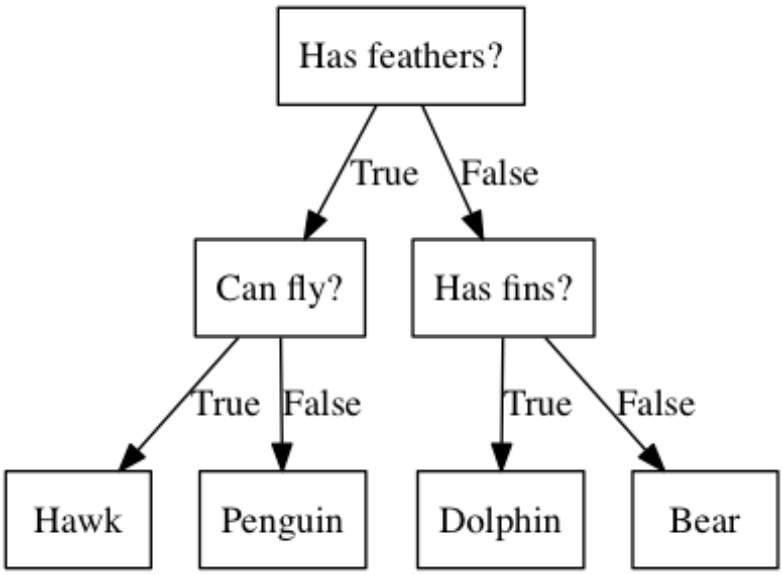
Trees and Ensembles

```
[6]: # 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

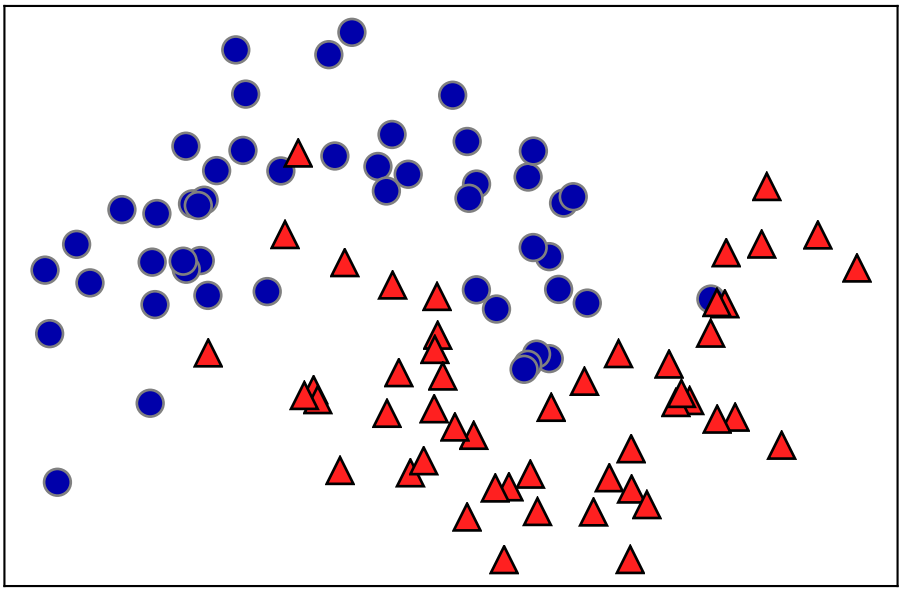
- Split the data in two (or more) parts
- Search over all possible splits and choose the one that is most *informative*
  - Many heuristics
  - E.g. *information gain*: how much does the entropy of the class labels decrease after the split (purer 'leafs')
- Repeat recursive partitioning

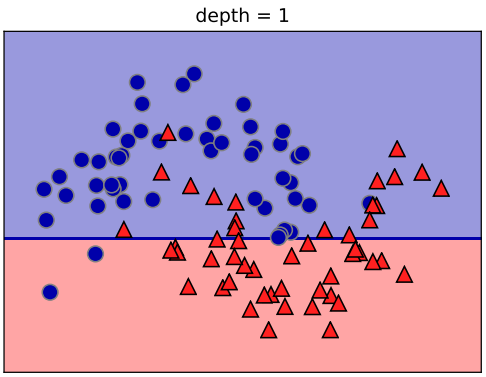
Making predictions:

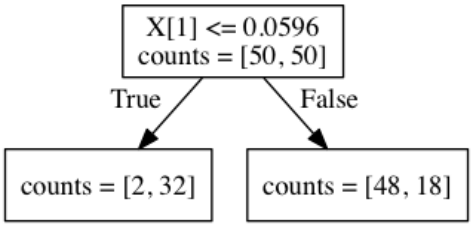
- Classification: find leaf for new data point, predict majority class (or class distribution)
- Regression: idem, but predict the *mean* of all values

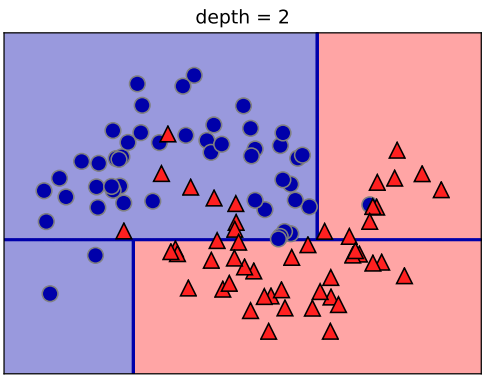
Decision Tree classification

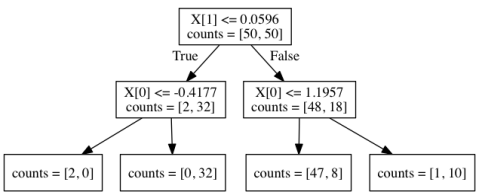
[3]: `mglearn.plots.plot_tree_progressive()`

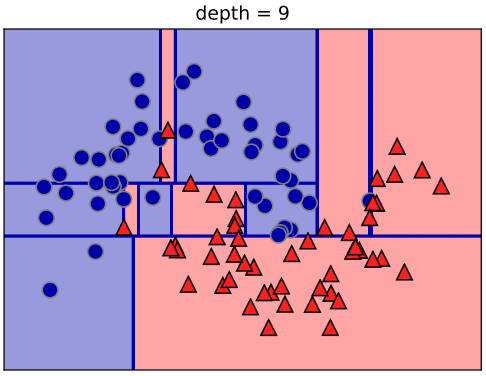


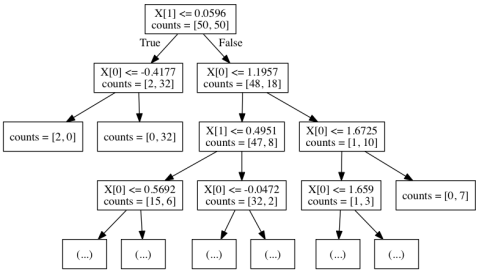












Heuristics

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:

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

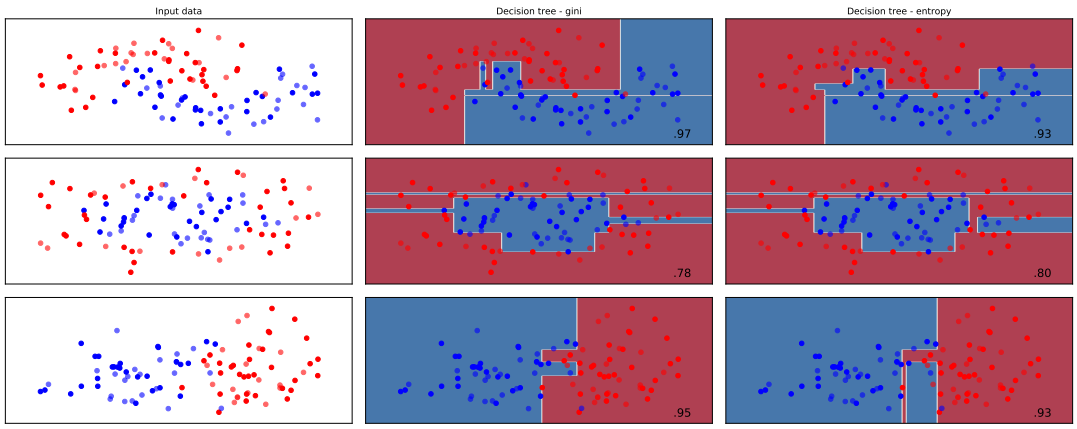
with $\hat{p}_k$ = the relative frequency of class k in the leaf node, X = the training set, containing i features (variables) X_i, v a specific value for X_i, $X_{i=v}$ is the set of examples having value v for feature X_i: $\{x \in X | X_i = v\}$

Heuristics 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

```
[8]: from sklearn.tree import DecisionTreeClassifier
     names = ["Decision tree - gini", "Decision tree - entropy"]

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

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



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

```
[9]: 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_train
    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
```

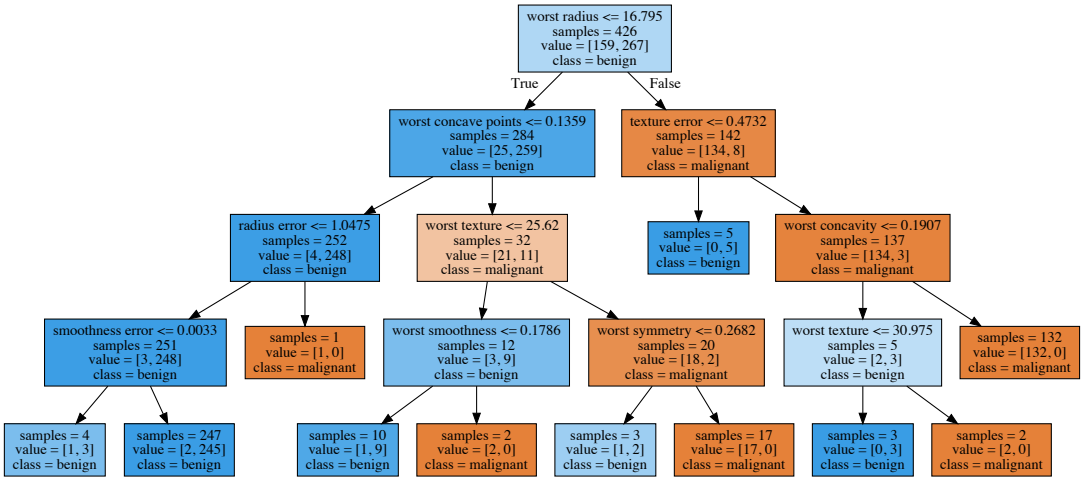
```
[10]: tree = DecisionTreeClassifier(max_depth=4, random_state=0)
      tree.fit(X_train, y_train)
      print("Accuracy on training set: {:.3f}".format(tree.score(X_train, y_trai
      print("Accuracy on test set: {:.3f}".format(tree.score(X_test, y_test)))
```

```
Accuracy on training set: 0.988
Accuracy on test set: 0.951
```

Analyzing Decision Trees manually

- Visualize and find the path that most data takes

```
[11]: # 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))
```



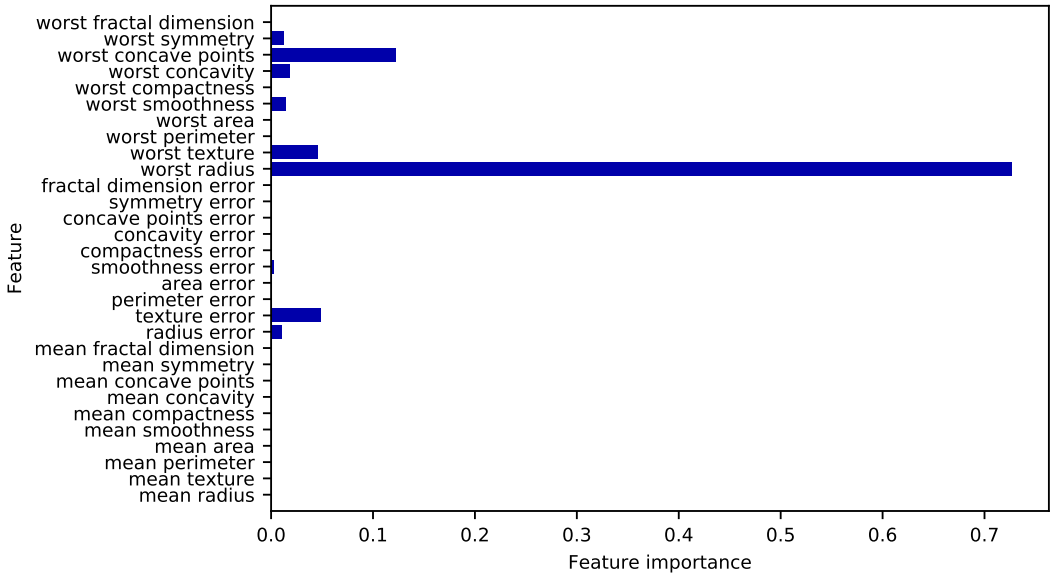
`DecisionTreeClassifier` also returns *feature importances*

- 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

```
[12]: # 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.    ]
```

```
[13]: 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 ($x_i \to y_i \in \mathbb{R}$): *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:

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

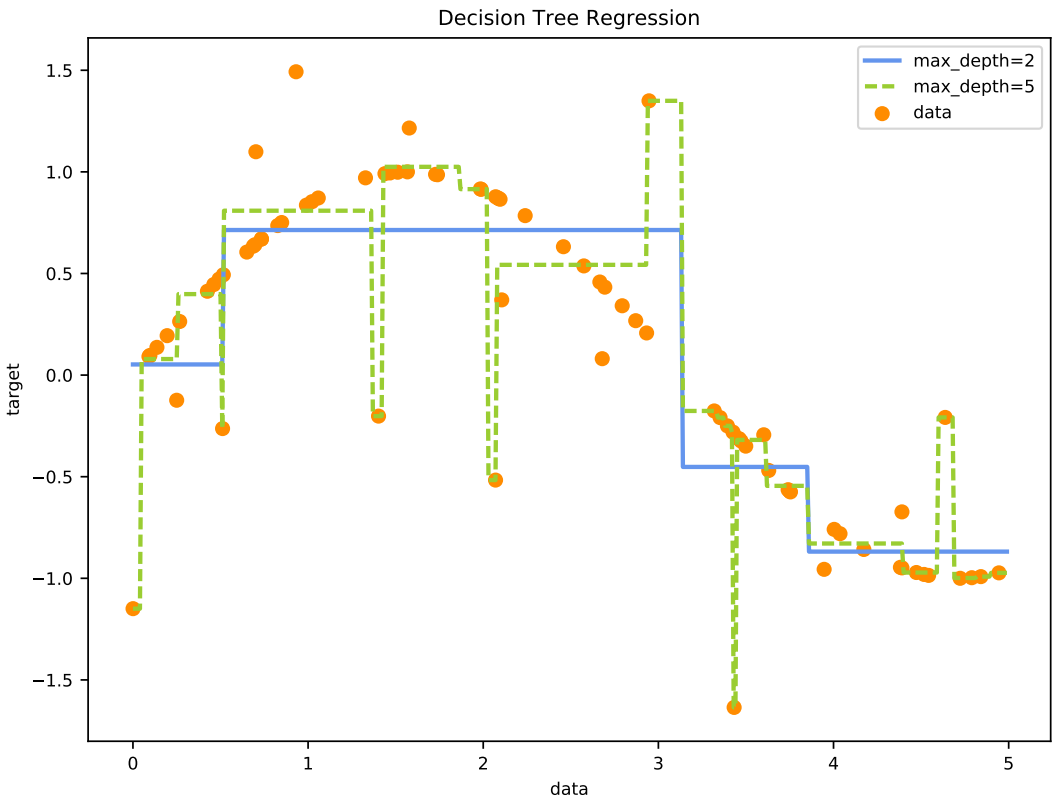
- Assuming that the tree predicts y_i as the average of all x_i in the leaf:

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

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

In scikit-learn Regression is done with `DecisionTreeRegressor`

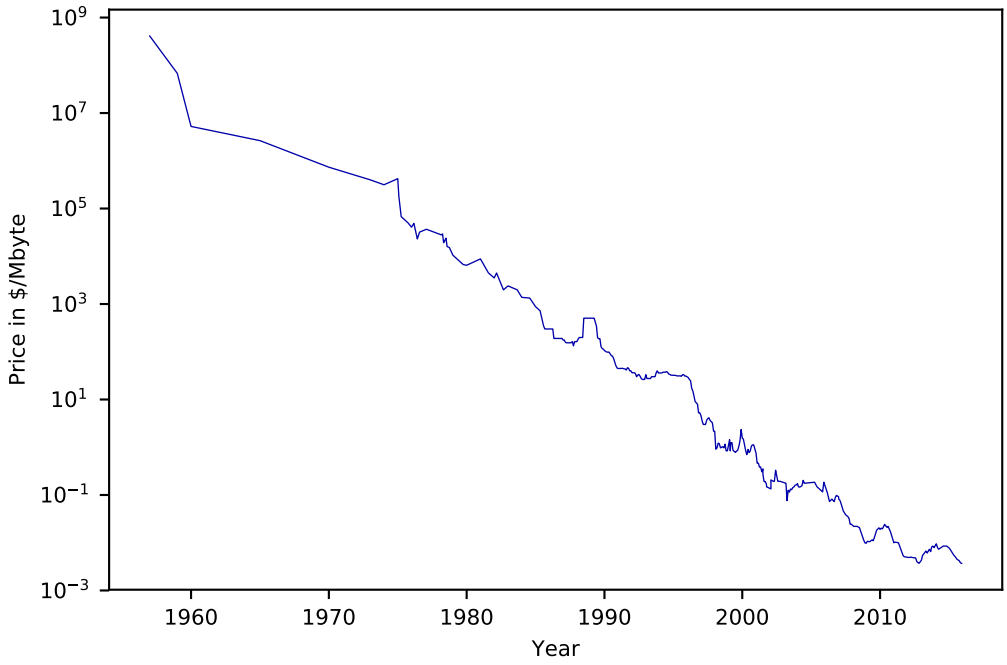
```
[14]: def plot_decision_tree_regression(regr_1, regr_2):
          # Create a random dataset
          rng = np.random.RandomState(1)
          X = np.sort(5 * rng.rand(80, 1), axis=0)
          y = np.sin(X).ravel()
          y[::5] += 3 * (0.5 - rng.rand(16))

          # 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()

[15]: 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

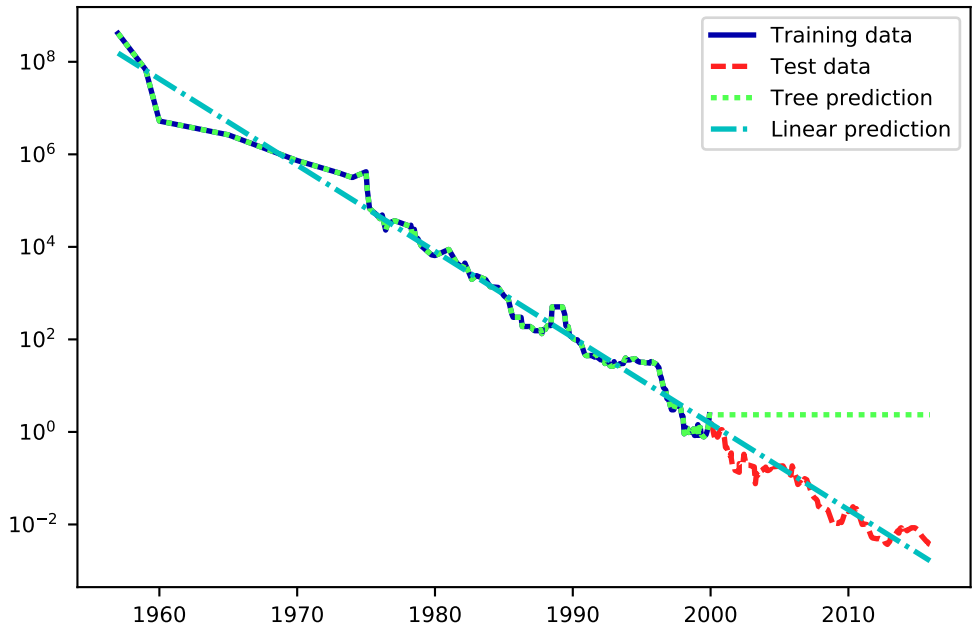
[16]:
```
ram_prices = pd.read_csv('data/ram_price.csv')

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



[17]:
```
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)
```

[18]:
```
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.

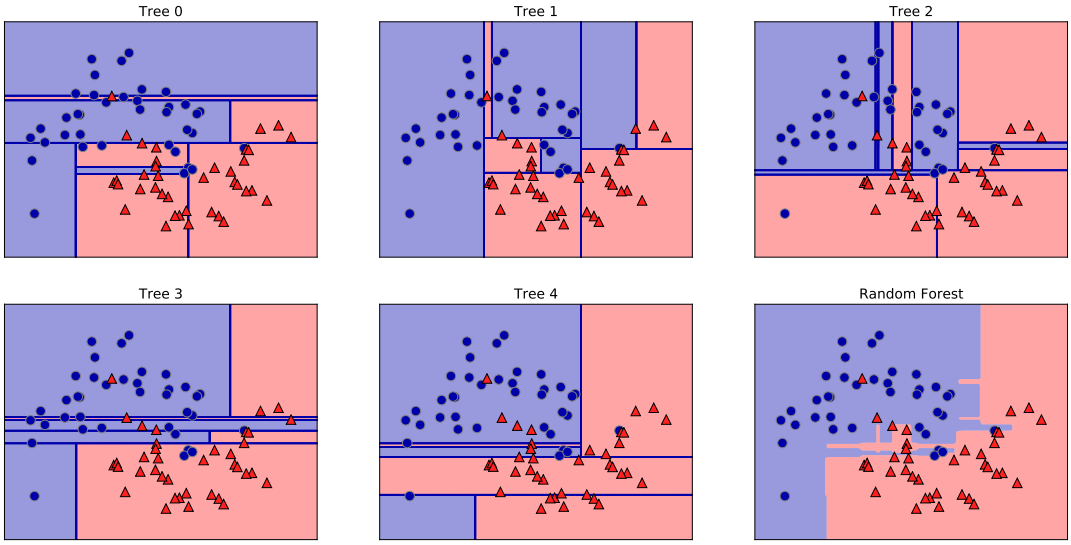
RandomForests

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 * Every member returns probability for each class * After averaging, the class with highest probability wins * Regression:
* Return the *mean* of all predictions

[19]:
```
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=5, 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)
- `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

```
[20]: 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)
```

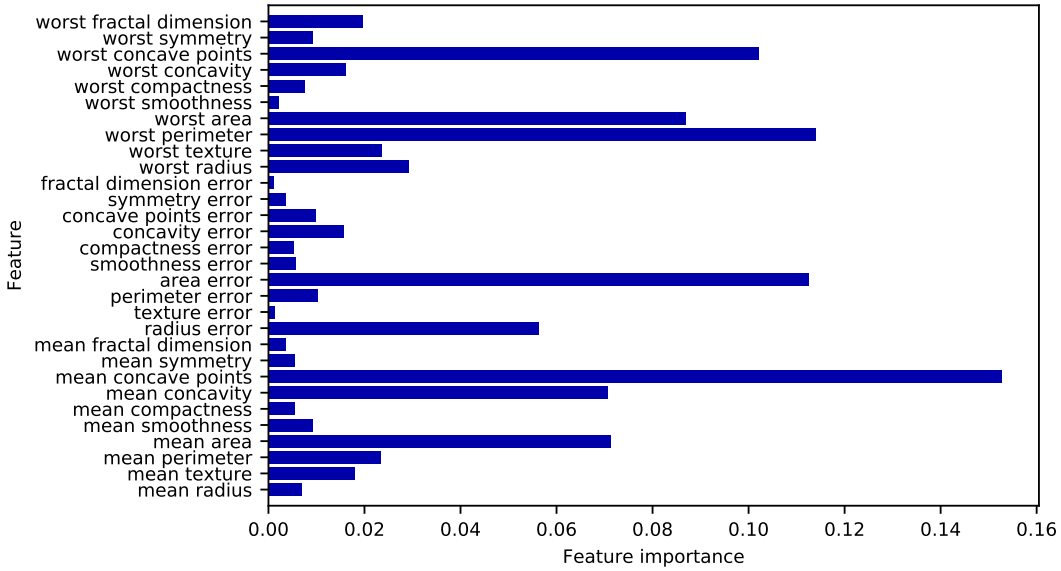
```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=100, n_jobs=1, oob_score=False, random_state=0,
            verbose=0, warm_start=False)
```

```
[21]: forest = RandomForestClassifier(n_estimators=10, 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: 0.951
```

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

```
[23]: 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

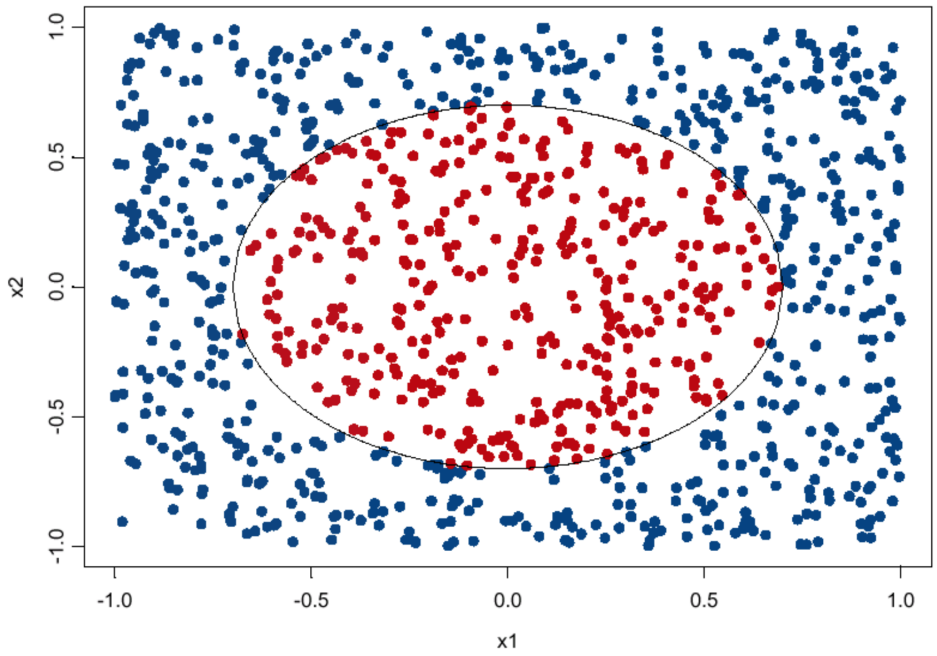
Downsides:

- 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)

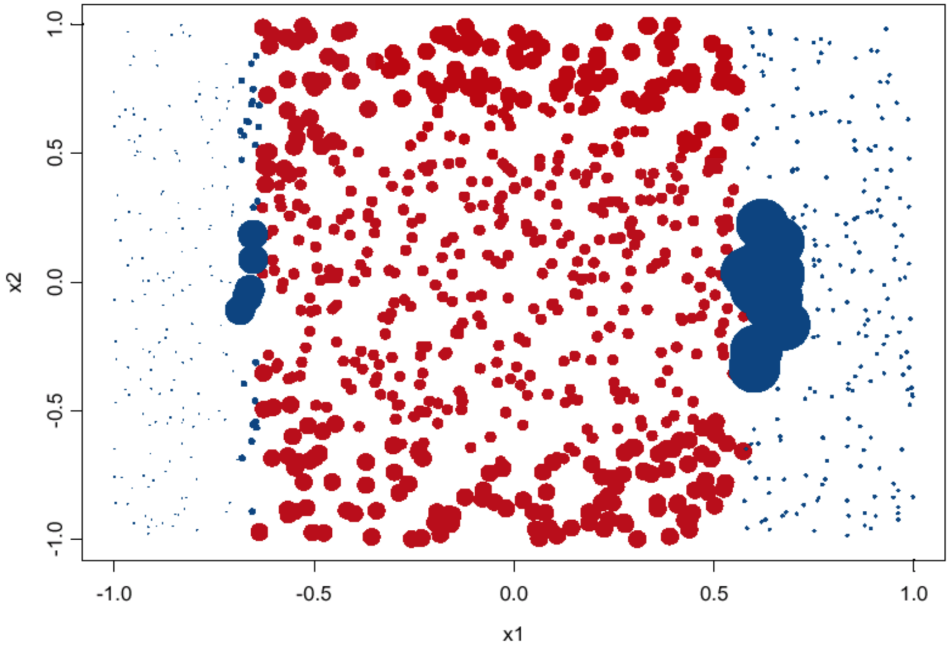
Instead of reducing the variance of overfitted models, reduce the bias of underfitted models

- 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
  - `learning rate` controls how strongly the weights are altered in each iteration (default 0.1)
  - Gradient descent (covered later) finds optimal set of weights
- Repeat `n_estimators` times (default 100)



Example:
After 1 iteration

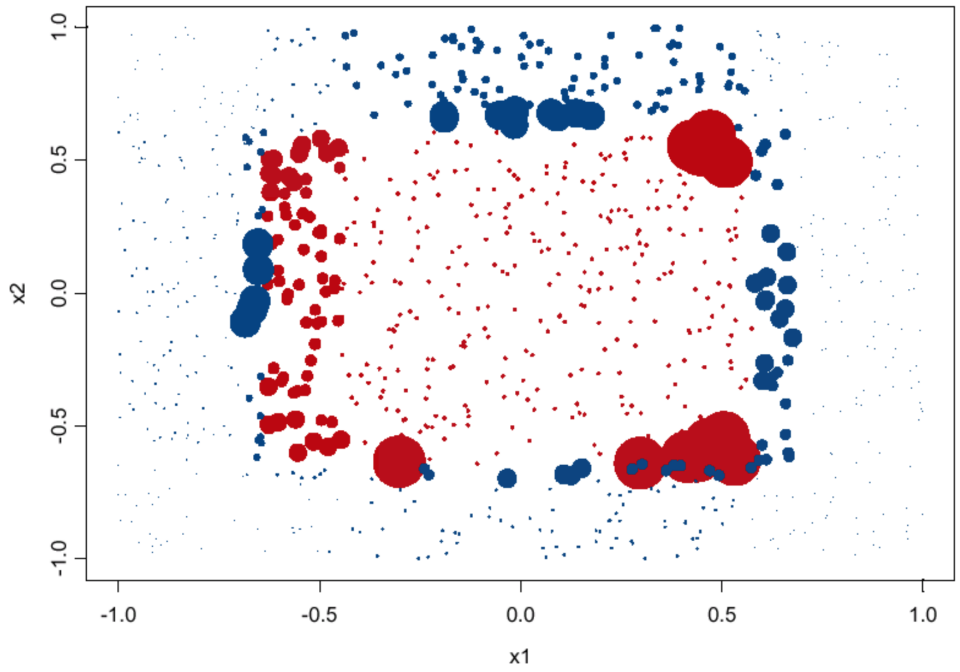
- The simple decision tree divides space
- Misclassified points get higher weight (larger dots)



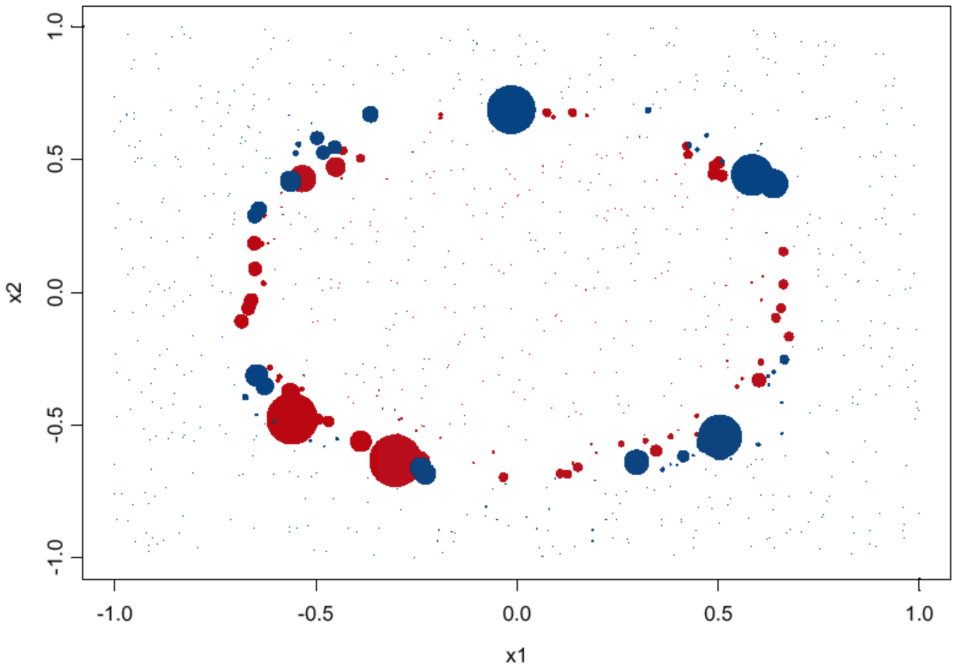
boosting

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

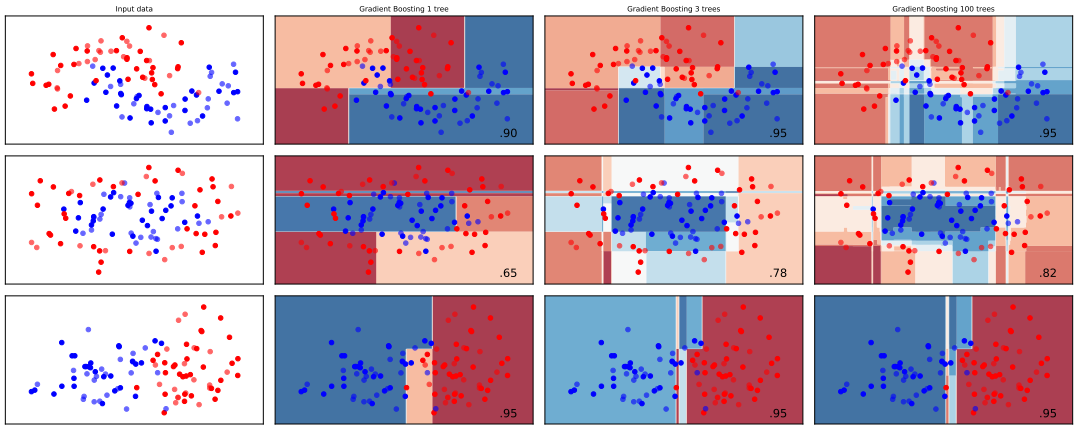


boosting



boosting

[29]:
```
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_
    ]

morelearn.plots.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)

[30]:
```
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
```

```
[31]: # 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)))
```

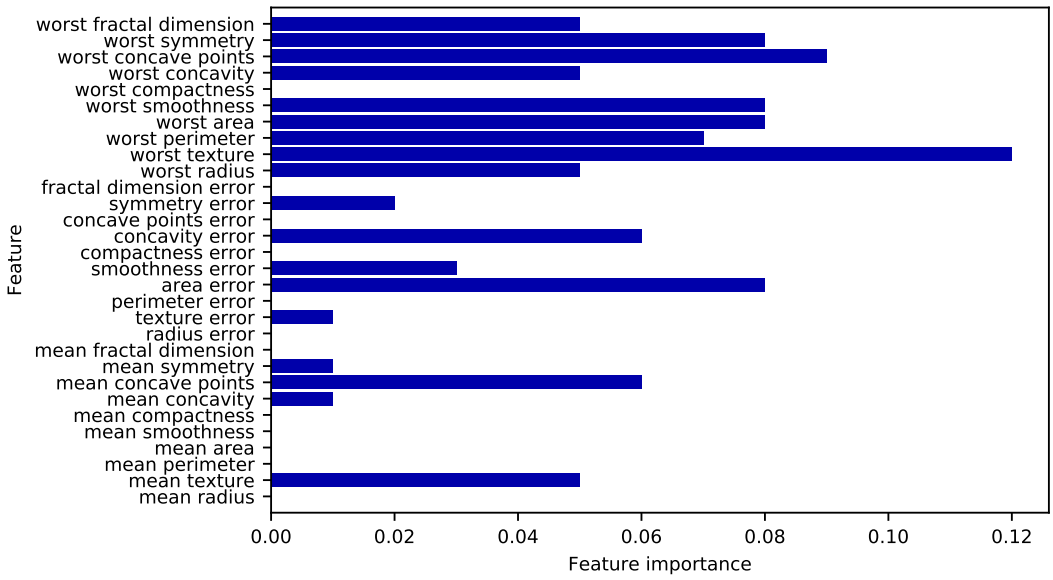
```
Accuracy on training set: 0.991
Accuracy on test set: 0.972
```

```
[32]: # 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

```
[33]: 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

[34]:
```
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))
```

```
---------------------------------------------------------------------------

ImportError                               Traceback (most recent call la

<ipython-input-34-819ed9e4a017> in <module>()
----> 1 import plot_classifiers as pc
      2 names = ["Decision tree", "Random Forest 10", "Gradient Boosting"]
      3
      4 classifiers = [
      5     DecisionTreeClassifier(),
```

```
ImportError: No module named 'plot_classifiers'
```

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