Supervised Learning

Tree-based methods

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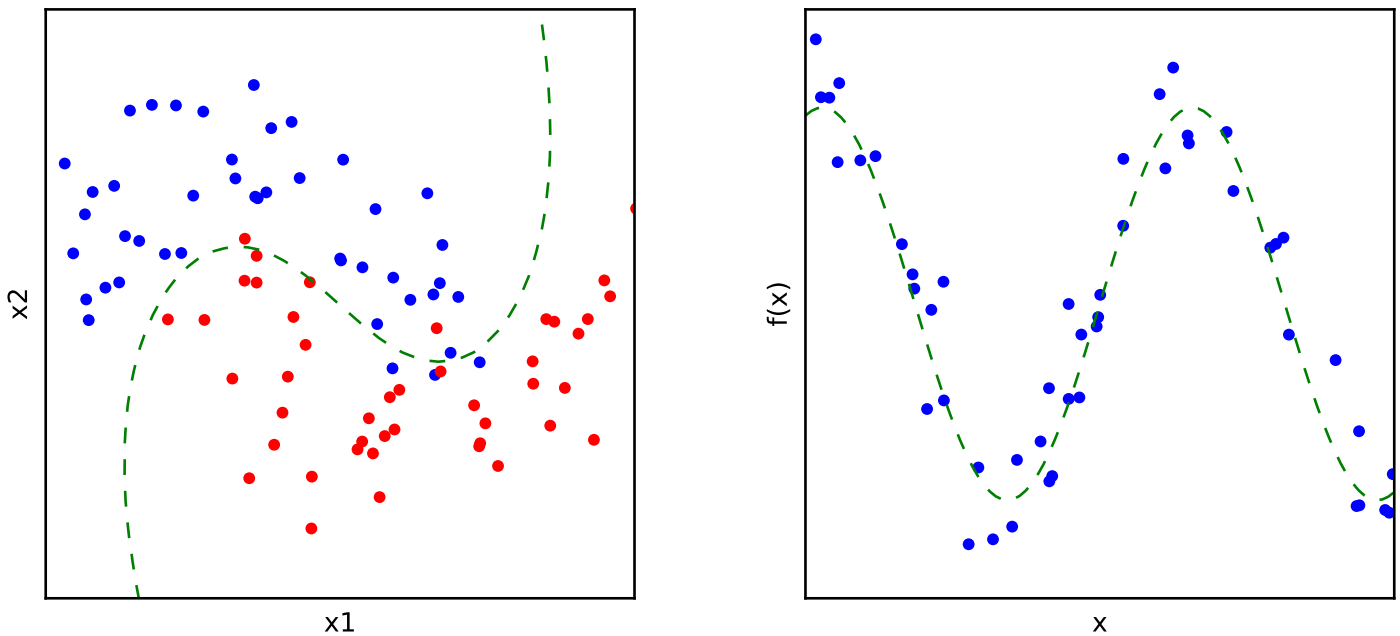
Outline

Problem statement



Classification vs. regression

Running example

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

learn a **model**

to predict **wine taste preferences**.

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,)`

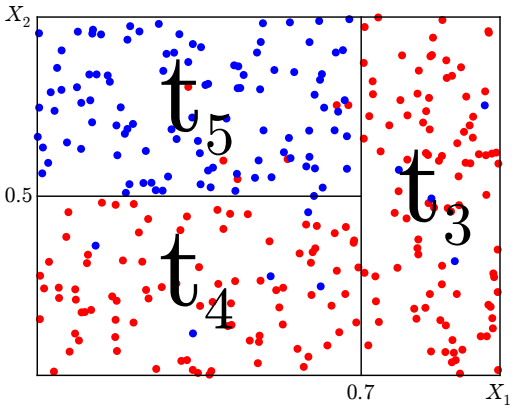
    E.g., wine taste preferences (from 0 to 10):

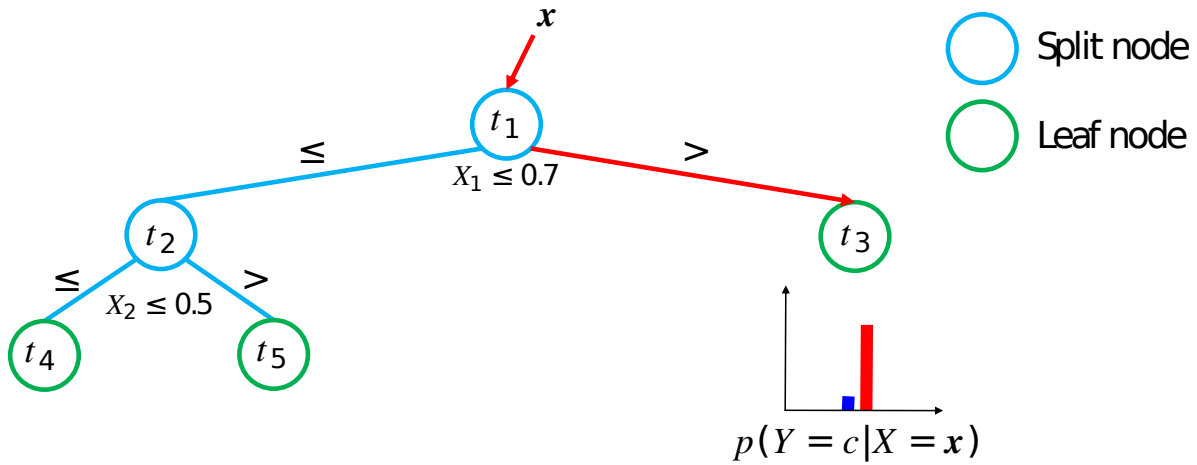
```
y = [5 5 5 ... 6 7 6]
```

- The goal is to build an estimator $f : \mathcal{X} \mapsto \mathcal{Y}$ minimizing

$$Err(f) = \mathbb{E}_{X,Y}\{L(Y, f(X))\}.$$

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

(Demo)

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

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

Sample weights

Sample weights can be accounted for by adapting the impurity and leaf model functions.

Weighted mean squared error

$\widehat{y}_t = \frac{1}{\sum_w w} \sum_{\mathbf{x},y,w \in \mathcal{L}_t} wy$

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

Weights are assumed to be non-negative since these quantities may otherwise be undefined. (E.g., what if $\sum_w w < 0$?)

sklearn.tree

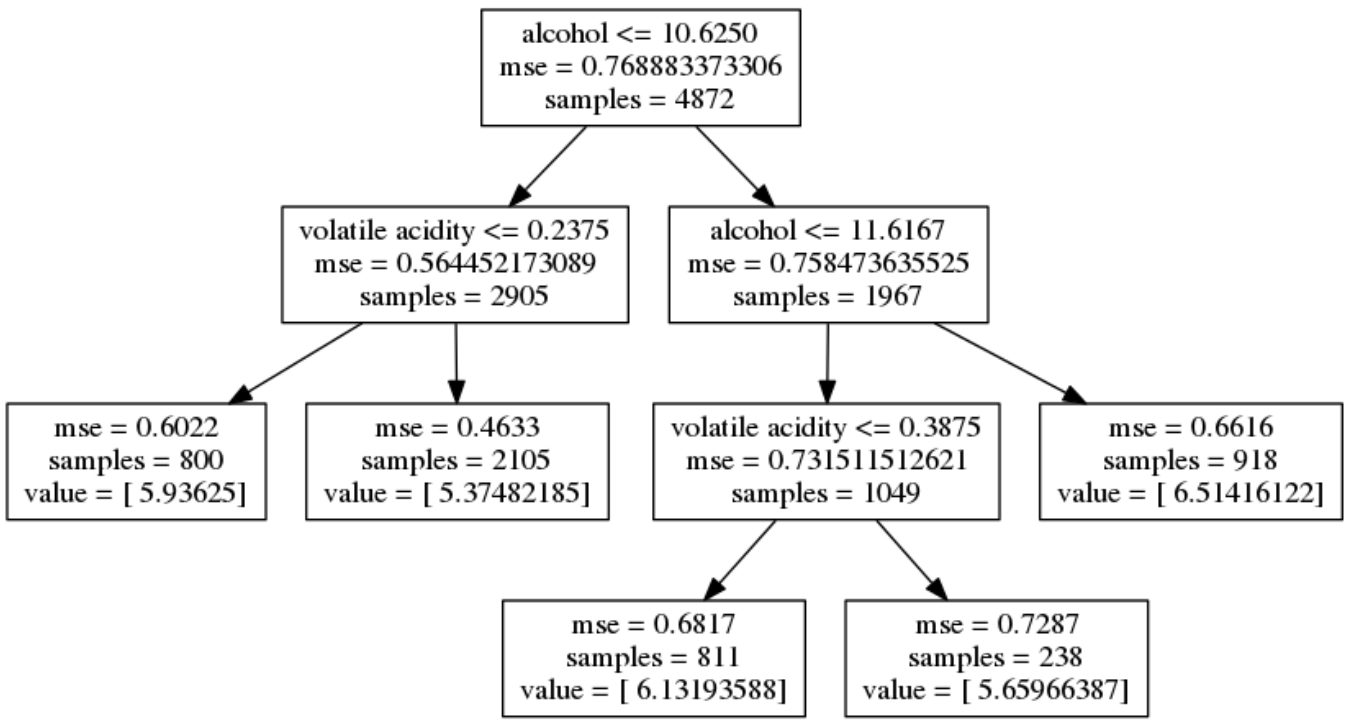
```
# Fit a decision tree
from sklearn.tree import DecisionTreeRegressor
estimator = DecisionTreeRegressor(criterion="mse",    # Set i(t) function
                                  max_leaf_nodes=5)
estimator.fit(X_train, y_train)

# 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

Bias-variance decomposition in regression

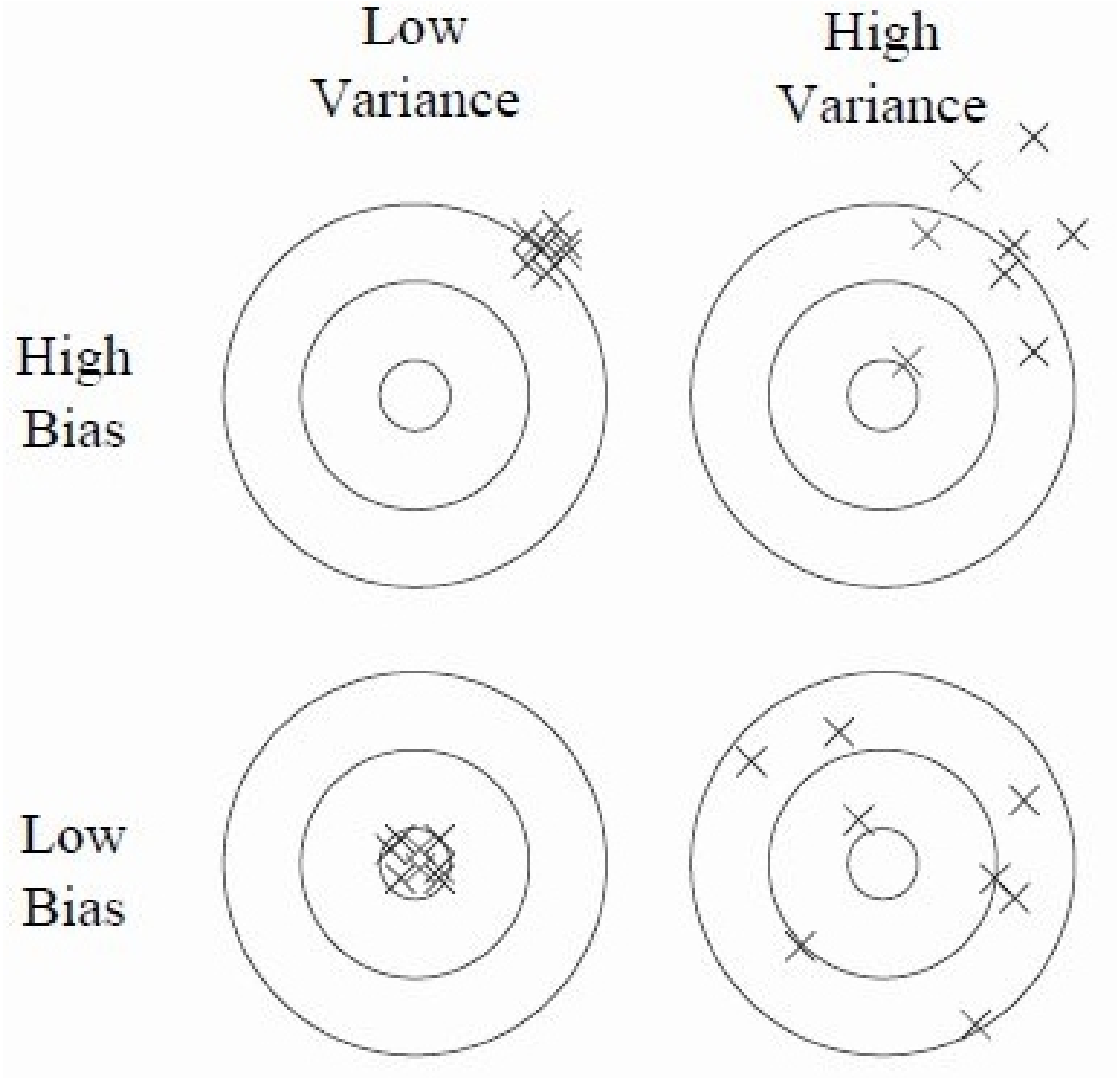
Theorem. For the *squared error loss*, the bias-variance decomposition of the expected generalization error at $X = \mathbf{x}$ is

$$\mathbb{E}_{\mathcal{L}}\{Err(f_{\mathcal{L}}(\mathbf{x}))\} = \text{noise}(\mathbf{x}) + \text{bias}^2(\mathbf{x}) + \text{var}(\mathbf{x})$$

where

$$\begin{aligned}
\text{noise}(\mathbf{x}) &= Err(f_B(\mathbf{x})), \\
\text{bias}^2(\mathbf{x}) &= (f_B(\mathbf{x}) - \mathbb{E}_{\mathcal{L}}\{f_{\mathcal{L}}(\mathbf{x})\})^2, \\
\text{var}(\mathbf{x}) &= \mathbb{E}_{\mathcal{L}}\{(\mathbb{E}_{\mathcal{L}}\{f_{\mathcal{L}}(\mathbf{x})\} - f_{\mathcal{L}}(\mathbf{x}))^2\}.
\end{aligned}$$

Bias-variance decomposition

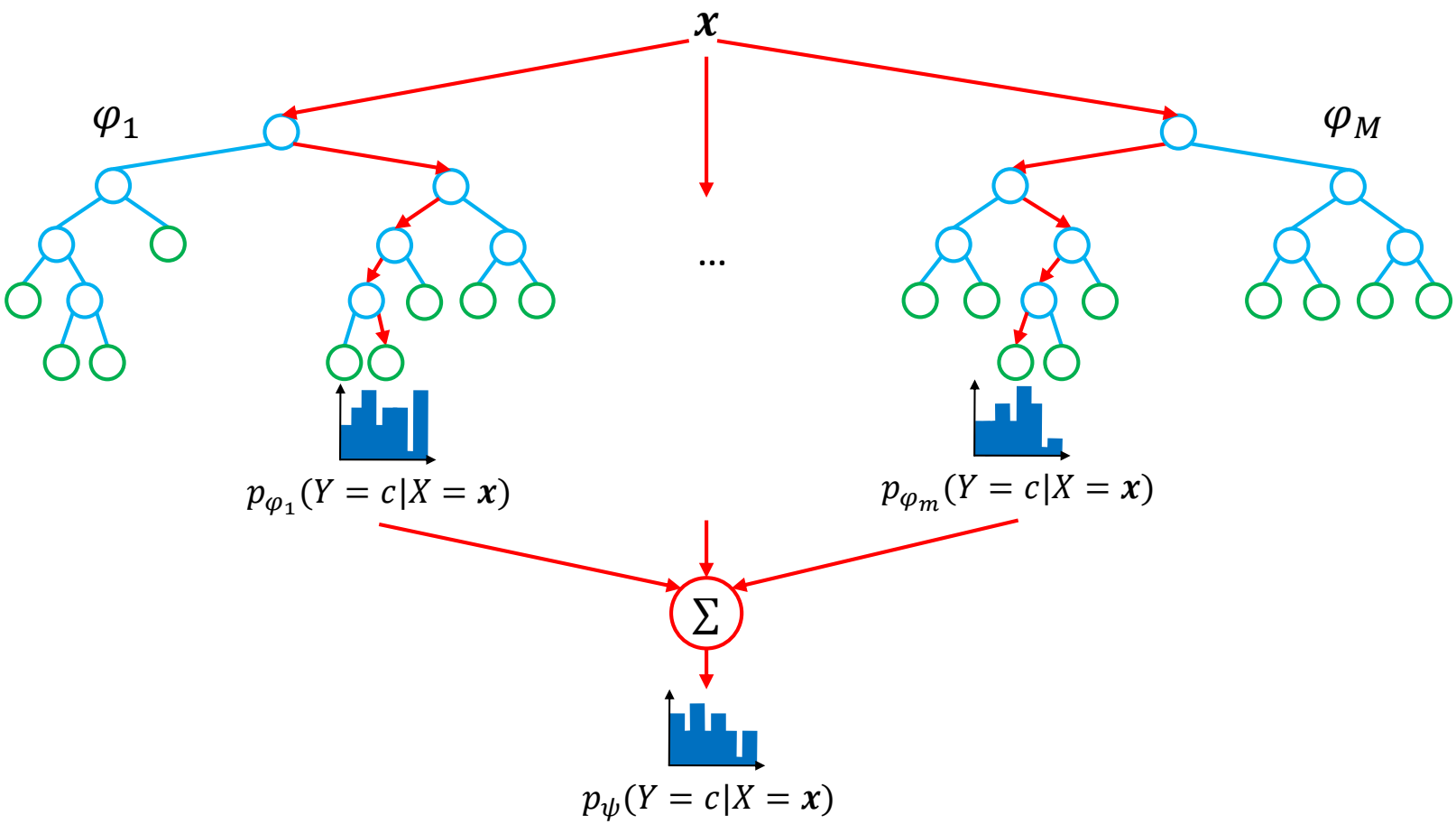


Diagnosing the generalization error of a decision tree

- (Residual error: Lowest achievable error, independent of $f_{\mathcal{L}}$.)
- Bias: Decision trees usually have low bias.
- Variance: They often suffer from high variance.

- Solution: *Combine the predictions of several randomized trees into a single model.*

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-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 $f_{\mathcal{L},\theta_m}$ 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

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

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

Interpretation of $\rho(\mathbf{x})$ (Louppe, 2014)

Theorem. $\rho(\mathbf{x}) = \frac{\mathbb{V}_{\mathcal{L}}\{\mathbb{E}_{\theta|\mathcal{L}}\{f_{\mathcal{L},\theta}(\mathbf{x})\}\}}{\mathbb{V}_{\mathcal{L}}\{\mathbb{E}_{\theta|\mathcal{L}}\{f_{\mathcal{L},\theta}(\mathbf{x})\}\}+\mathbb{E}_{\mathcal{L}}\{\mathbb{V}_{\theta|\mathcal{L}}\{f_{\mathcal{L},\theta}(\mathbf{x})\}\}}$

In other words, it is the ratio between

- the variance due to the learning set and
- the total variance, accounting for random effects due to both the learning set and the random perturbations.

$\rho(\mathbf{x}) \to 1$ when variance is mostly due to the learning set;
$\rho(\mathbf{x}) \to 0$ when variance is mostly due to the random perturbations;
$\rho(\mathbf{x}) \geqslant 0$.

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

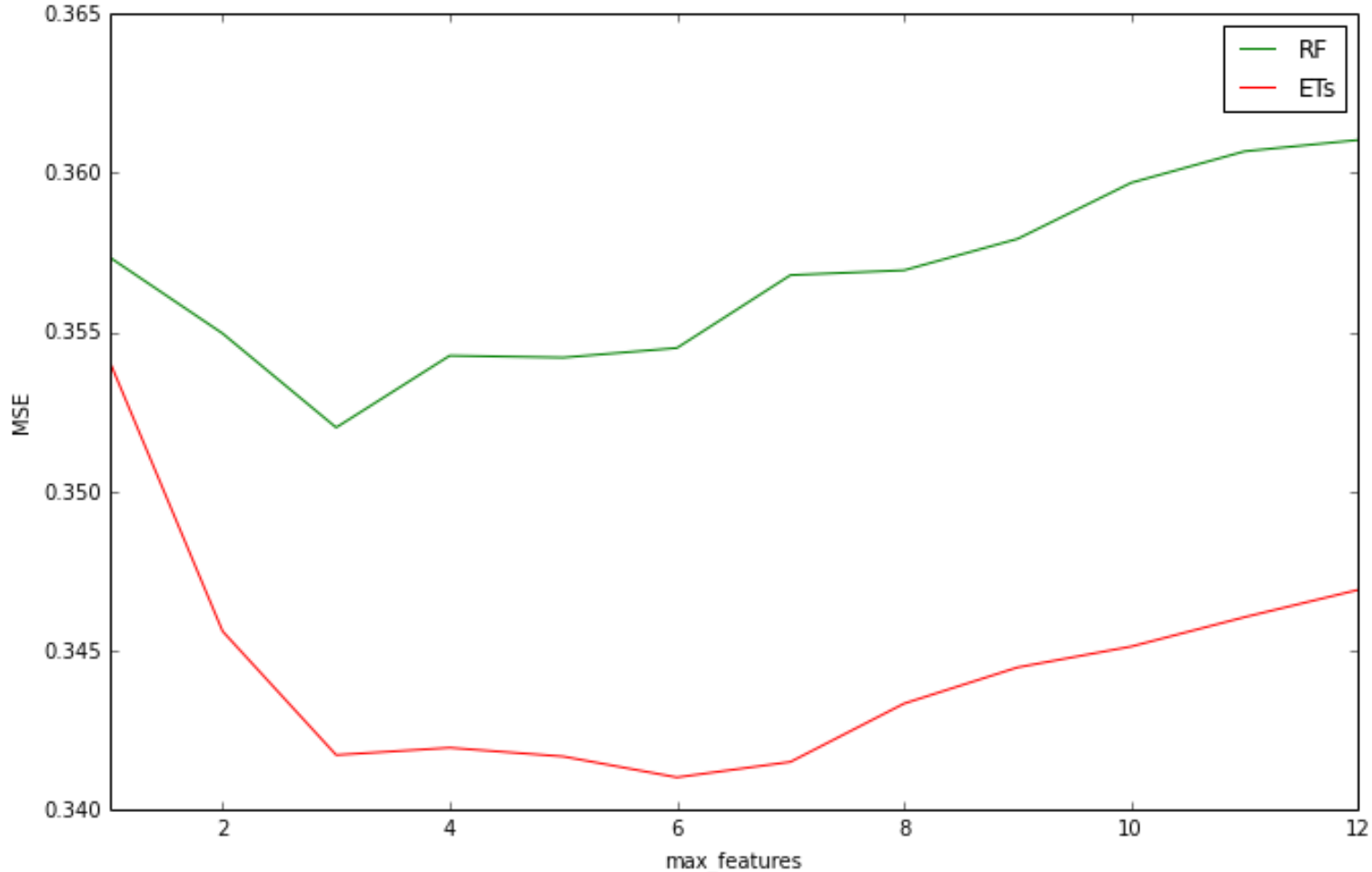
```
from sklearn.ensemble import RandomForestRegressor, ExtraTreesRegressor
from sklearn.cross_validation import ShuffleSplit
from sklearn.learning_curve import validation_curve

# Validation of max_features, controlling randomness in forests
param_range = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]

_, test_scores = validation_curve(
    RandomForestRegressor(n_estimators=100, n_jobs=-1), X, y,
    cv=ShuffleSplit(n=len(X), n_iter=10, test_size=0.25),
    param_name="max_features", 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="RF", color="g")

_, test_scores = validation_curve(
    ExtraTreesRegressor(n_estimators=100, n_jobs=-1), X, y,
    cv=ShuffleSplit(n=len(X), n_iter=10, test_size=0.25),
    param_name="max_features", 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="ETs", color="r")
```

Tuning randomization in `sklearn.ensemble`



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

Strengths and weaknesses of forests

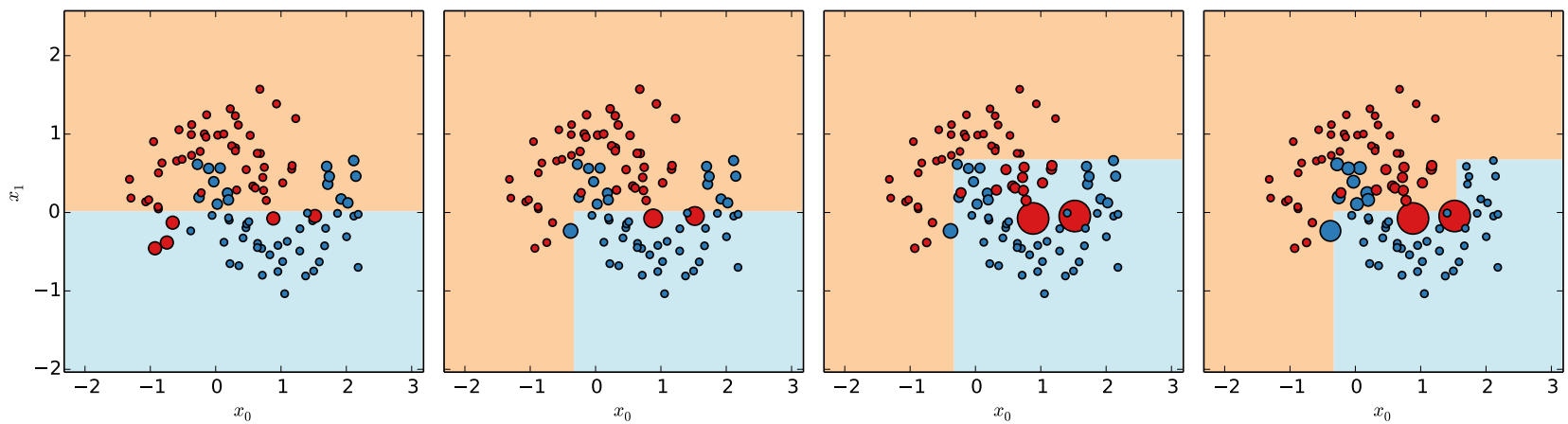
- One of the best off-the-self learning algorithm, requiring almost no tuning.
- Fine control of bias and variance through averaging and randomization, resulting in better performance.
- Moderately fast to train and to predict.
  - $\Theta(MK\widetilde{N}\log^2\widetilde{N})$ for RFs (where $\widetilde{N}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

Outline

AdaBoost (Freund and Schapire, 1995)

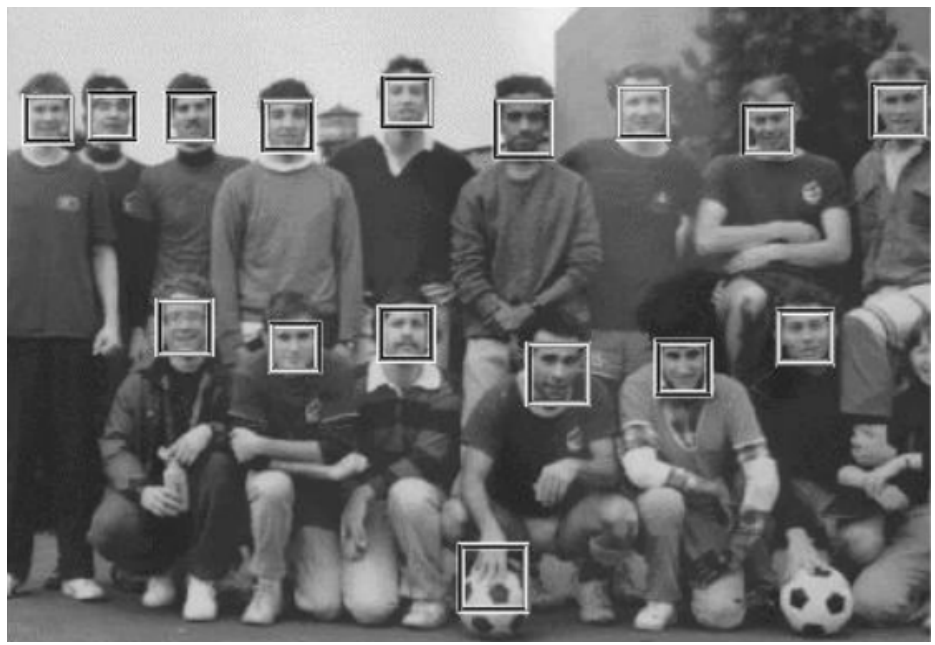
Can we build a strong learner from multiple weak learners?

- Ensemble: each member is an expert on the errors of its predecessor;
- Iteratively re-weights training examples based on errors.



Huge success

- Viola-Jones Face Detector (2001)



- Freund & Schapire won the Gödel prize (2003)

Gradient Boosted Machines (Friedman, 2001)

Statistical view of boosting:

- Ultimately, we are interested in finding

$$f^* = \arg\min_f \mathbb{E}_{X,Y}[L(Y, f(X))]$$

  for an arbitrary loss L;
- Under the boosting assumption that f^* can be expressed as an additive model $\hat{f}$ of the form

$$\hat{f} = c + \sum_{m=1}^{M} \rho_m h_m.$$

Greedy approximation

- The ensemble is built in a forward stage-wise fashion:

$$f_m = f_{m-1} + \rho_m h_m$$

- In accordance with the empirical risk minimization principle, the weak learner $\rho_m h_m$ is chosen to minimize the loss L on the training set, given the current model f_{m-1}:

$$f_m = f_{m-1} + \arg\min_{\rho, h} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \rho h(x_i))$$

$$f_0 = \arg\min_{c} \sum_{i=1}^{N} L(y_i, c)$$

- Solving for ρ, h at each step for an arbitrary loss L and/or arbitrary family $\mathcal{H}$ is a difficult optimization problem.

Steepest descent in function space

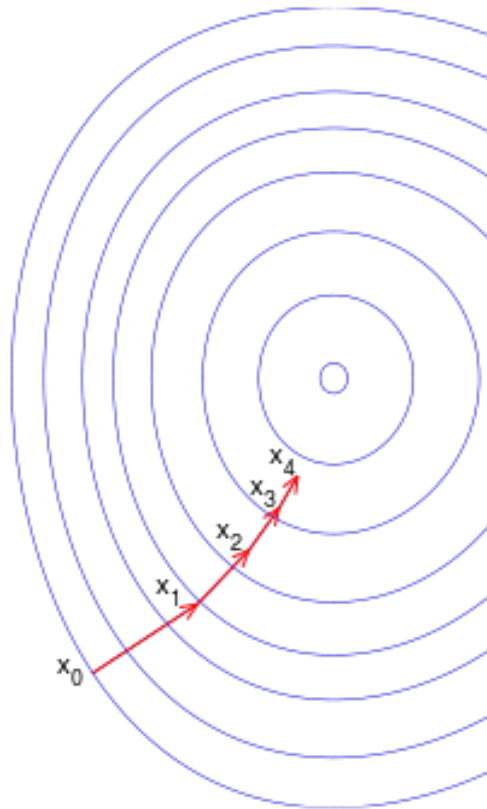
Solution: approximate using steepest descent in function space, by choosing a function h that is the most parallel to the negative gradient $\{g_m(x_i)\}_{i=1}^N$ on the training data:

$$g_m(x) = \mathbb{E}_{Y|X=x}\left[\frac{\partial L(Y, f(x))}{\partial f(x)}\right]_{f(x)=f_{m-1}(x)}$$

$$h_m = \arg\min_h \sum_{i=1}^{N} (-g_m(x_i) - h(x_i))^2$$

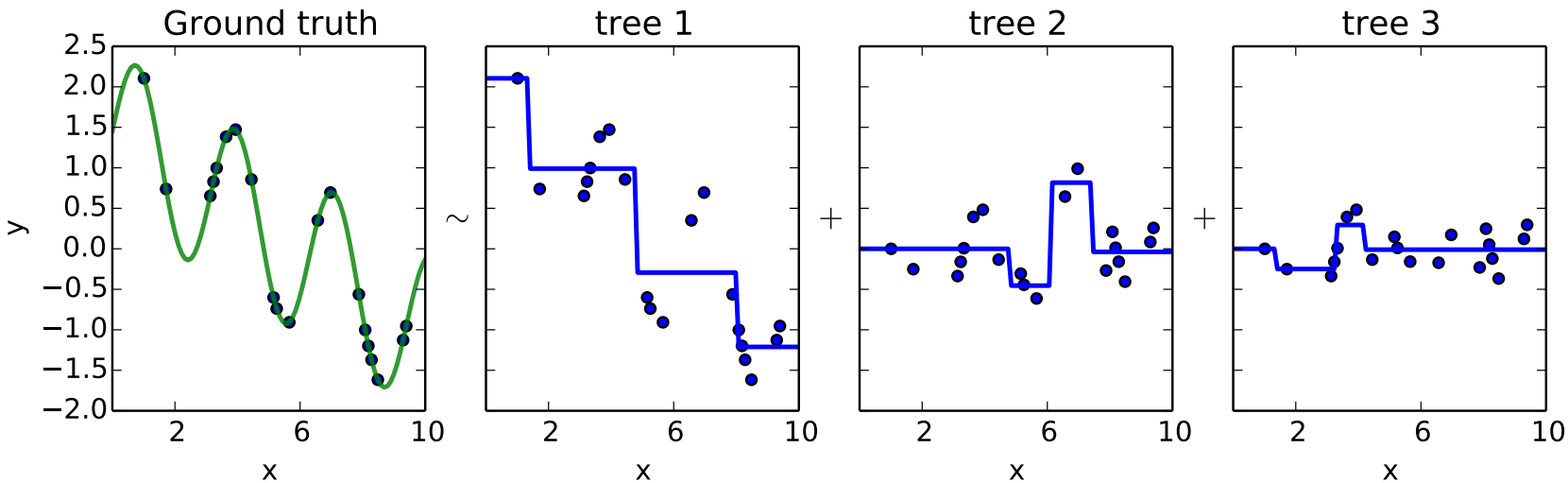
$$\rho_m = \arg\min_\gamma L(y_i, f_{m-1}(x_i) + \rho h_m(x_i))$$

where the second equation is solved using a standard regression algorithm (e.g. decision trees) and the third using line search.



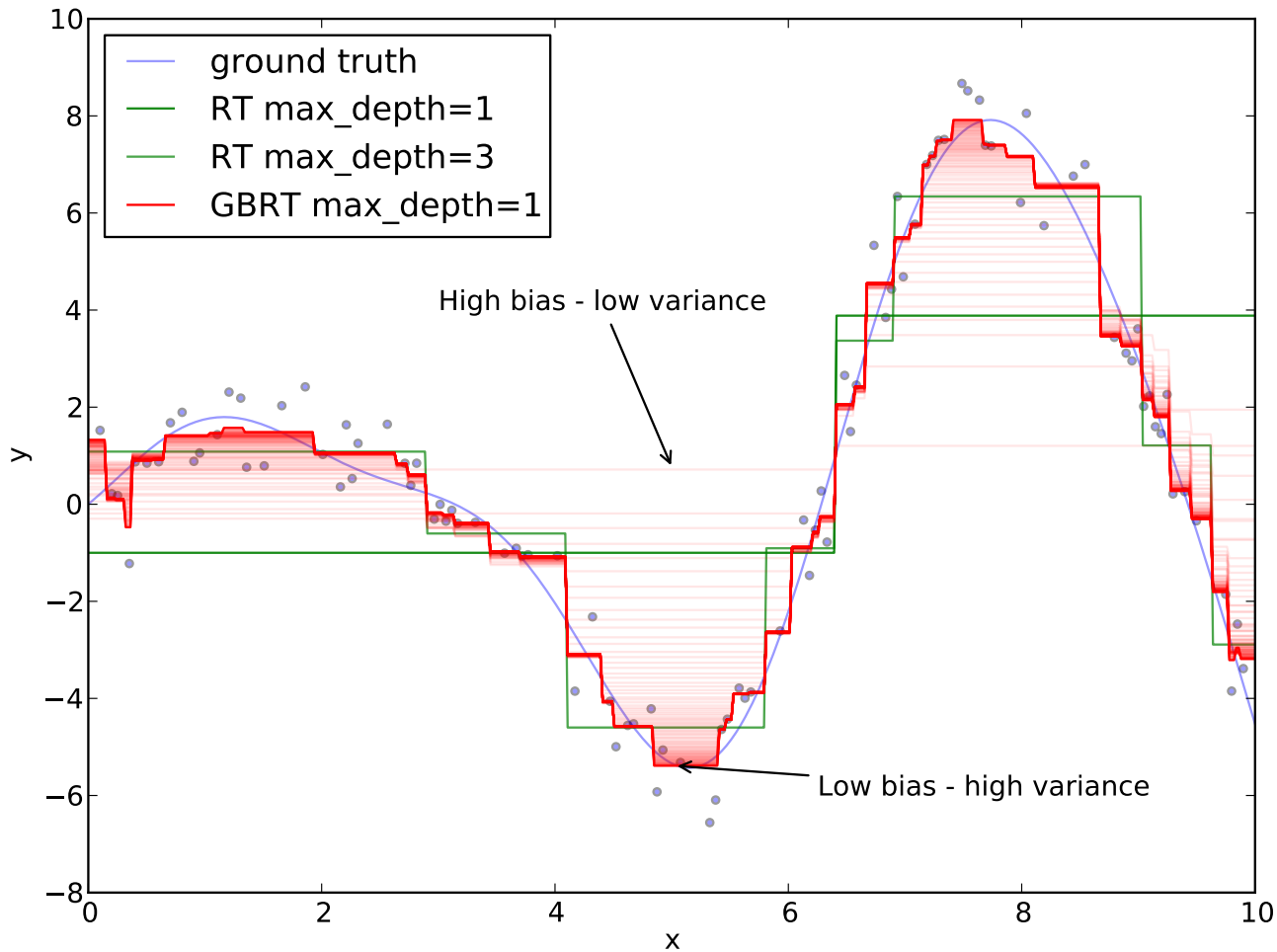
In short

- GBM fits an additive model of the form $\hat{f} = c + \sum_{m=1}^{M} \rho_m h_m$.
- Where h_m are regression trees approximating the negative gradient step $-\left[\frac{\partial L(Y, f(x))}{\partial f(x)}\right]_{f(x)=f_{m-1}(x)}$.
- For $L(Y, f(X)) = (Y - f(X))^2$, regression trees h_m approximate the residuals $y_i - f_{m-1}(x_i)$.

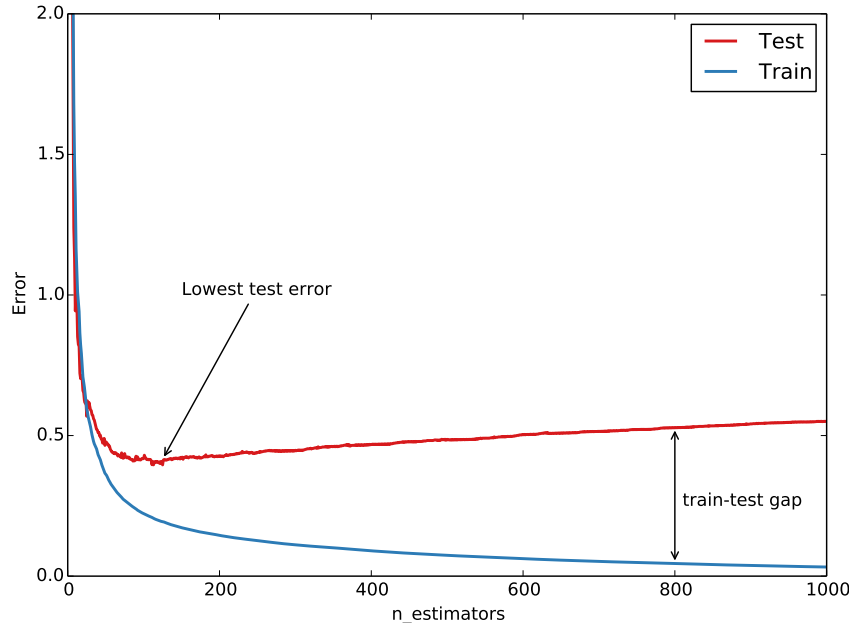


Example

```
from sklearn.ensemble import GradientBoostingRegressor
est = GradientBoostingRegressor(n_estimators=100).fit(X, y)
```



Model complexity and over-fitting

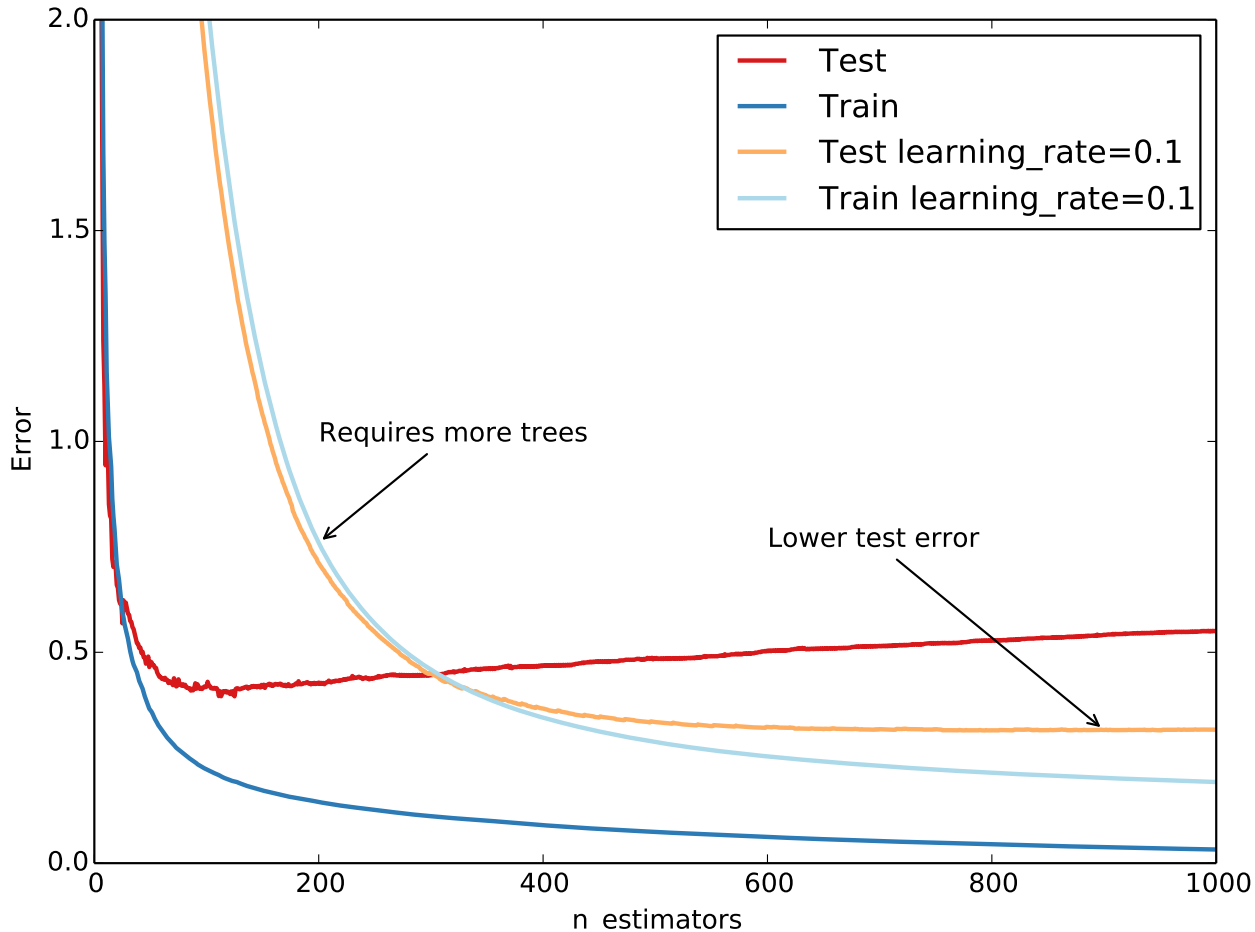


GBM provides a number of knobs to control over-fitting:

- Shrinkage
- Tree structure
- Stochastic Gradient Boosting

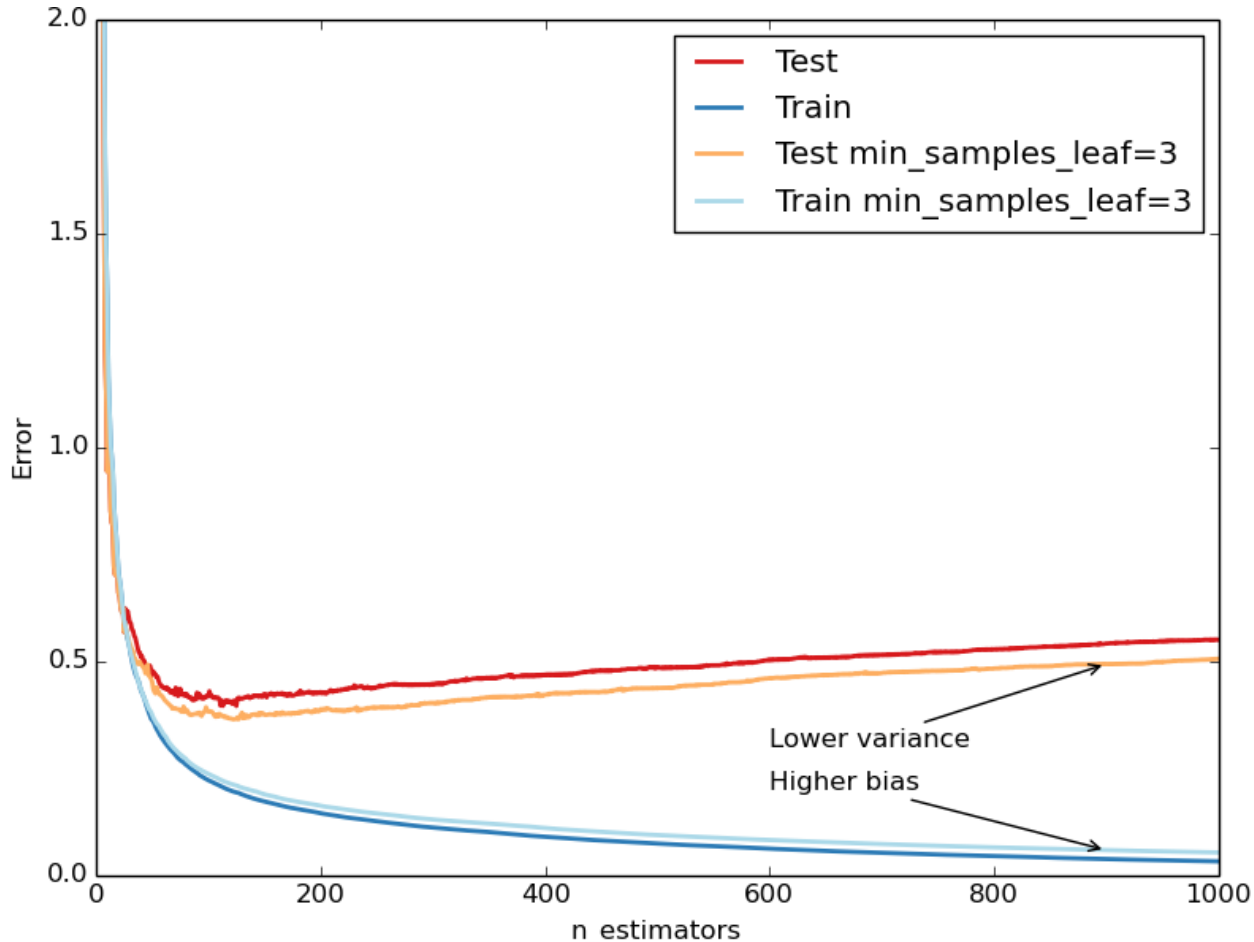
Regularization: shrinkage

- Slow learning by shrinking tree predictions with $0 < \text{learning\_rate} <= 1$
- Lower `learning_rate` requires higher `n_estimators`



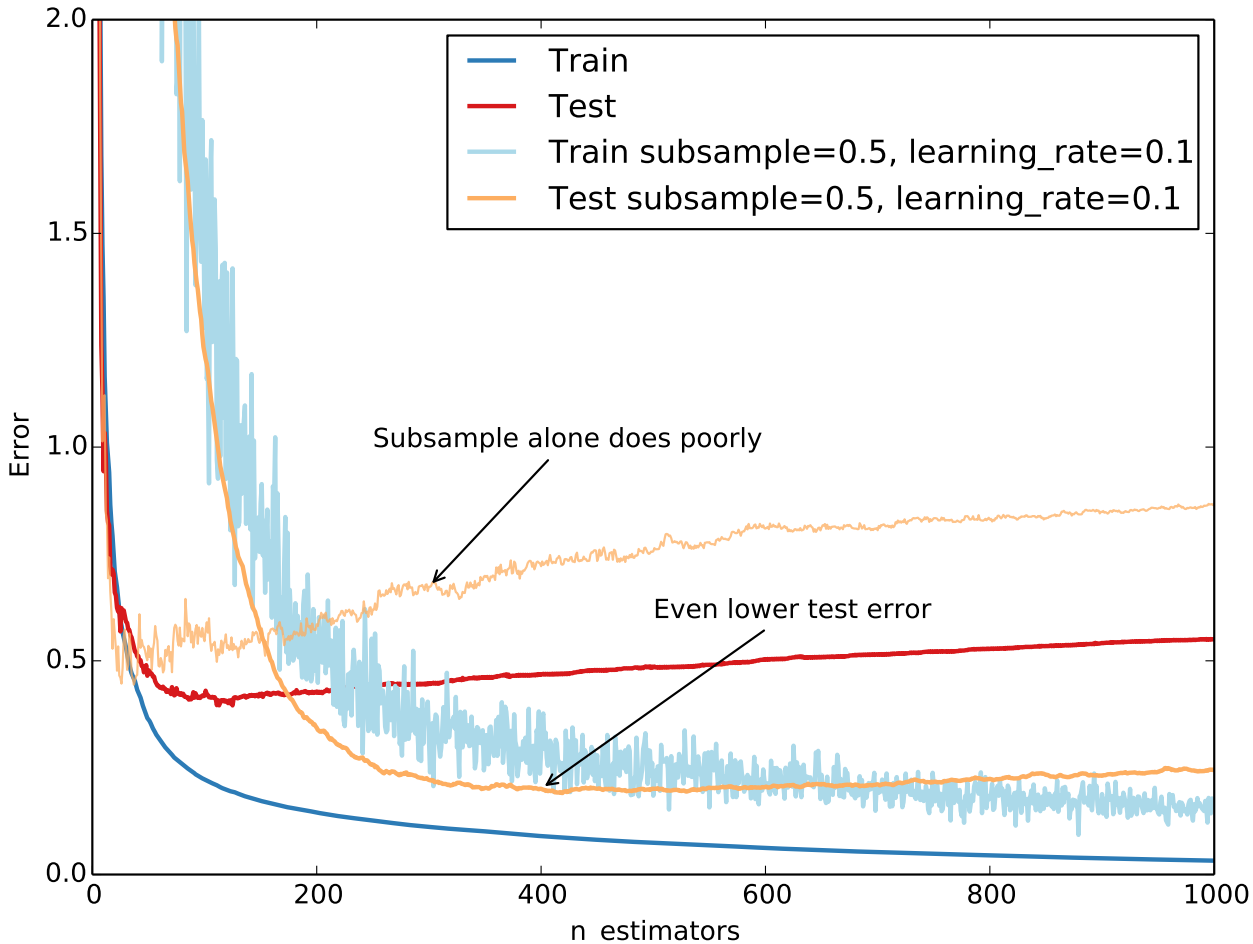
Regularization: tree structure

- The `max_depth` of the trees controls the degree of features interactions
- Use `min_samples_leaf` to have a sufficient nr. of samples per leaf.



Regularization: stochastic gradient boosting

- Samples: random subset of the training set (`subsample`)
- Features: random subset of features (`max_features`)
- Improved accuracy – reduced run-time



Hyper-parameter tuning

1. Set `n_estimators` as high as possible (eg. 3000)
2. Tune hyper-parameters via grid search.

```
from sklearn.grid_search import GridSearchCV
param_grid = {'learning_rate': [0.1, 0.05, 0.02, 0.01],
              'max_depth': [4, 6],
              'min_samples_leaf': [3, 5, 9, 17],
              'max_features': [1.0, 0.3, 0.1]}
est = GradientBoostingRegressor(n_estimators=3000)
gs_cv = GridSearchCV(est, param_grid).fit(X, y)
# best hyper-parameter setting
gs_cv.best_params_
```

3. Finally, set `n_estimators` even higher and tune `learning_rate`.

Strengths and weaknesses of Boosting

- Often more accurate than random forests.
- Flexible framework, that can adapt to arbitrary loss functions.
- Fine control of under/over-fitting 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 selection/ranking/exploration

Tree-based models come with built-in methods for variable selection, ranking or exploration.

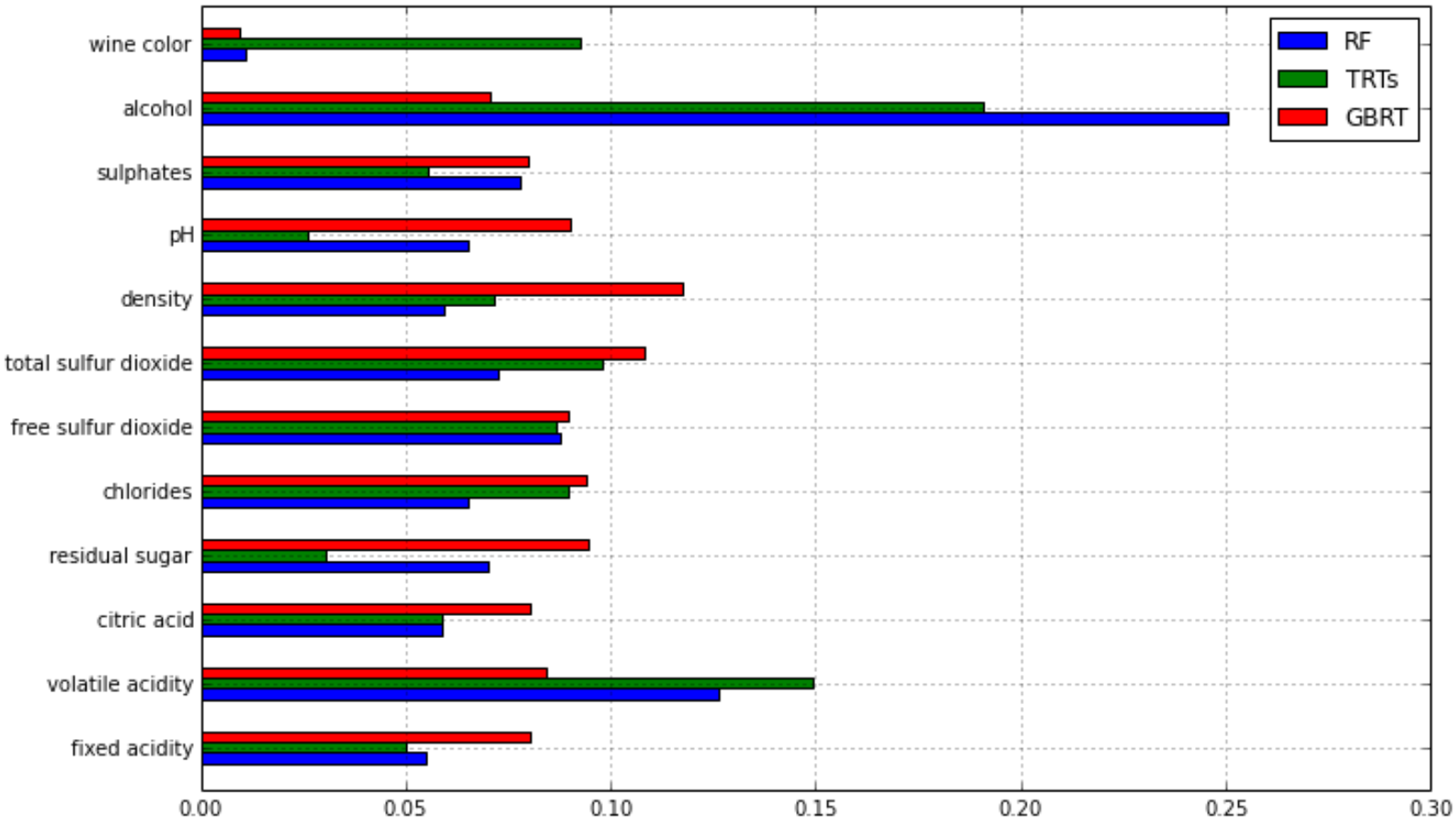
The main goals are:

- To reduce training times;
- To enhance generalization by reducing over-fitting;
- To uncover relations between variables and ease model interpretation.

Variable importances

```
# Variable importances with Random Forest, default parameters
forest = RandomForestRegressor(n_estimators=10000, n_jobs=-1).fit(X, y)
forest.feature_importances_
```

Variable importances

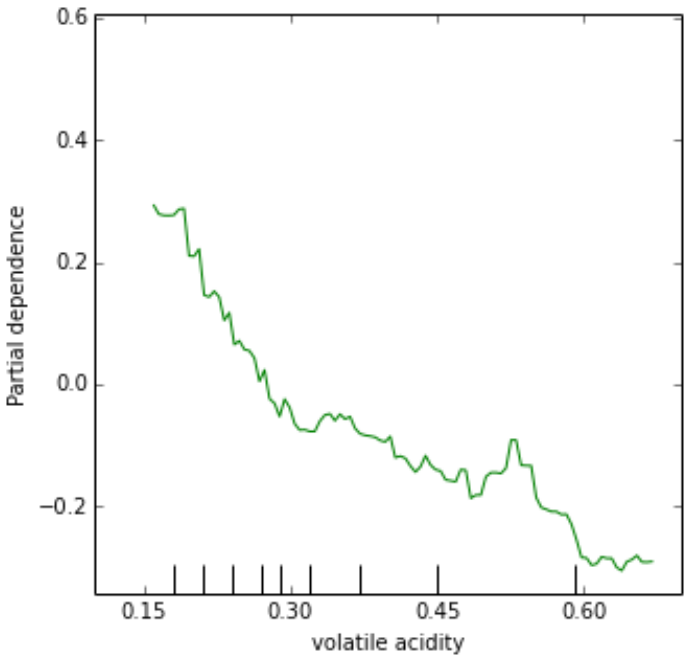


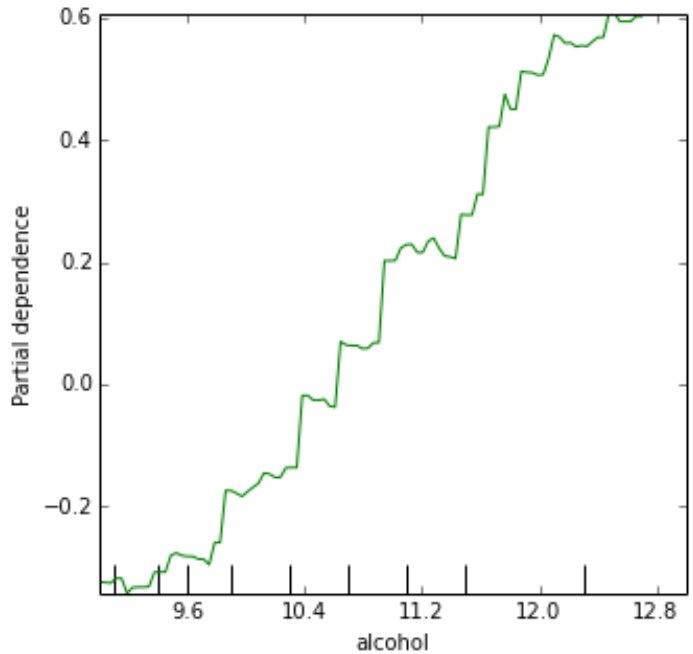
Importances are measured only through the eyes of the model. They may not tell the entire nor the same story! (Louppe et al., 2013)

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)
```





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