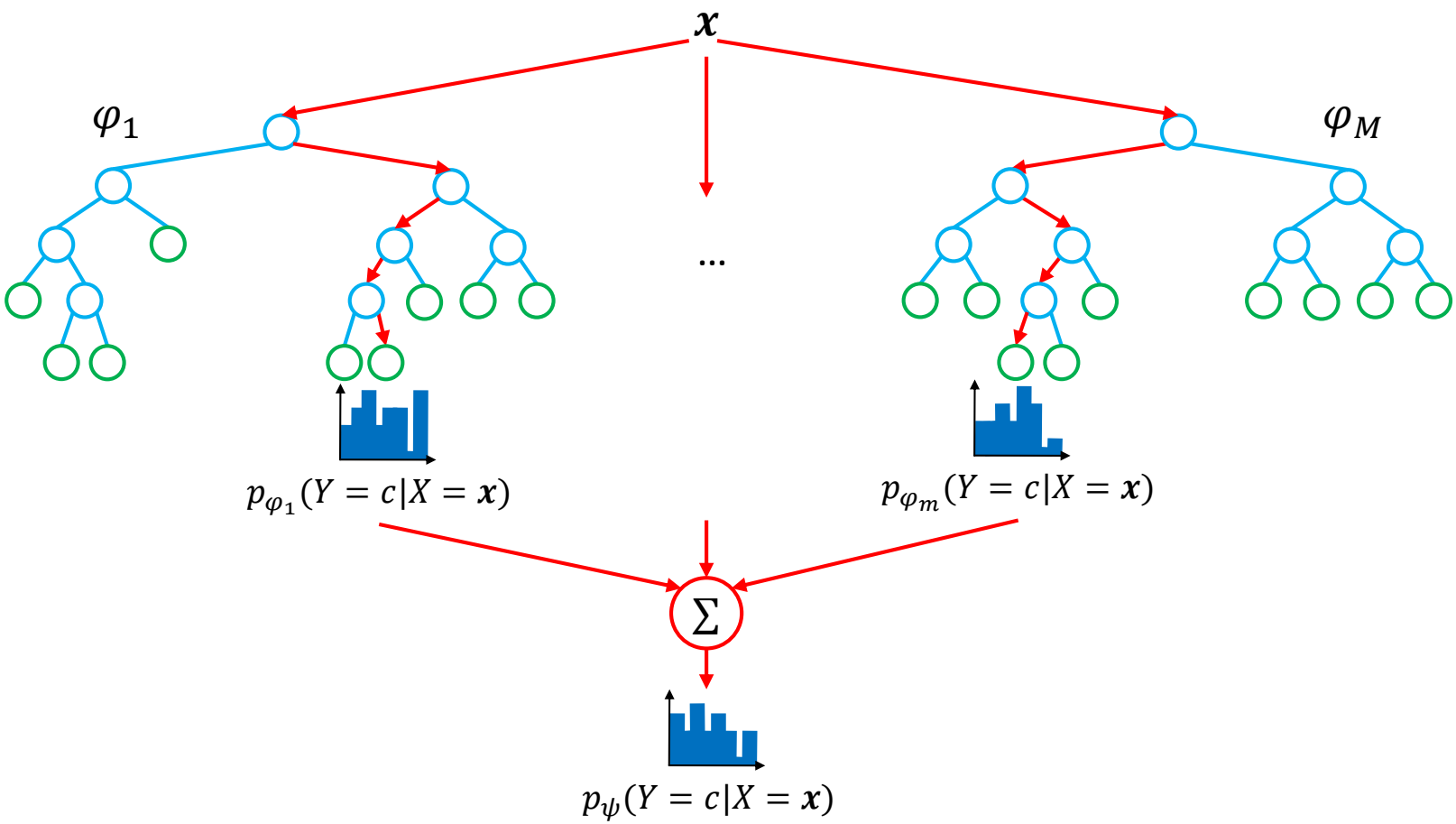


Strengths and weaknesses of decision trees

- Non-parametric model, proved to be consistent.
- Support heterogeneous data (continuous, ordered or categorical variables).
- Flexibility in loss functions (but choice is limited).
- Fast to train, fast to predict.
  - In the average case, complexity of training is $\Theta(pN \log^2 N)$.
- Easily interpretable.
- Low bias, but usually high variance
  - Solution: Combine the predictions of several randomized trees into a single model.

Outline

Random Forests (Breiman, 2001; Geurts et al., 2006)



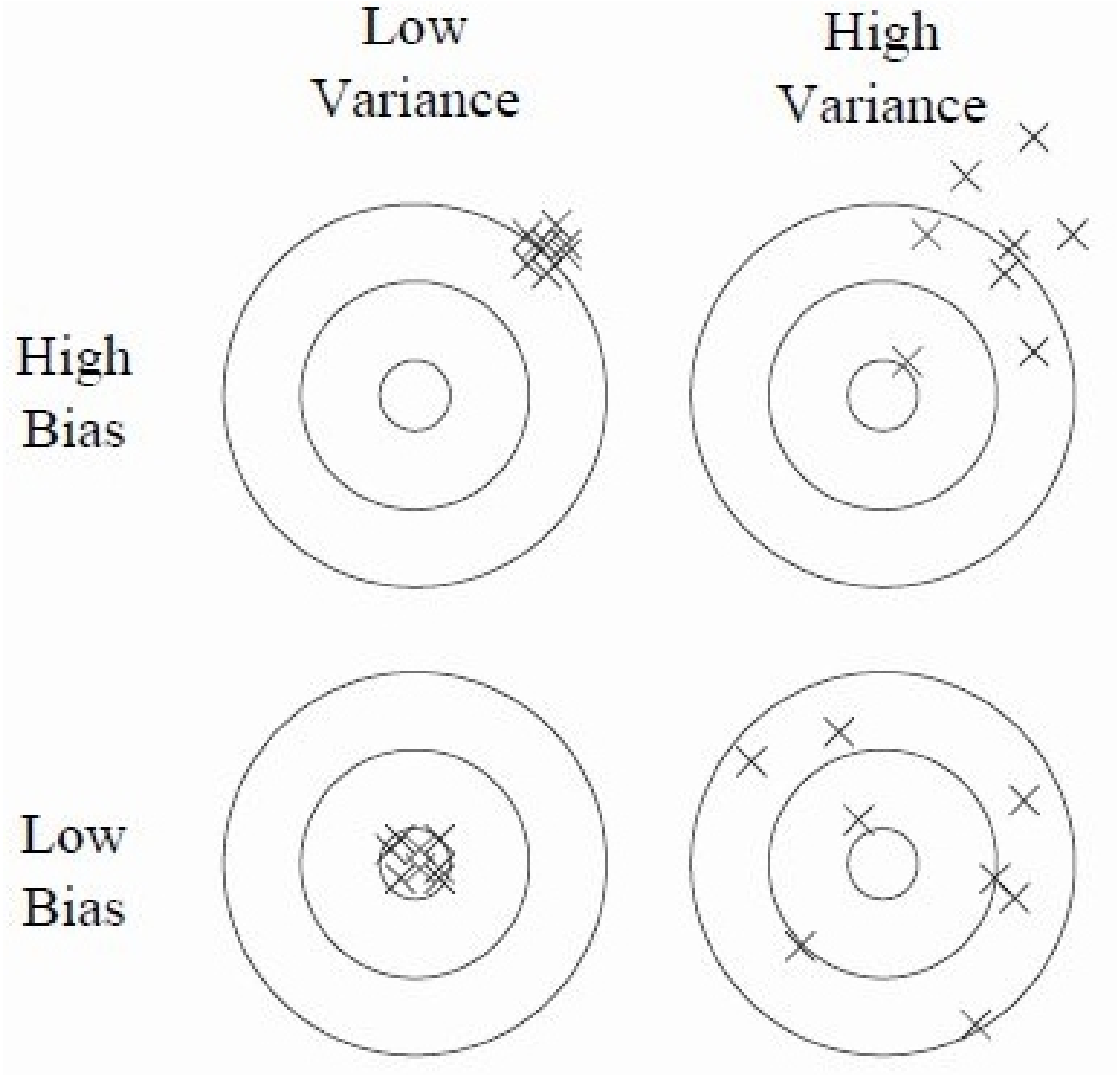
Randomization

- Bootstrap samples
- Random selection of $K \leqslant p$ split variables
- Random selection of the threshold

} Random Forests

} Extra-Trees

Bias and variance



Bias-variance decomposition

Theorem. For the squared error loss, the bias-variance decomposition of the expected generalization error $\mathbb{E}_{\mathcal{L}}\{Err(\psi_{\mathcal{L},\theta_1,\ldots,\theta_M}(\mathbf{x}))\}$ at $X = \mathbf{x}$ of an ensemble of M randomized models $\varphi_{\mathcal{L},\theta_m}$ is

$$\mathbb{E}_{\mathcal{L}}\{Err(\psi_{\mathcal{L},\theta_1,\ldots,\theta_M}(\mathbf{x}))\} = \text{noise}(\mathbf{x}) + \text{bias}^2(\mathbf{x}) + \text{var}(\mathbf{x}),$$

where

$$\begin{aligned}
\text{noise}(\mathbf{x}) &= Err(\varphi_B(\mathbf{x})), \\
\text{bias}^2(\mathbf{x}) &= (\varphi_B(\mathbf{x}) - \mathbb{E}_{\mathcal{L},\theta}\{\varphi_{\mathcal{L},\theta}(\mathbf{x})\})^2, \\
\text{var}(\mathbf{x}) &= \rho(\mathbf{x})\sigma^2_{\mathcal{L},\theta}(\mathbf{x}) + \frac{1-\rho(\mathbf{x})}{M}\sigma^2_{\mathcal{L},\theta}(\mathbf{x}).
\end{aligned}$$

and where $\rho(\mathbf{x})$ is the Pearson correlation coefficient between the predictions of two randomized trees built on the same learning set.

Diagnosing the error of random forests (Louppe, 2014)

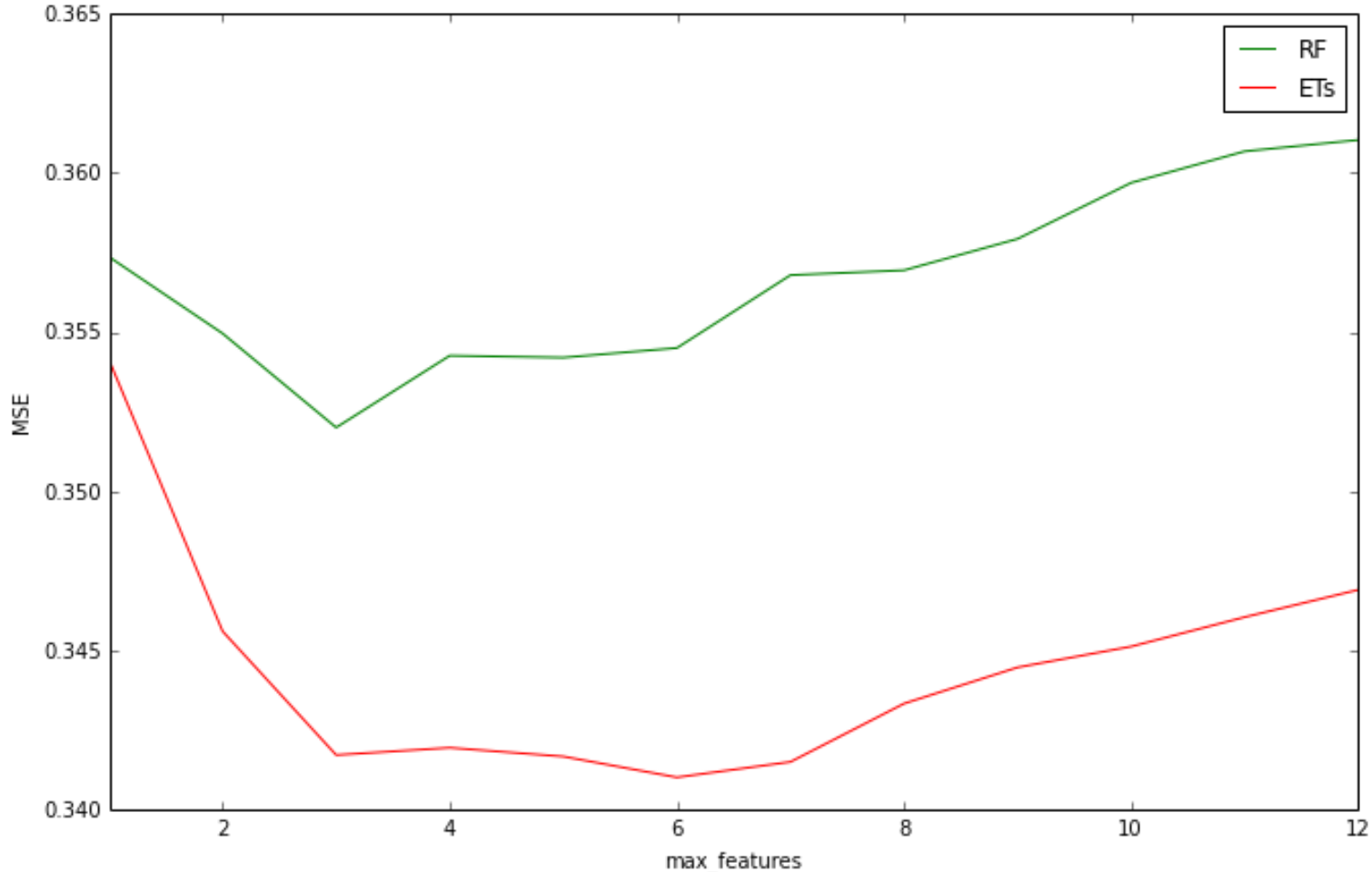
- Bias: Identical to the bias of a single randomized tree.
- Variance: $\text{var}(\mathbf{x}) = \rho(\mathbf{x})\sigma^2_{\mathcal{L},\theta}(\mathbf{x}) + \frac{1-\rho(\mathbf{x})}{M}\sigma^2_{\mathcal{L},\theta}(\mathbf{x})$
  As $M \to \infty$, $\text{var}(\mathbf{x}) \to \rho(\mathbf{x})\sigma^2_{\mathcal{L},\theta}(\mathbf{x})$
  - The stronger the randomization, $\rho(\mathbf{x}) \to 0$, $\text{var}(\mathbf{x}) \to 0$.
  - The weaker the randomization, $\rho(\mathbf{x}) \to 1$, $\text{var}(\mathbf{x}) \to \sigma^2_{\mathcal{L},\theta}(\mathbf{x})$

Bias-variance trade-off. Randomization increases bias but makes it possible to reduce the variance of the corresponding ensemble model. The crux of the problem is to find the right trade-off.

Tuning randomization in sklearn.ensemble

```
from sklearn.ensemble import RandomForestRegressor, ExtraTreesRegressor
from sklearn.cross_validation import ShuffleSplit
from sklearn.learning_curve import validation_curve

# Validation of max_features, controlling randomness in forests
param_name = "max_features"
param_range = range(1, X.shape[1]+1)

for Forest, color, label in [(RandomForestRegressor, "g", "RF"),
                             (ExtraTreesRegressor, "r", "ETs")]:
    _, test_scores = validation_curve(
        Forest(n_estimators=100, n_jobs=-1), X, y,
        cv=ShuffleSplit(n=len(X), n_iter=10, test_size=0.25),
        param_name=param_name, param_range=param_range,
        scoring="mean_squared_error")
    test_scores_mean = np.mean(-test_scores, axis=1)
    plt.plot(param_range, test_scores_mean, label=label, color=color)

plt.xlabel(param_name)
plt.xlim(1, max(param_range))
plt.ylabel("MSE")
plt.legend(loc="best")
plt.show()
```

Tuning randomization in `sklearn.ensemble`



Best-tradeoff: ExtraTrees, for `max_features=6`.

Strengths and weaknesses of forests

- One of the best off-the-self learning algorithm, requiring almost no tuning.
- Fine control of bias and variance through averaging and randomization, resulting in better performance.
- Moderately fast to train and to predict.
  - $\Theta(MK\widetilde{N}\log^2\widetilde{N})$ for RFs (where $\widetilde{N} = 0.632N$)
  - $\Theta(MKN\log N)$ for ETs
- Embarrassingly parallel (use `n_jobs`).
- Less interpretable than decision trees.

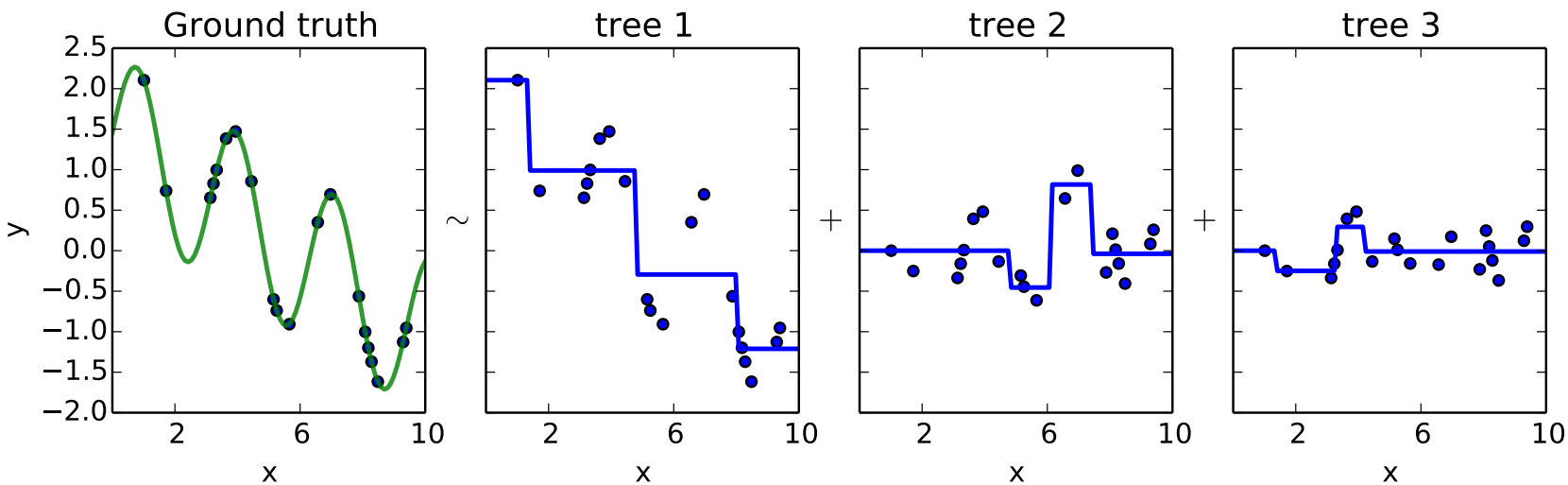
Outline

Gradient Boosted Regression Trees (Friedman, 2001)

- GBRT fits an additive model of the form

$$\varphi(x) = \sum_{m=1}^{M} \gamma_m h_m(x)$$

- The ensemble is built in a forward stagewise manner, where each regression tree h_m is an approximate successive gradient step.



Careful tuning required

```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.cross_validation import ShuffleSplit
from sklearn.grid_search import GridSearchCV

# Careful tuning is required to obtained good results
param_grid = {"learning_rate": [0.1, 0.01, 0.001],
              "subsample": [1.0, 0.9, 0.8],
              "max_depth": [3, 5, 7],
              "min_samples_leaf": [1, 3, 5]}

est = GradientBoostingRegressor(n_estimators=1000)
grid = GridSearchCV(est, param_grid,
                    cv=ShuffleSplit(n=len(X), n_iter=10, test_size=0.25),
                    scoring="mean_squared_error",
                    n_jobs=-1).fit(X, y)

gbrt = grid.best_estimator_
```

See our PyData 2014 tutorial for further guidance

https://github.com/pprett/pydata-gbrt-tutorial

Strengths and weaknesses of GBRT

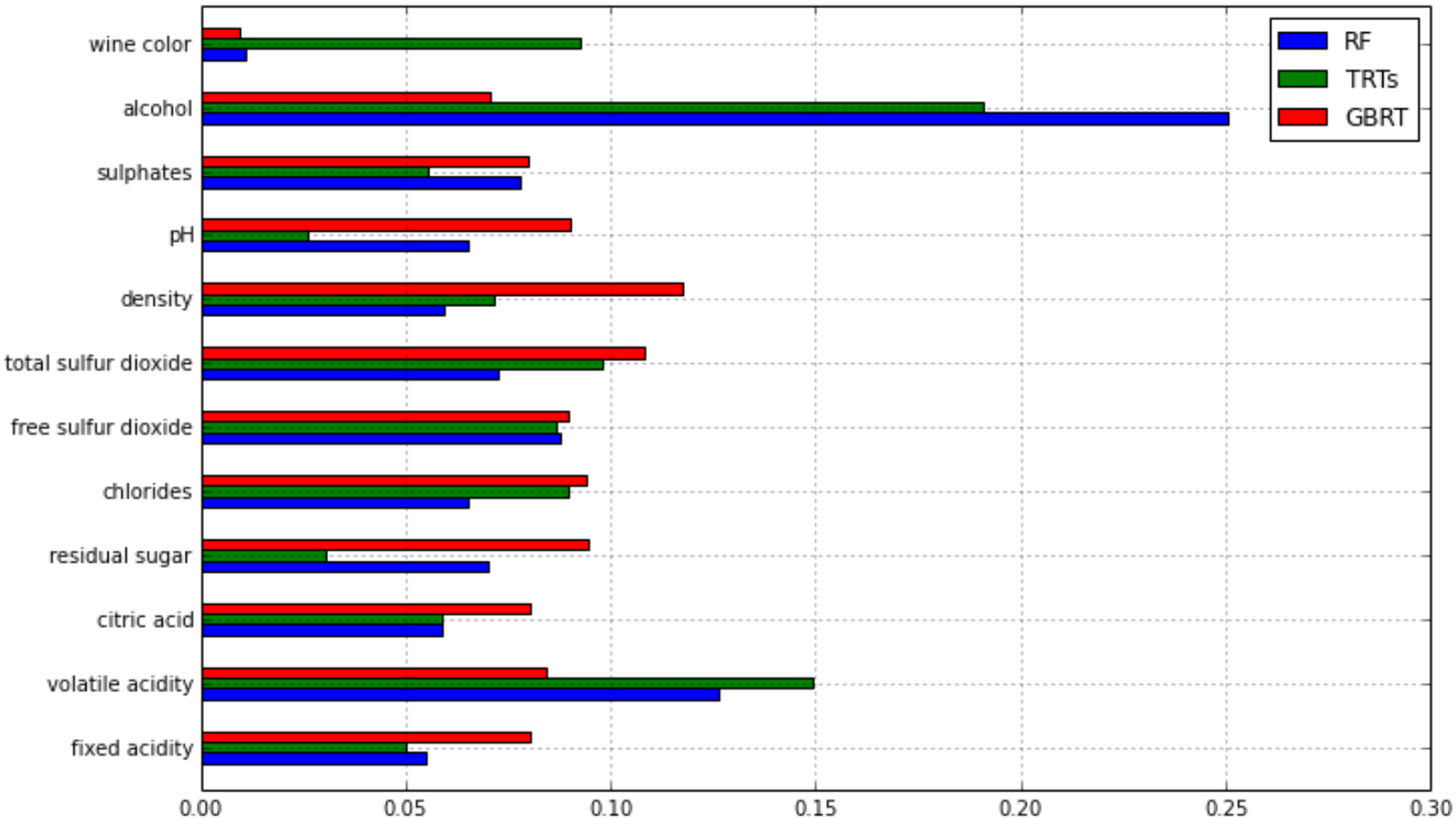
- Flexible framework, that can adapt to arbitrary loss functions.
- Fine control of under/overfitting through regularization (e.g., learning rate, subsampling, tree structure, penalization term in the loss function, etc).
- Careful tuning required.
- Slow to train, fast to predict.

Outline

Variable importances

```
importances = pd.DataFrame()

# Variable importances with Random Forest, default parameters
est = RandomForestRegressor(n_estimators=10000, n_jobs=-1).fit(X, y)
importances["RF"] = pd.Series(est.feature_importances_,
                              index=feature_names)

# Variable importances with Totally Randomized Trees
est = ExtraTreesRegressor(max_features=1, max_depth=3,
                          n_estimators=10000, n_jobs=-1).fit(X, y)
importances["TRTs"] = pd.Series(est.feature_importances_,
                                index=feature_names)

# Variable importances with GBRT
importances["GBRT"] = pd.Series(gbrt.feature_importances_,
                                index=feature_names)

importances.plot(kind="barh")
```

Variable importances

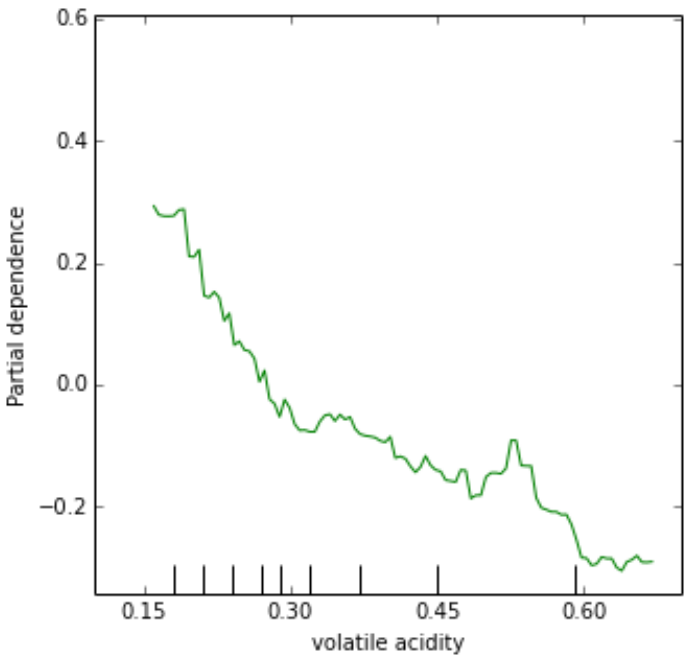


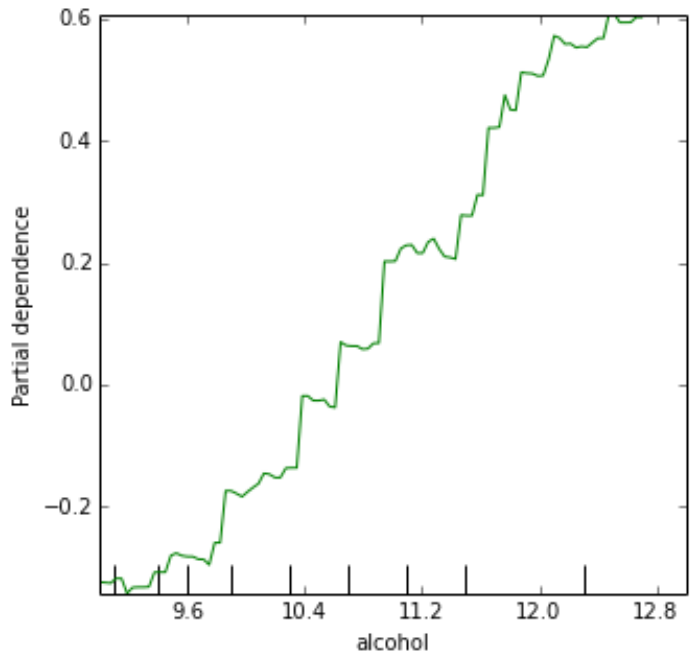
Importances are measured only through the eyes of the model. They may not tell the entire nor the same story! (Louppe et al., 2013)

Partial dependence plots

Relation between the response Y and a subset of features, marginalized over all other features.

```
from sklearn.ensemble.partial_dependence import plot_partial_dependence
plot_partial_dependence(gbrt, X,
                        features=[1, 10], feature_names=feature_names)
```

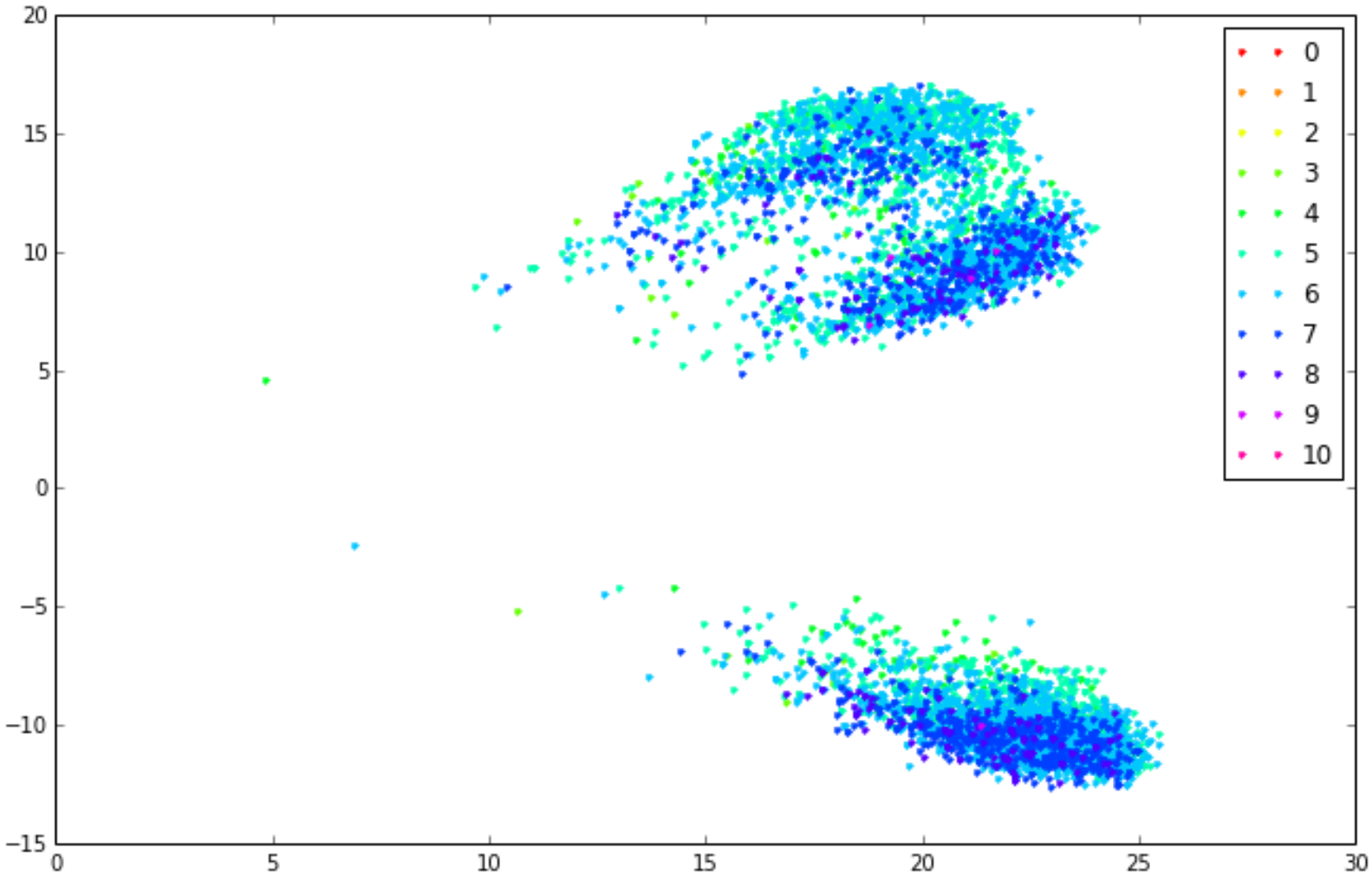




Embedding

```
from sklearn.ensemble import RandomTreesEmbedding
from sklearn.decomposition import TruncatedSVD

# Project wines through a forest of totally randomized trees
# and use the leafs the samples end into as a high-dimensional representation
hasher = RandomTreesEmbedding(n_estimators=1000)
X_transformed = hasher.fit_transform(X)

# Plot wines on a plane using the 2 principal components
svd = TruncatedSVD(n_components=2)
coords = svd.fit_transform(X_transformed)

n_values = 10 + 1  # Wine preferences are from 0 to 10
cm = plt.get_cmap("hsv")
colors =  (cm(1. * i / n_values) for i in range(n_values))

for k, c in zip(range(n_values), colors):
    plt.plot(coords[y == k, 0], coords[y == k, 1], '.', label=k, color=c)

plt.legend()
plt.show()
```

Embedding



Can you guess what these 2 clusters correspond to?

Outline

Summary

- Tree-based methods offer a flexible and efficient non-parametric framework for classification and regression.
- Applicable to a wide variety of problems, with a fine control over the model that is learned.
- Assume a good feature representation – i.e., tree-based methods are often not that good on very raw input data, like pixels, speech signals, etc.
- Insights on the problem under study (variable importances, dependence plots, embedding, ...).
- Efficient implementation in Scikit-Learn.

Join us on
https://github.com/
scikit-learn/scikit-learn

References

Breiman, L. (2001). Random Forests. *Machine learning*, 45(1):5–32.

Breiman, L., Friedman, J. H., Olshen, R. A., and Stone, C. J. (1984). *Classification and regression trees*.

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