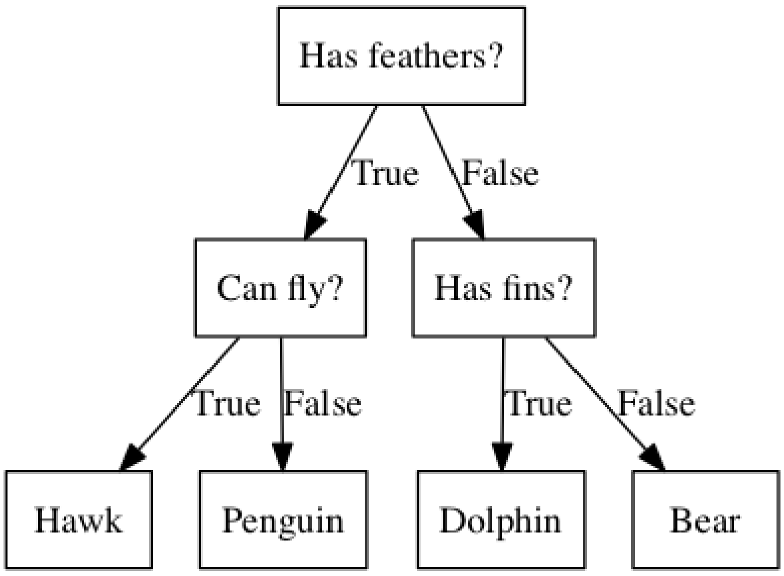
Trees and Ensembles

```
[1]: # Global imports and settings
     from preamble import *
     %matplotlib inline
     plt.rcParams['savefig.dpi'] = 120 # Use 300 for PDF, 100 for slides
     # InteractiveShell.ast_node_interactivity = "all"
     HTML('''<style>html, body{overflow-y: visible !important} .CodeMirror{min-w
```

```
<IPython.core.display.HTML object>
```

Trees

```
[2]: mglearn.plots.plot_animal_tree()
```



Building Decision Trees

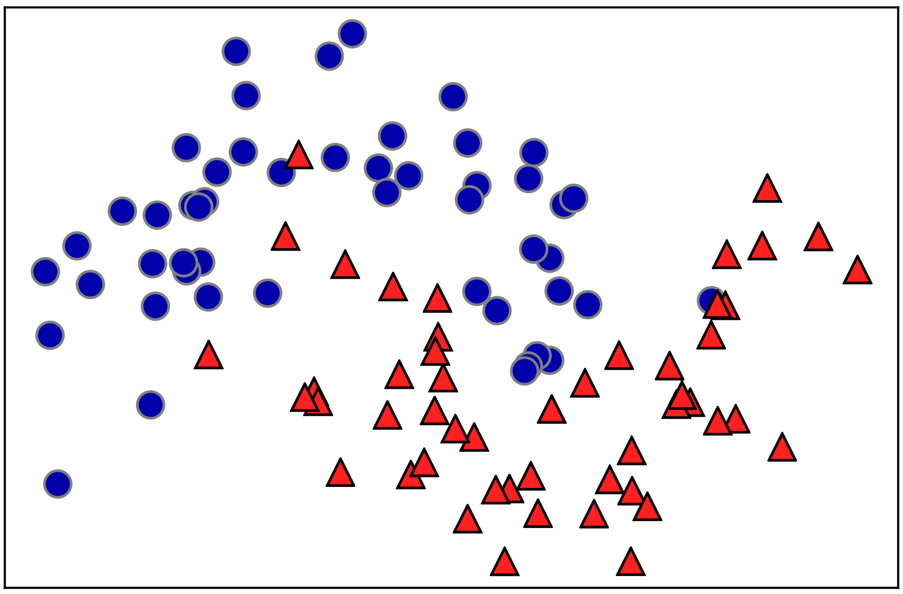
- Split the data in two (or more) parts
- Search over all possible splits and choose the one that is most *informative*
  - Many heuristics
  - E.g. *information gain*: how much does the entropy of the class labels decrease after the split (purer 'leafs')
- Repeat recursive partitioning

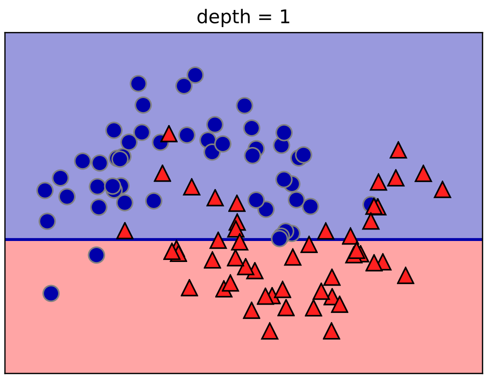
Making predictions:

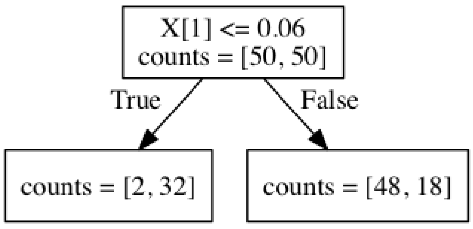
- Classification: find leaf for new data point, predict majority class (or class distribution)
- Regression: idem, but predict the *mean* of all values

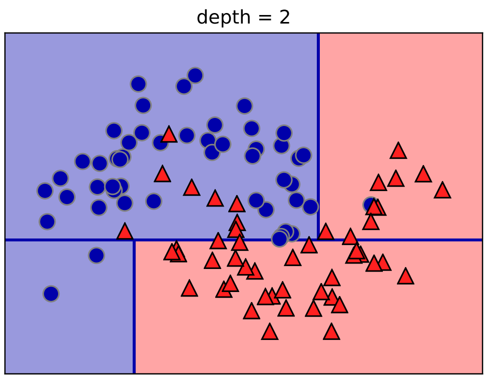
Decision Tree classification

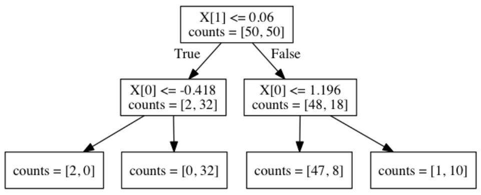
```
[3]: mglearn.plots.plot_tree_progressive()
```

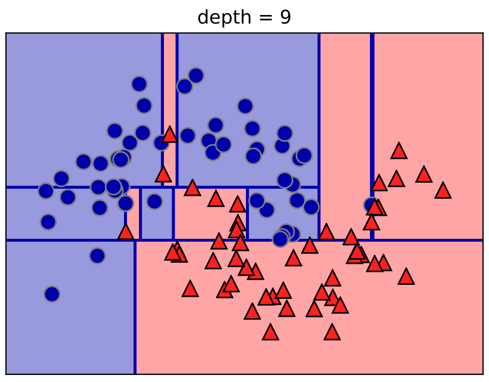


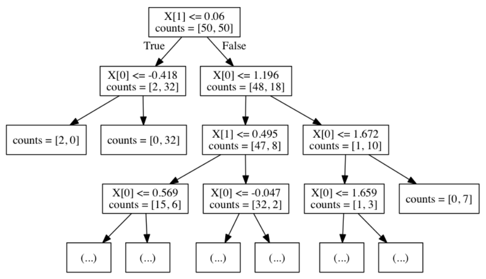












Heuristics

For classification ($X_i \rightarrow class_k$): *Impurity measures*:

- Misclassification Error (leads to larger trees):

$$1 - \underset{k}{\operatorname{argmax}} \hat{p}_k$$

- Gini-Index (probabilistic predictions):

$$\sum_{k \neq k'} \hat{p}_k \hat{p}_{k'} = \sum_{k=1}^{K} \hat{p}_k (1 - \hat{p}_k)$$

with $\hat{p}_k$ = the relative frequency of class k in the leaf node

- Entropy (of the class attribute) measures *unpredictability* of the data:
  - How likely will random example have class k?

$$E(X) = -\sum_{k=1}^{K} \hat{p}_k \log_2 \hat{p}_k$$

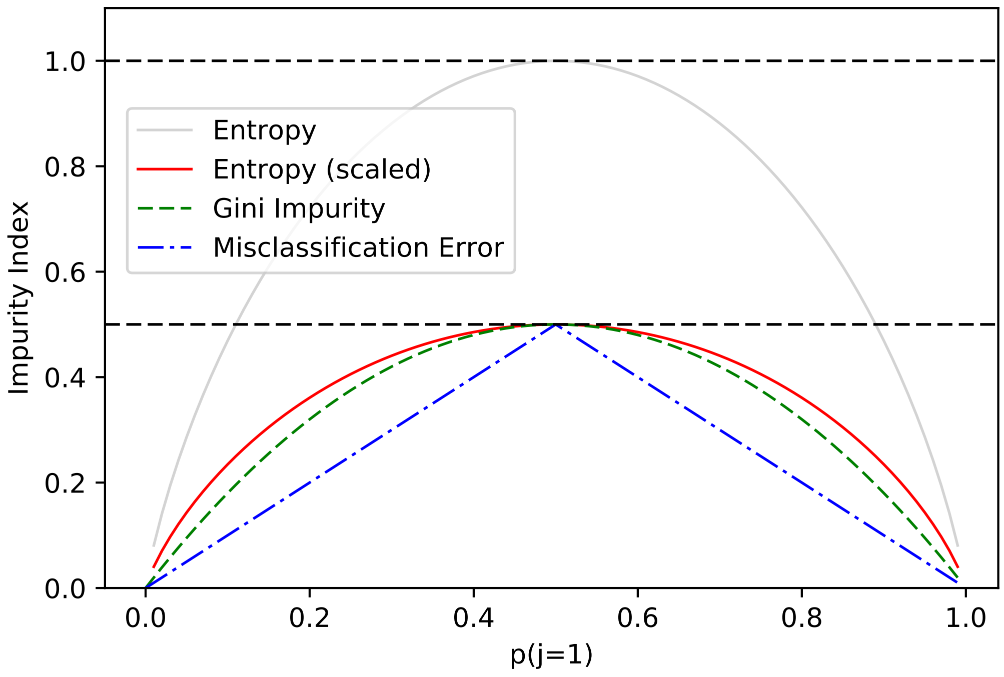
- Information Gain (a.k.a. Kullback–Leibler divergence) for choosing attribute X_i to split the data:

$$G(X, X_i) = E(X) - \sum_{v=1}^{V} \frac{|X_{i=v}|}{|X_i|} E(X_{i=v})$$

with $\hat{p}_k$ = the relative frequency of class k in the leaf node, X = the training set, containing i features (variables) X_i, v a specific value for X_i, $X_{i=v}$ is the set of examples having value v for feature X_i: $\{x \in X | X_i = v\}$

Heuristics visualized (binary class) - Note that `gini != entropy/2`

```
[4]: def gini(p):
        return (p)*(1 - (p)) + (1 - p)*(1 - (1-p))

     def entropy(p):
        return - p*np.log2(p) - (1 - p)*np.log2((1 - p))

     def classification_error(p):
        return 1 - np.max([p, 1 - p])

     x = np.arange(0.0, 1.0, 0.01)
     ent = [entropy(p) if p != 0 else None for p in x]
     scaled_ent = [e*0.5 if e else None for e in ent]
     c_err = [classification_error(i) for i in x]

     fig = plt.figure()
     ax = plt.subplot(111)

     for j, lab, ls, c, in zip(
           [ent, scaled_ent, gini(x), c_err],
           ['Entropy', 'Entropy (scaled)', 'Gini Impurity', 'Misclassification E
           ['-', '-', '--', '-.'],
           ['lightgray', 'red', 'green', 'blue']):
        line = ax.plot(x, j, label=lab, linestyle=ls, lw=1, color=c)

     ax.legend(loc='upper left', bbox_to_anchor=(0.01, 0.85),
               ncol=1, fancybox=True, shadow=False)
     ax.axhline(y=0.5, linewidth=1, color='k', linestyle='--')
     ax.axhline(y=1.0, linewidth=1, color='k', linestyle='--')

     plt.ylim([0, 1.1])
     plt.xlabel('p(j=1)')
     plt.ylabel('Impurity Index')
     plt.show()
```



Example

Ex.	1	2	3	4	5	6
a1	T	T	T	F	F	F
a2	T	T	F	F	T	T
class	+	+	-	+	-	-

$E(X)$?
$G(X, X_{a2})$?
$G(X, X_{a1})$?
$E(X) = -(\frac{1}{2} * log_2(\frac{1}{2}) + \frac{1}{2} * log_2(\frac{1}{2})) = 1$ (classes have equal probabilities)
$G(X, X_{a2}) = 0$ (after split, classes still have equal probabilities, entropy stays 1)

Ex.	1	2	3	4	5	6
a1	T	T	T	F	F	F
a2	T	T	F	F	T	T
class	+	+	-	+	-	-

$$E(X) = -\sum_{k=1}^{K} \hat{p}_k \log \hat{p}_k \quad , \quad G(X, X_i) = E(X) - \sum_{v=1}^{V} \frac{|X_{i=v}|}{|X_i|} E(X_{i=v})$$

$$E(X_{a1=T}) = -\frac{2}{3}\log_2(\frac{2}{3}) - \frac{1}{3}\log_2(\frac{1}{3}) = 0.9183 \quad (= E(X_{a1=F}))$$

$$G(X, X_{a1}) = 1 - \frac{1}{2}0.9183 - \frac{1}{2}0.9183 = 0.0817$$

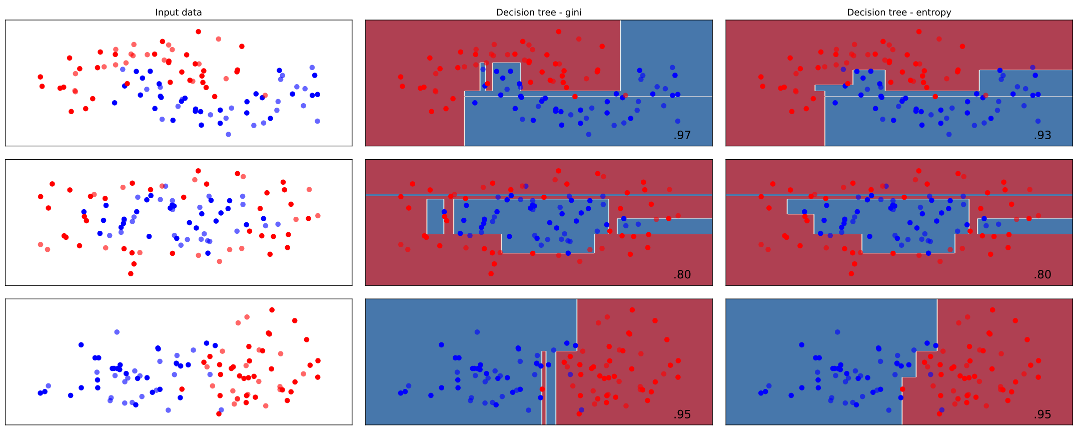
hence we split on a1

Heuristics in scikit-learn The splitting criterion can be set with the `criterion` option in `DecisionTreeClassifier`

- `gini` (default): gini impurity index
- `entropy`: information gain

Best value depends on dataset, as well as other hyperparameters

```
[7]: from sklearn.tree import DecisionTreeClassifier
     import plot_classifiers as pc
     names = ["Decision tree - gini", "Decision tree - entropy"]

     classifiers = [
         DecisionTreeClassifier(),
         DecisionTreeClassifier(criterion="entropy")
         ]

     pc.plot_classifiers(names, classifiers, figuresize=(20,8))
```



Handling many-valued features

What happens when a feature has (almost) as many values as examples? - Information Gain will select it

One approach: use Gain Ratio instead (not available scikit-learn):

$$GainRatio(X, X_i) = \frac{Gain(X, X_i)}{SplitInfo(X, X_i)}$$

$$SplitInfo(X, X_i) = -\sum_{v=1}^{V} \frac{|X_{i=v}|}{|X|} log_2 \frac{|X_{i=v}|}{|X|}$$

where $X_{i=v}$ is the subset of examples for which feature X_i has value v.

SplitInfo will be big if X_i fragments the data into many small subsets, resulting in a smaller Gain Ratio.

Overfitting: Controlling complexity of Decision Trees

Decision trees can very easily overfit the data. Regularization strategies:

- Pre-pruning: stop creation of new leafs at some point
  - Limiting the depth of the tree, or the number of leafs
  - Requiring a minimal leaf size (number of instances)
- Post-pruning: build full tree, then prune (join) leafs
  - Reduced error pruning: evaluate against held-out data
  - Many other strategies exist.
  - scikit-learn supports none of them (yet)

Effect of pre-pruning: default tree overfits, setting `max_depth=4` is better

```
[42]: from sklearn.datasets import load_breast_cancer
      from sklearn.tree import DecisionTreeClassifier
      from sklearn.model_selection import train_test_split

      cancer = load_breast_cancer()
      X_train, X_test, y_train, y_test = train_test_split(
          cancer.data, cancer.target, stratify=cancer.target, random_state=42)
      tree = DecisionTreeClassifier(random_state=0)
      tree.fit(X_train, y_train)
      print("Accuracy on training set: {:.3f}".format(tree.score(X_train, y_trai
      print("Accuracy on test set: {:.3f}".format(tree.score(X_test, y_test)))
```

```
Accuracy on training set: 1.000
Accuracy on test set: 0.937
```

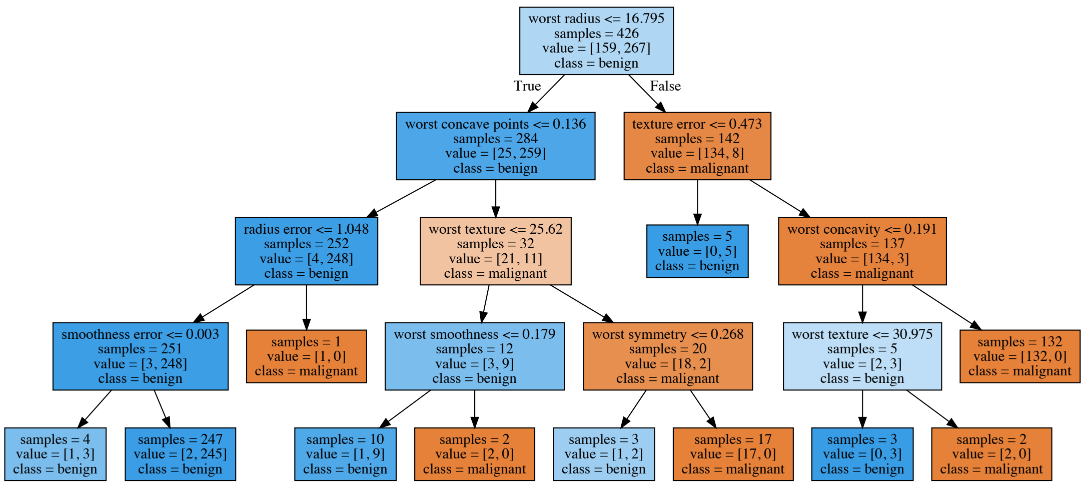
```
[43]: tree = DecisionTreeClassifier(max_depth=5, random_state=0)
      tree.fit(X_train, y_train)
      print("Accuracy on training set: {:.3f}".format(tree.score(X_train, y_trai
      print("Accuracy on test set: {:.3f}".format(tree.score(X_test, y_test)))
```

```
Accuracy on training set: 0.995
Accuracy on test set: 0.951
```

Analyzing Decision Trees manually

- Visualize and find the path that most data takes

```
[10]: # Creates a .dot file
      from sklearn.tree import export_graphviz
      export_graphviz(tree, out_file="tree.dot", class_names=["malignant", "beni
                      feature_names=cancer.feature_names, impurity=False, filled
      # Open and display
      import graphviz
      with open("tree.dot") as f:
          dot_graph = f.read()
      display(graphviz.Source(dot_graph))
```



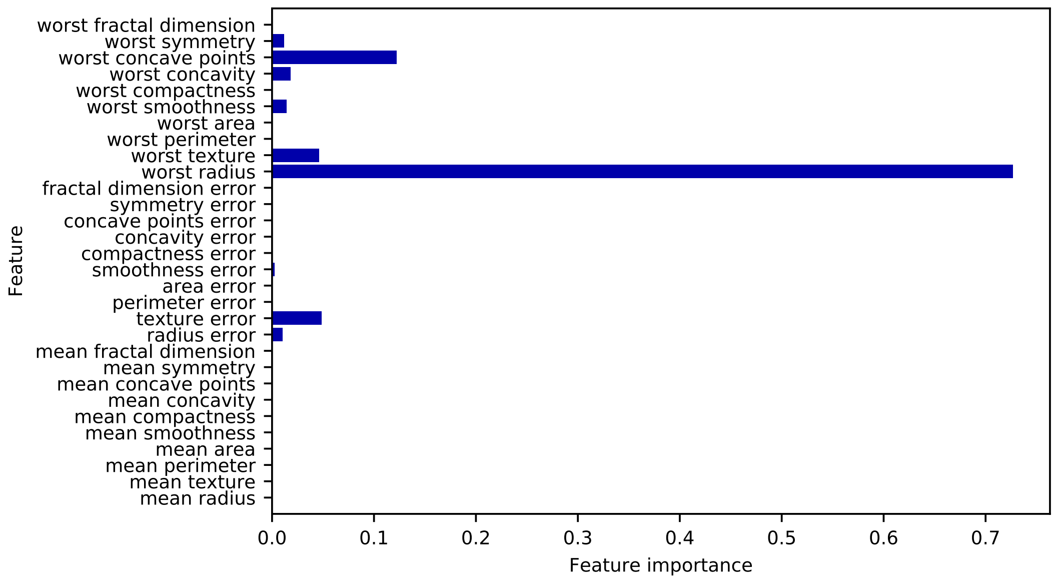
`DecisionTreeClassifier` also returns *feature importances*

- In [0,1], sum up to 1
- High values for features selected by the algorithm
- Other features may also be relevant, but don't contribute new information given the selected features

```
[11]: # Feature importances sum up to 1
      print("Feature importances:\n{}".format(tree.feature_importances_))
```

```
Feature importances:
[0.    0.    0.    0.    0.    0.    0.    0.    0.    0.    0.01  0.048
 0.    0.    0.002 0.    0.    0.    0.    0.    0.727 0.046 0.    0.
 0.014 0.    0.018 0.122 0.012 0.   ]
```

```
[12]: def plot_feature_importances_cancer(model):
          n_features = cancer.data.shape[1]
          plt.barh(range(n_features), model.feature_importances_, align='center'
          plt.yticks(np.arange(n_features), cancer.feature_names)
          plt.xlabel("Feature importance")
          plt.ylabel("Feature")
          plt.ylim(-1, n_features)

      plt.rcParams.update({'font.size': 8})
      plot_feature_importances_cancer(tree)
```



Decision tree regression

Heuristic for regression ($x_i \to y_i \in I\!R$): *Minimal quadratic distance*

- Consider splits at every data point for every variable (or halfway between data points)
- Dividing the data on split variable X_j at splitpoint s leads to the following half-spaces:

$$R_1(j,s) = X : X_j \leq s \quad and \quad R_2(j,s) = X : X_j > s$$

- The best split variable and the corresponding splitpoint, with predicted value c_i and actual value Y_i:

$$\min_{j,s}\left(\min_{c_1}\sum_{x_i\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x_i\in R_2(j,s)}(y_i-c_2)^2\right)$$

- Assuming that the tree predicts y_i as the average of all x_i in the leaf:

$$\hat{c}_1 = \text{avg}(y_i|x_i \in R_1(j,s)) \quad and \quad \hat{c}_2 = \text{avg}(y_i|x_i \in R_2(j,s))$$

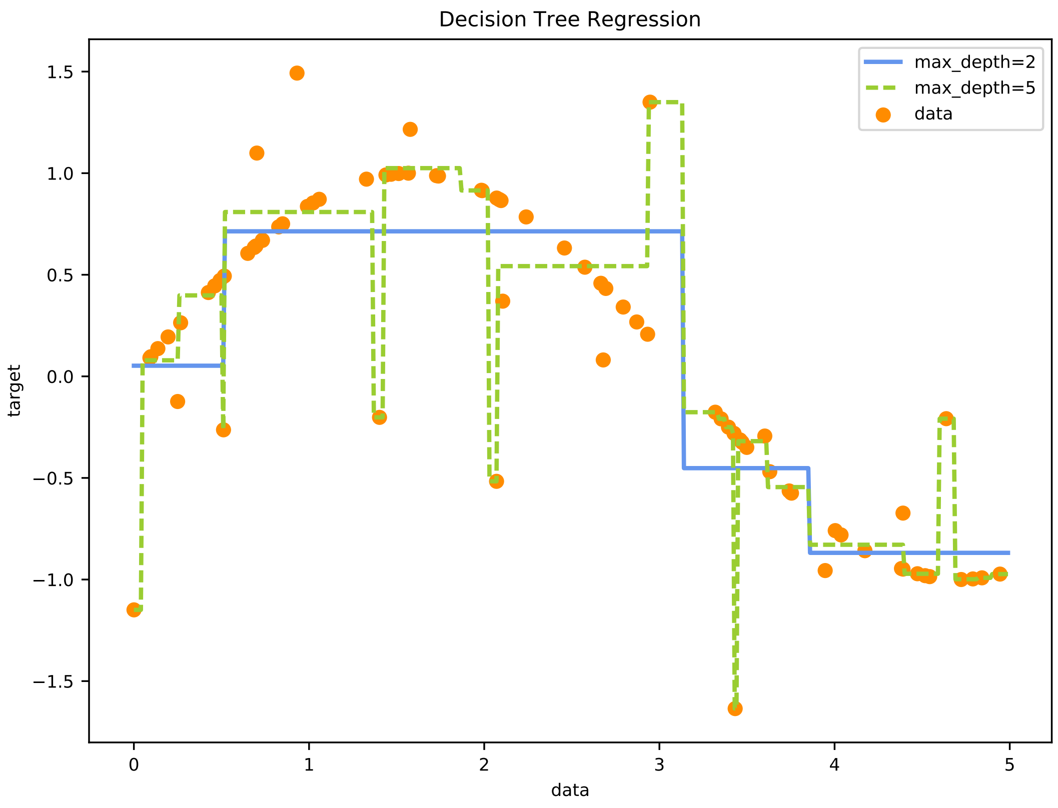
with x_i being the i-th example in the data, with target value y_i

In scikit-learn Regression is done with `DecisionTreeRegressor`

```
[13]: def plot_decision_tree_regression(regr_1, regr_2):
          # Create a random dataset
          rng = np.random.RandomState(1)
          X = np.sort(5 * rng.rand(80, 1), axis=0)
          y = np.sin(X).ravel()
          y[::5] += 3 * (0.5 - rng.rand(16))
```

```
    # Fit regression model
    regr_1.fit(X, y)
    regr_2.fit(X, y)

    # Predict
    X_test = np.arange(0.0, 5.0, 0.01)[:, np.newaxis]
    y_1 = regr_1.predict(X_test)
    y_2 = regr_2.predict(X_test)

    # Plot the results
    plt.figure(figsize=(8,6))
    plt.scatter(X, y, c="darkorange", label="data")
    plt.plot(X_test, y_1, color="cornflowerblue", label="max_depth=2", lin
    plt.plot(X_test, y_2, color="yellowgreen", label="max_depth=5", linewi
    plt.xlabel("data")
    plt.ylabel("target")
    plt.title("Decision Tree Regression")
    plt.legend()
    plt.show()
```

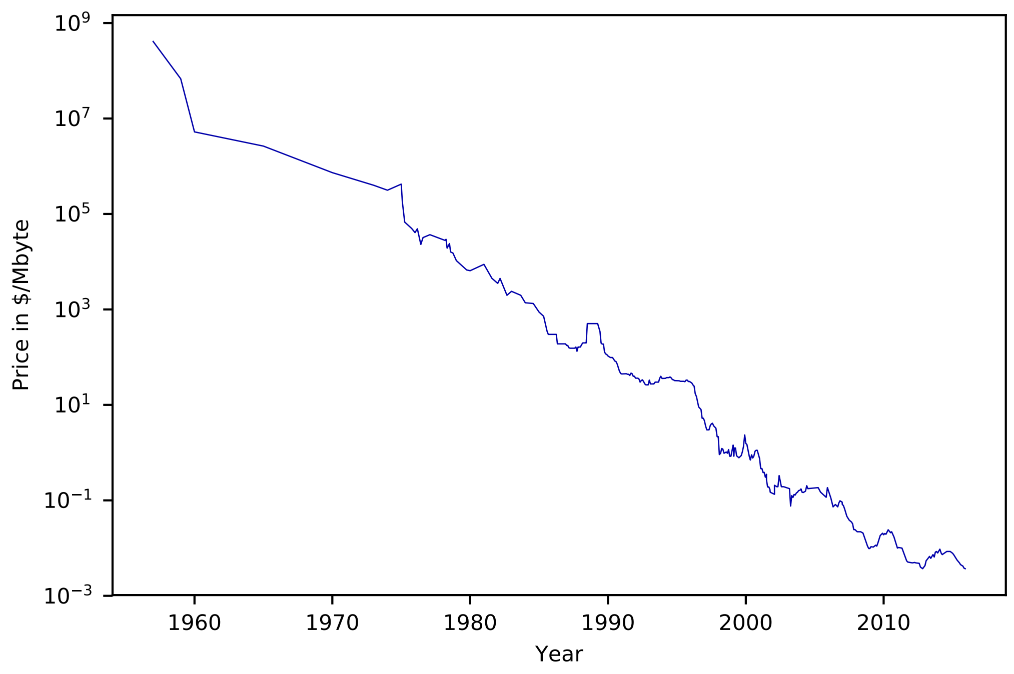
```
[46]: from sklearn.tree import DecisionTreeRegressor
      regr_1 = DecisionTreeRegressor(max_depth=2)
      regr_2 = DecisionTreeRegressor(max_depth=5)

      plot_decision_tree_regression(regr_1,regr_2)
```



Note that decision trees do not extrapolate well.

- The leafs return the same *mean* value no matter how far the new data point lies from the training examples.
- Example on the `ram_price` forecasting dataset

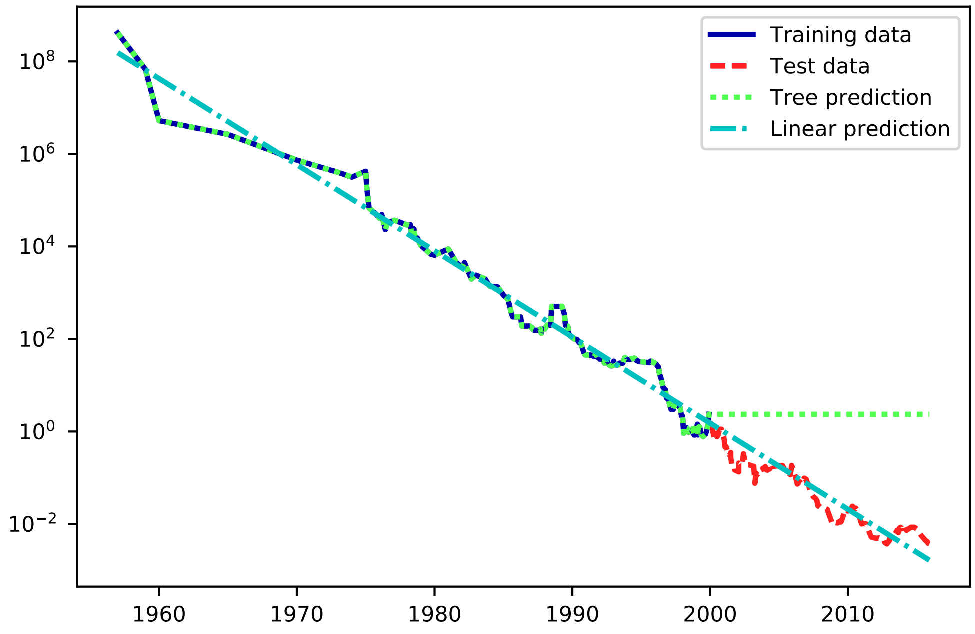
```
[15]: ram_prices = pd.read_csv('data/ram_price.csv')

      plt.semilogy(ram_prices.date, ram_prices.price)
      plt.xlabel("Year")
      plt.ylabel("Price in $/Mbyte");
```



```
[16]: from sklearn.tree import DecisionTreeRegressor
      from sklearn.linear_model import LinearRegression

      # Use historical data to forecast prices after the year 2000
      data_train = ram_prices[ram_prices.date < 2000]
      data_test = ram_prices[ram_prices.date >= 2000]

      # predict prices based on date:
      X_train = data_train.date[:, np.newaxis]
      # we use a log-transform to get a simpler relationship of data to target
      y_train = np.log(data_train.price)

      tree = DecisionTreeRegressor().fit(X_train, y_train)
      linear_reg = LinearRegression().fit(X_train, y_train)

      # predict on all data
      X_all = ram_prices.date[:, np.newaxis]
```

```
pred_tree = tree.predict(X_all)
pred_lr = linear_reg.predict(X_all)

# undo log-transform
price_tree = np.exp(pred_tree)
price_lr = np.exp(pred_lr)
```

```
[17]: plt.rcParams['lines.linewidth'] = 2
      plt.semilogy(data_train.date, data_train.price, label="Training data")
      plt.semilogy(data_test.date, data_test.price, label="Test data")
      plt.semilogy(ram_prices.date, price_tree, label="Tree prediction")
      plt.semilogy(ram_prices.date, price_lr, label="Linear prediction")
      plt.legend();
```



Strengths, weaknesses and parameters Pre-pruning: regularize by:

- Setting a low `max_depth`, `max_leaf_nodes`
- Setting a higher `min_samples_leaf` (default=1)

Decision trees:

- Work well with features on completely different scales, or a mix of binary and continuous features
  - Does not require normalization
- Interpretable, easily visualized
- Still tend to overfit easily. Use ensembles of trees.

Ensemble learning

Ensembles are methods that combine multiple machine learning models to create more powerful models. Most popular are:

- **RandomForests**: Build randomized trees on random samples of the data
- **Gradient boosting machines**: Build trees iteratively, giving higher weights to the points misclassified by previous trees

In both cases, predictions are made by doing a vote over the members of the example. **Stacking** is another technique that builds a (meta)model over the predictions of each member.

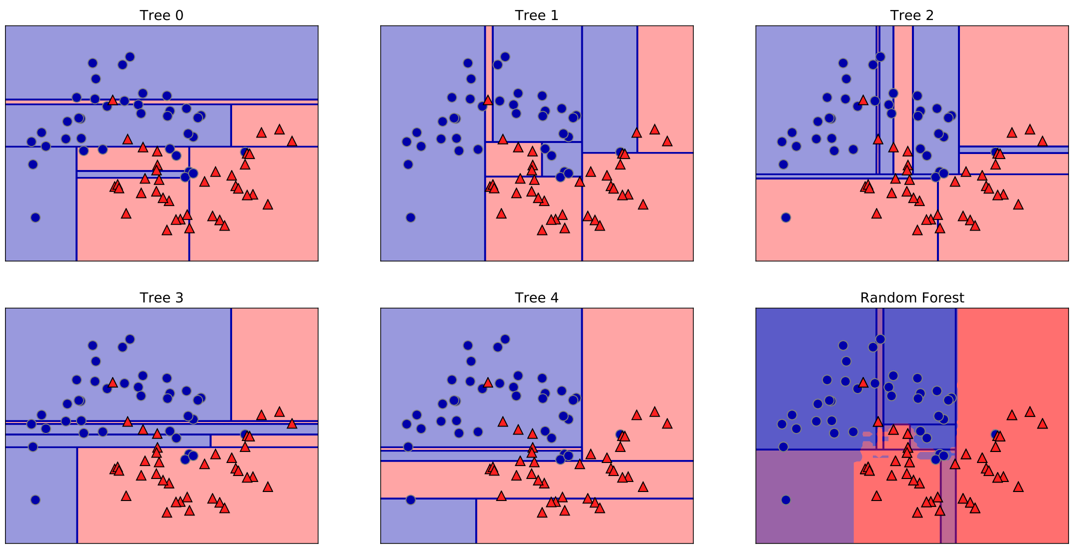
RandomForests

Reduce overfitting by averaging out individual predictions (variance reduction)

- Take a *bootstrap sample* of your data
  - Randomly sample with replacement
  - Build a tree on each bootstrap
- Repeat `n_estimators` times
  - Higher values: more trees, more smoothing
  - Make prediction by aggrating the individual tree predictions
    - a.k.a. Bootstrap aggregating (Bagging)
- RandomForest: Randomize trees by considering only a random subset of features of size `max_features` *in each node*
  - Small `max_features` yields more different trees, more smoothing
  - Default: $sqrt(n\_features)$ for classification, $log2(n\_features)$ for regression

Making predictions: * Classification: soft voting (softmax) * Every member returns probability for each class * After averaging, the class with highest probability wins * Regression: * Return the *mean* of all predictions

```
[47]: from sklearn.ensemble import RandomForestClassifier
      from sklearn.datasets import make_moons

      X, y = make_moons(n_samples=100, noise=0.25, random_state=3)
      X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y,
                                                          random_state=42)

      forest = RandomForestClassifier(n_estimators=10, random_state=2)
      forest.fit(X_train, y_train)

      plt.rcParams.update({'font.size': 12})
      fig, axes = plt.subplots(2, 3, figsize=(20, 10))
      for i, (ax, tree) in enumerate(zip(axes.ravel(), forest.estimators_)):
          ax.set_title("Tree {}".format(i))
          mglearn.plots.plot_tree_partition(X_train, y_train, tree, ax=ax)

      mglearn.plots.plot_2d_separator(forest, X_train, fill=True, ax=axes[-1, -1
                                      alpha=.4)
      axes[-1, -1].set_title("Random Forest")
      mglearn.discrete_scatter(X_train[:, 0], X_train[:, 1], y_train);
```



Scikit-learn algorithms:

- `RandomForestClassifier` (or Regressor)
- `ExtraTreesClassifier`: Grows deeper trees, faster

Most important parameters:

- `n_estimators` (higher is better, but diminishing returns)
  - Will start to underfit (bias error component increases slightly)
- `max_features` (default is typically ok)
  - Set smaller to reduce space/time requirements
- parameters of trees, e.g. `max_depth` (less effect)

`n_jobs` sets the number of parallel cores to run
`random_state` should be fixed for reproducibility

```
[67]: X_train, X_test, y_train, y_test = train_test_split(
          cancer.data, cancer.target, random_state=0)
      forest = RandomForestClassifier(n_estimators=100, random_state=0)
      forest.fit(X_train, y_train)
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_decrease=0.0, min_impurity_split=None,
            min_samples_leaf=1, min_samples_split=2,
            min_weight_fraction_leaf=0.0, n_estimators=100, n_jobs=1,
            oob_score=False, random_state=0, verbose=0, warm_start=False)
```

```
[68]: forest = RandomForestClassifier(n_estimators=100, random_state=0) # Vary n
      forest.fit(X_train, y_train)
      print("Accuracy on training set: {:.3f}".format(forest.score(X_train, y_tr
      print("Accuracy on test set: {:.3f}".format(forest.score(X_test, y_test)))
```

```
Accuracy on training set: 1.000
Accuracy on test set: 0.972
```

RandomForest allow another way to evaluate performance: out-of-bag (OOB) error

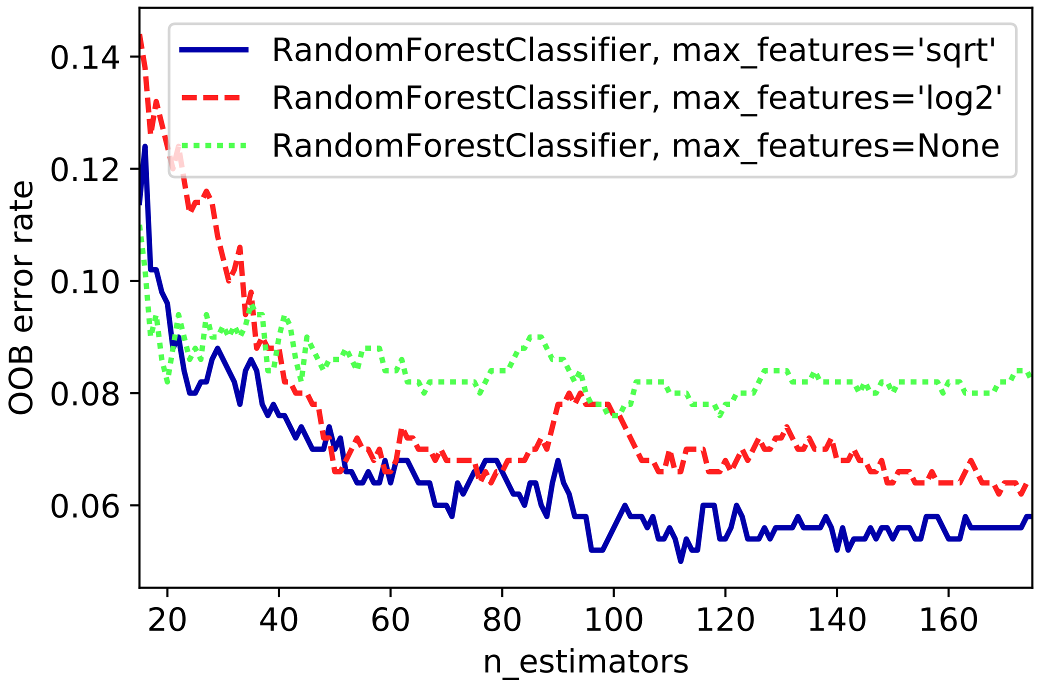
- While growing forest, estimate test error from training samples
- For each tree grown, 33-36% of samples are not selected in bootstrap
  - Called the 'out of bootstrap' (OOB) samples
  - Predictions are made as if they were novel test samples
  - Through book-keeping, majority vote is computed for all OOB samples from all trees
- OOB estimated test error is rather accurate in practice
  - As good as CV estimates, but can be computed on the fly (without repeated model fitting)
  - Tends to be slightly pessimistic

In scikit-learn OOB error are returned as follows:

```
oob_error = 1 - clf.oob_score_
```

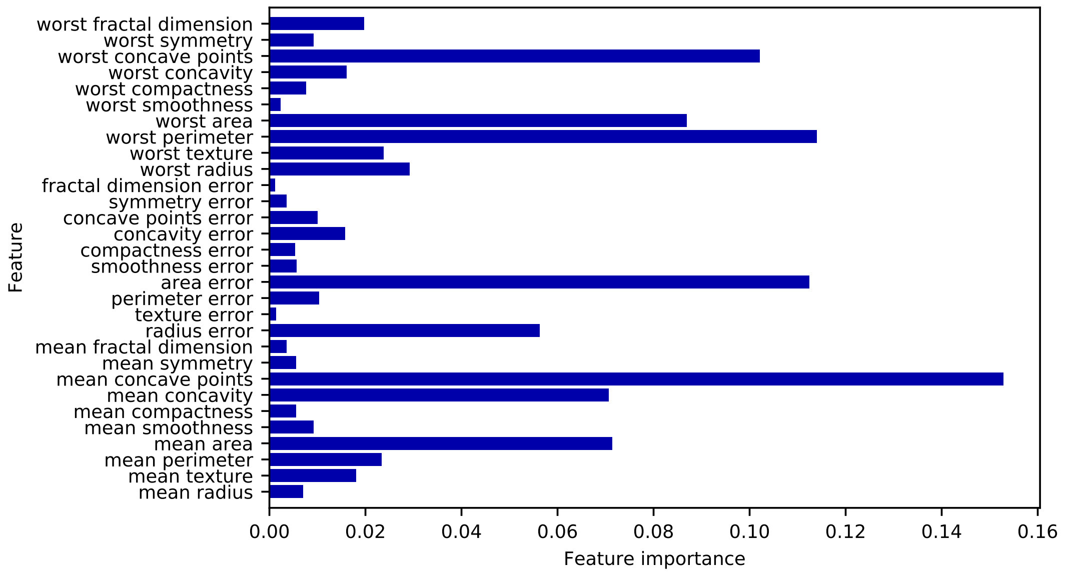
```
[21]: from collections import OrderedDict
      from sklearn.datasets import make_classification
      from sklearn.ensemble import RandomForestClassifier, ExtraTreesClassifier

      RANDOM_STATE = 123

      # Generate a binary classification dataset.
      X, y = make_classification(n_samples=500, n_features=25,
                                 n_clusters_per_class=1, n_informative=15,
                                 random_state=RANDOM_STATE)

      # NOTE: Setting the `warm_start` construction parameter to `True` disables
      # support for parallelized ensembles but is necessary for tracking the OOB
      # error trajectory during training.
      ensemble_clfs = [
          ("RandomForestClassifier, max_features='sqrt'",
              RandomForestClassifier(warm_start=True, oob_score=True,
                                     max_features="sqrt",
                                     random_state=RANDOM_STATE)),
          ("RandomForestClassifier, max_features='log2'",
              RandomForestClassifier(warm_start=True, max_features='log2',
                                     oob_score=True,
                                     random_state=RANDOM_STATE)),
          ("RandomForestClassifier, max_features=None",
              RandomForestClassifier(warm_start=True, max_features=None,
                                     oob_score=True,
                                     random_state=RANDOM_STATE))
      ]

      # Map a classifier name to a list of (<n_estimators>, <error rate>) pairs.
```

```
error_rate = OrderedDict((label, []) for label, _ in ensemble_clfs)

# Range of `n_estimators` values to explore.
min_estimators = 15
max_estimators = 175

for label, clf in ensemble_clfs:
    for i in range(min_estimators, max_estimators + 1):
        clf.set_params(n_estimators=i)
        clf.fit(X, y)

        # Record the OOB error for each `n_estimators=i` setting.
        oob_error = 1 - clf.oob_scor e_
        error_rate[label].append((i, oob_error))

# Generate the "OOB error rate" vs. "n_estimators" plot.
for label, clf_err in error_rate.items():
    xs, ys = zip(*clf_err)
    plt.plot(xs, ys, label=label)

plt.xlim(min_estimators, max_estimators)
plt.xlabel("n_estimators")
plt.ylabel("OOB error rate")
plt.legend(loc="upper right")
plt.show()
```



Feature importance RandomForests provide more reliable feature importances, based on many alternative hypotheses (trees)

```
[22]: plt.rcParams.update({'font.size':8})
      plot_feature_importances_cancer(forest)
```



Strengths, weaknesses and parameters RandomForest are among most widely used algorithms:

- Don't require a lot of tuning
- Typically very accurate models
- Handles heterogeneous features well
- Implictly selects most relevant features

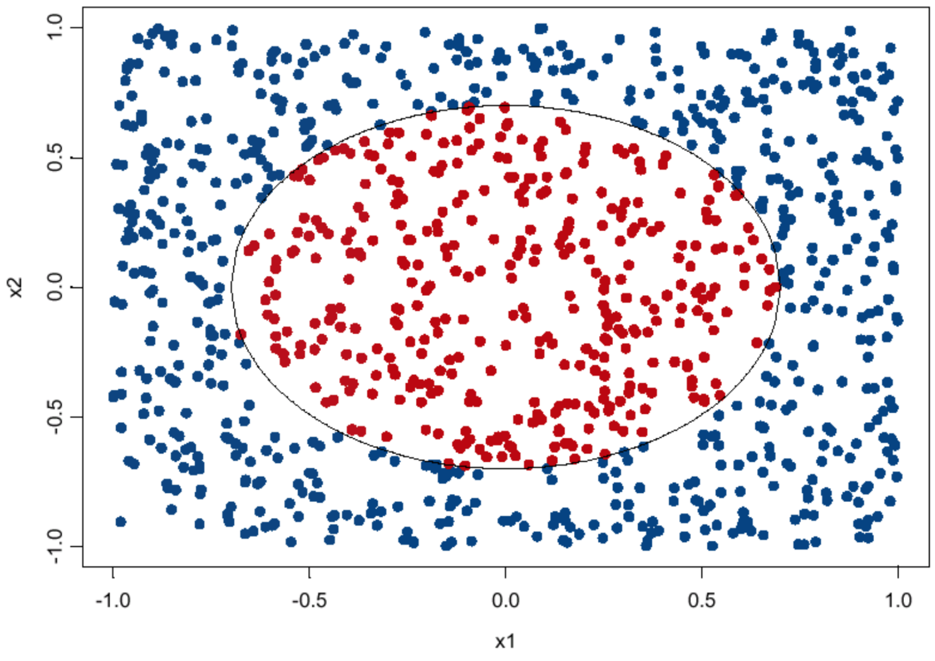
Downsides:

- less interpretable, slower to train (but parallellizable)
- don't work well on high dimensional sparse data (e.g. text)

Gradient Boosted Regression Trees (Gradient Boosting Machines)

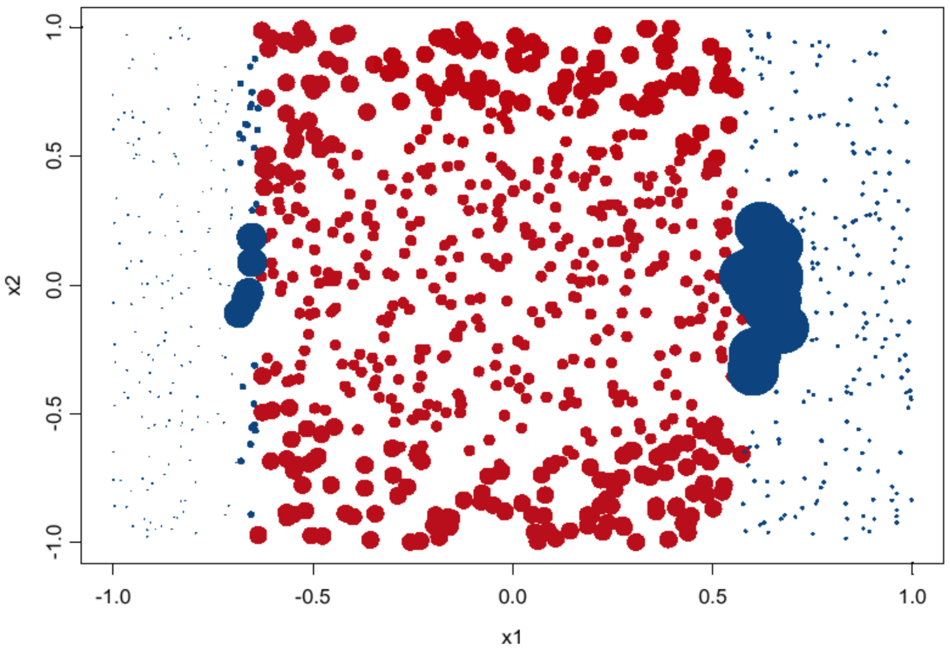
Instead of reducing the variance of overfitted models, reduce the bias of underfitted models

- Use strong pre-pruning to build very shallow trees
  - Default `max_depth`=3
- Iteratively build new trees by increasing weights of points that were badly predicted
- Example of *additive modelling*: each tree depends on the outcome of previous trees
- Optimization: find optimal weights for all data points
  - Gradient descent (covered later) finds optimal set of weights
  - `learning rate` controls how strongly the weights are altered in each iteration (default 0.1)
- Repeat `n_estimators` times (default 100)



Example:
After 1 iteration

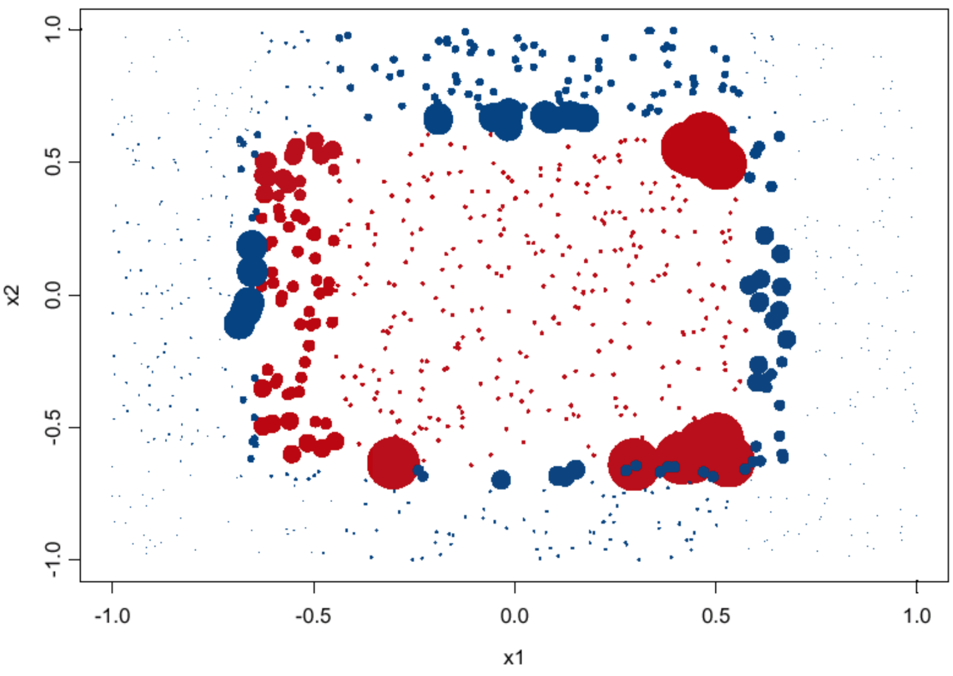
- The simple decision tree divides space
- Misclassified points get higher weight (larger dots)



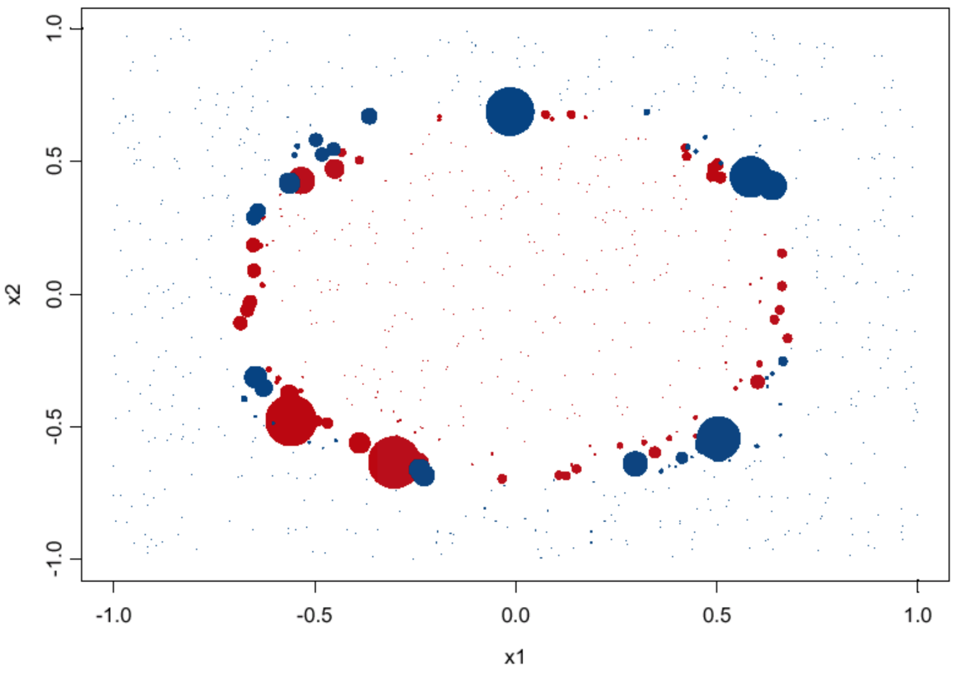
boosting

After 3 iterations
After 20 iterations
Each tree provides good predictions on part of the data, use voting for final prediction

- Soft voting for classification, mean values for regression

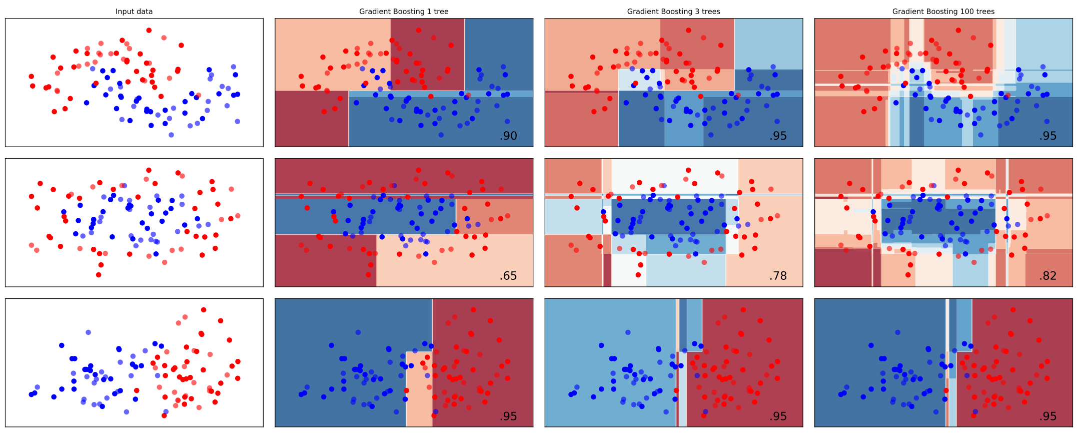


boosting



boosting

```
[25]: import plot_classifiers as pc
      from sklearn.ensemble import GradientBoostingClassifier
      names = ["Gradient Boosting 1 tree", "Gradient Boosting 3 trees", "Gradien

      classifiers = [
          GradientBoostingClassifier(n_estimators=1, random_state=0, learning_ra
          GradientBoostingClassifier(n_estimators=3, random_state=0, learning_ra
          GradientBoostingClassifier(n_estimators=100, random_state=0, learning_
          ]

      pc.plot_classifiers(names, classifiers, figuresize=(20,8))
```



Tuning

- n_estimators: Higher is better, but will start to overfit
- learning_rate: Lower rates mean more trees are needed to get more complex models
  - Main regularizer, also known as 'shrinkage'
  - Set n_estimators as high as possible, then tune learning_rate
- max_depth: typically kept low (<5), reduce when overfitting
- loss: Loss function used for gradient descent (defaults OK)
  - Classification:
    * `deviance` (default): log-likelihood loss (as in logistic regression)
    * `exponential`: exponential loss (AdaBoost algorithm)
  - Regression:
    * `ls`: Least squares (typically the best option)

```
[70]: from sklearn.ensemble import GradientBoostingClassifier

      X_train, X_test, y_train, y_test = train_test_split(
          cancer.data, cancer.target, random_state=0)

      gbrt = GradientBoostingClassifier(random_state=0)
      gbrt.fit(X_train, y_train)
```

```
print("Accuracy on training set: {:.3f}".format(gbrt.score(X_train, y_trai
print("Accuracy on test set: {:.3f}".format(gbrt.score(X_test, y_test)))
```

```
Accuracy on training set: 1.000
Accuracy on test set: 0.958
```

```
[71]: # We are overfitting. We can decrease max_depth
      gbrt = GradientBoostingClassifier(random_state=0, max_depth=1)
      gbrt.fit(X_train, y_train)

      print("Accuracy on training set: {:.3f}".format(gbrt.score(X_train, y_trai
      print("Accuracy on test set: {:.3f}".format(gbrt.score(X_test, y_test)))
```

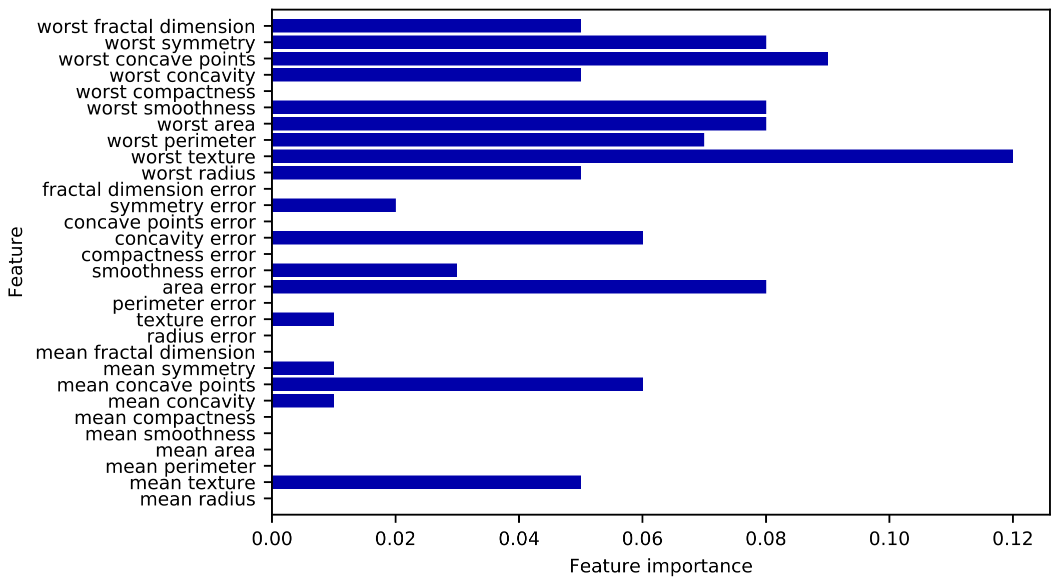
```
Accuracy on training set: 0.991
Accuracy on test set: 0.972
```

```
[75]: # or decrease the learning rate (less effect)
      gbrt = GradientBoostingClassifier(random_state=0, learning_rate=0.01)
      gbrt.fit(X_train, y_train)

      print("Accuracy on training set: {:.3f}".format(gbrt.score(X_train, y_trai
      print("Accuracy on test set: {:.3f}".format(gbrt.score(X_test, y_test)))
```

```
Accuracy on training set: 0.988
Accuracy on test set: 0.965
```

Gradient boosting machines use much simpler trees - Hence, tends to completely ignore some of the features

```
[29]: gbrt = GradientBoostingClassifier(random_state=0, max_depth=1)
      gbrt.fit(X_train, y_train)

      plot_feature_importances_cancer(gbrt)
```



Strengths, weaknesses and parameters

- Among the most powerful and widely used models
- Work well on heterogeneous features and different scales
- Require careful tuning, take longer to train.
- Does not work well on high-dimensional sparse data

Main hyperparameters:

- `n_estimators`: Higher is better, but will start to overfit
- `learning_rate`: Lower rates mean more trees are needed to get more complex models
    - Set `n_estimators` as high as possible, then tune `learning_rate`
- `max_depth`: typically kept low (<5), reduce when overfitting

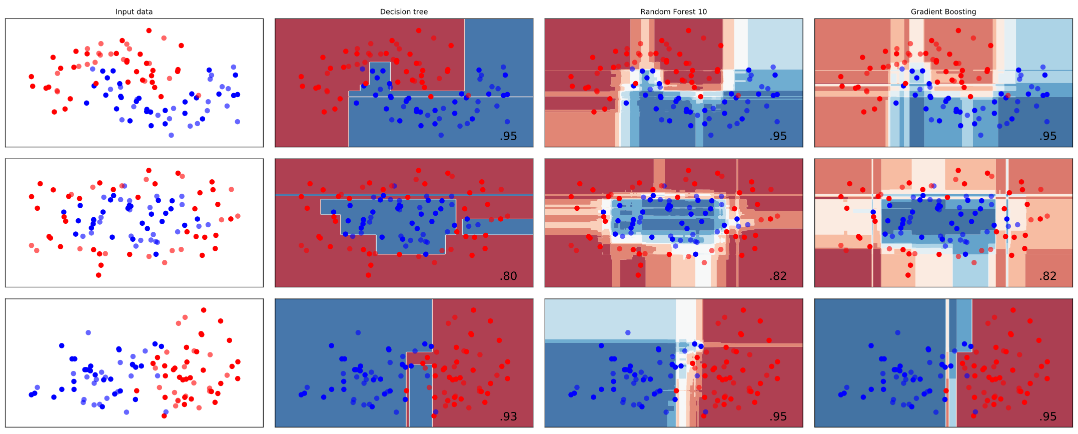
XGBoost

XGBoost is another python library for gradient boosting (install separately).

- The main difference lies the use of approximation techniques to make it faster.
    - Hence, you can do 10x (or 100x) more boosting iterations in same amount of time
- Sketching: Given 10000 possible splits, it will only consider 300 "good enough" splits by default
    - Controlled by the `sketch_eps` parameter (default 0.03)
- Loss function approximation with Taylor Expansion: more efficient way to evaluate splits

Further reading: XGBoost Documentation Paper
Comparison

[30]:
```
import plot_classifiers as pc
names = ["Decision tree", "Random Forest 10", "Gradient Boosting"]

classifiers = [
    DecisionTreeClassifier(),
    RandomForestClassifier(max_depth=5, n_estimators=100, max_features=1),
    GradientBoostingClassifier(random_state=0, learning_rate=0.5)
    ]

pc.plot_classifiers(names, classifiers, figuresize=(20,8))
```



Summary

- Bagging / RandomForest is a variance-reduction technique
  - Build many high-variance (overfitting) models
    - Typically deep (randomized) decision trees
    - The more different the models, the better
  - Aggregation (soft voting or averaging) reduces variance
  - Parallellizes easily
- Boosting is a bias-reduction technique
  - Build many high-bias (underfitting) models
    - Typically shallow decision trees
    - Sample weights are updated to create different trees
  - Aggregation (soft voting or averaging) reduces bias
  - Doesn't parallelize easily
    - Approximation techniques exist to speed up calculation
- You can build ensembles with other models as well
  - Especially if they show high variance or bias
- It is also possible to build *heterogeneous* ensembles
  - Models from different algorithms
  - Are combined by letting each algorithm predict
  - Often a meta-classifier/regressor is trained on the predictions: Stacking