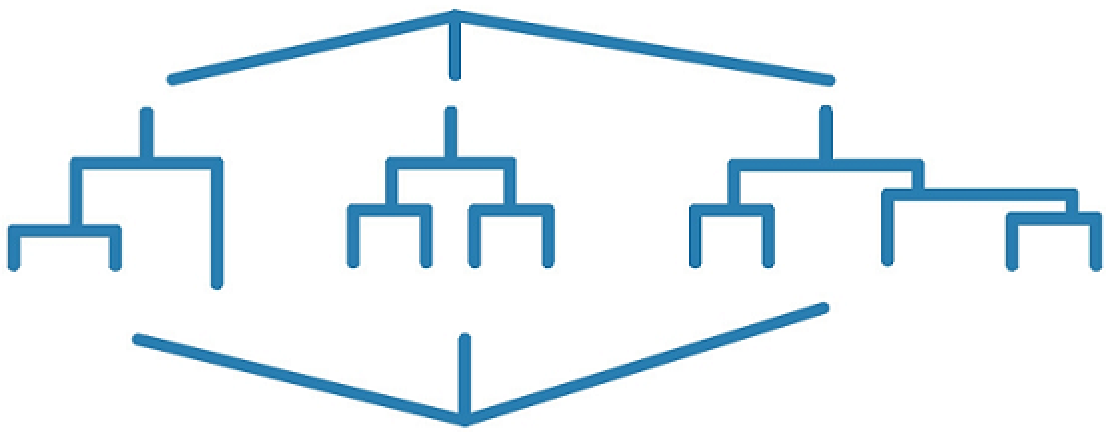
シングル・バギング・ブースティング



目的

3つのモデリング（決定木・ランダムフォレスト・勾配ブースティング）における、精度と特徴量選択を比較する。

データの準備

今回はTitanic（Kaggle）のデータを使用します。

・[https://www.kaggle.com/c/titanic (https://www.kaggle.com/c/titanic)](https://www.kaggle.com/c/titanic)

In [1]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import graphviz
import optuna
import lightgbm as lgb
import xgboost as xgb

from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_auc_score
from sklearn.tree import DecisionTreeClassifier
from sklearn.tree import plot_tree
from sklearn.tree import export_graphviz
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import GradientBoostingClassifier
from catboost import CatBoostClassifier
```

In [2]:

```
train = pd.read_csv('train.csv')
test = pd.read_csv('test.csv')

print('train:',train.shape)
print('test:',test.shape)
```

```
train: (891, 12)
test: (418, 11)
```

In [3]:

```
y = train['Survived']
train = train[[col for col in train.columns if col != 'Survived']]
PassengerId = test['PassengerId']

print('train:',train.shape)
print('test:',test.shape)
```

```
train: (891, 11)
test: (418, 11)
```

In [4]:

```
X = pd.concat([train, test], axis=0)

print('X:',X.shape)
X.head()
```

```
X: (1309, 11)
```

Out[4]:

	PassengerId	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Em
0	1	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	
1	2	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C85	
2	3	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	
3	4	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	
4	5	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	

・Survived：生存したかどうか（0：助からない、1：助かる）

・PassengerId：乗客ID
・Pclass – チケットのクラス（1：上層クラス、2：中級クラス、3：下層クラス）
・Name：乗客の名前
・Sex：性別
・Age：年齢
・SibSp：船に同乗している兄弟・配偶者の数
・parch：船に同乗している親・子供の数
・ticket：チケット番号
・fare：料金
・cabin：客室番号
・Embarked：船に乗った港（C：Cherbourg、Q：Queenstown、S：Southampton）

In [5]:

```
features = ['Pclass', 'Sex', 'Age', 'SibSp', 'Parch', 'Fare', 'Embarked']
X = X[features]

X.head()
```

Out[5]:

	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
0	3	male	22.0	1	0	7.2500	S
1	1	female	38.0	1	0	71.2833	C
2	3	female	26.0	0	0	7.9250	S
3	1	female	35.0	1	0	53.1000	S
4	3	male	35.0	0	0	8.0500	S

後ほど各モデルにおける、特徴量の重要度を比較するため、今回はOne-Hot-Encodingではない前処理をします。

In [6]:

```
def code_transform(x):
    if x == 'male':
        y = 0
    else:
        y = 1
    return y

X['Sex'] = X['Sex'].apply(lambda x: code_transform(x))
```

In [7]:

```
X['Embarked'] = X['Embarked'].fillna(value='missing')

def code_transform(x):
    if x == 'S':
        y = 0
    elif x == 'C':
        y = 1
    elif x == 'Q':
        y = 2
    else:
        y = 3

    return y

X['Embarked'] = X['Embarked'].apply(lambda x: code_transform(x))
```

In [8]:

```
X['Age'] = X['Age'].fillna(X['Age'].median())
X['Fare'] = X['Fare'].fillna(X['Fare'].median())

print(X.dtypes)
print('Total null:',X.isnull().sum().sum())
X.head()
```

```
Pclass        int64
Sex           int64
Age         float64
SibSp         int64
Parch         int64
Fare        float64
Embarked      int64
dtype: object
Total null: 0
```

Out[8]:

	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
0	3	0	22.0	1	0	7.2500	0
1	1	1	38.0	1	0	71.2833	1
2	3	1	26.0	0	0	7.9250	0
3	1	1	35.0	1	0	53.1000	0
4	3	0	35.0	0	0	8.0500	0

In [9]:

```
train_rows = train.shape[0]
X = X[:train_rows]

print('X:', X.shape)
print('y:', y.shape)
```

```
X: (891, 7)
y: (891,)
```

決定木では個々の特徴量は独立に処理され、データの分割はスケールに依存しないため、正規化や標準化は不要である。

In [10]:

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=0)

print('X_train:', X_train.shape)
print('y_train:', y_train.shape)
print('X_test:', X_test.shape)
print('y_test:', y_test.shape)

X_train.head()
```

```
X_train: (712, 7)
y_train: (712,)
X_test: (179, 7)
y_test: (179,)
```

Out[10]:

	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
140	3	1	28.0	0	2	15.2458	1
439	2	0	31.0	0	0	10.5000	0
817	2	0	31.0	1	1	37.0042	1
378	3	0	20.0	0	0	4.0125	1
491	3	0	21.0	0	0	7.2500	0

※今回の発表で重要視するのは、モデルの精度ではなく、どのモデルでも対応できるデータの前処理ですので、ご了承下さい。

1. 決定木

In [11]:

```
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_train)))
print('Accuracy on test set: {:.3f}'.format(tree.score(X_test, y_test)))
```

```
Accuracy on training set: 0.843
Accuracy on test set: 0.816
```

In [12]:

```
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_train)))
print('Accuracy on test set: {:.3f}'.format(tree.score(X_test, y_test)))
```

```
Accuracy on training set: 0.850
Accuracy on test set: 0.816
```

In [13]:

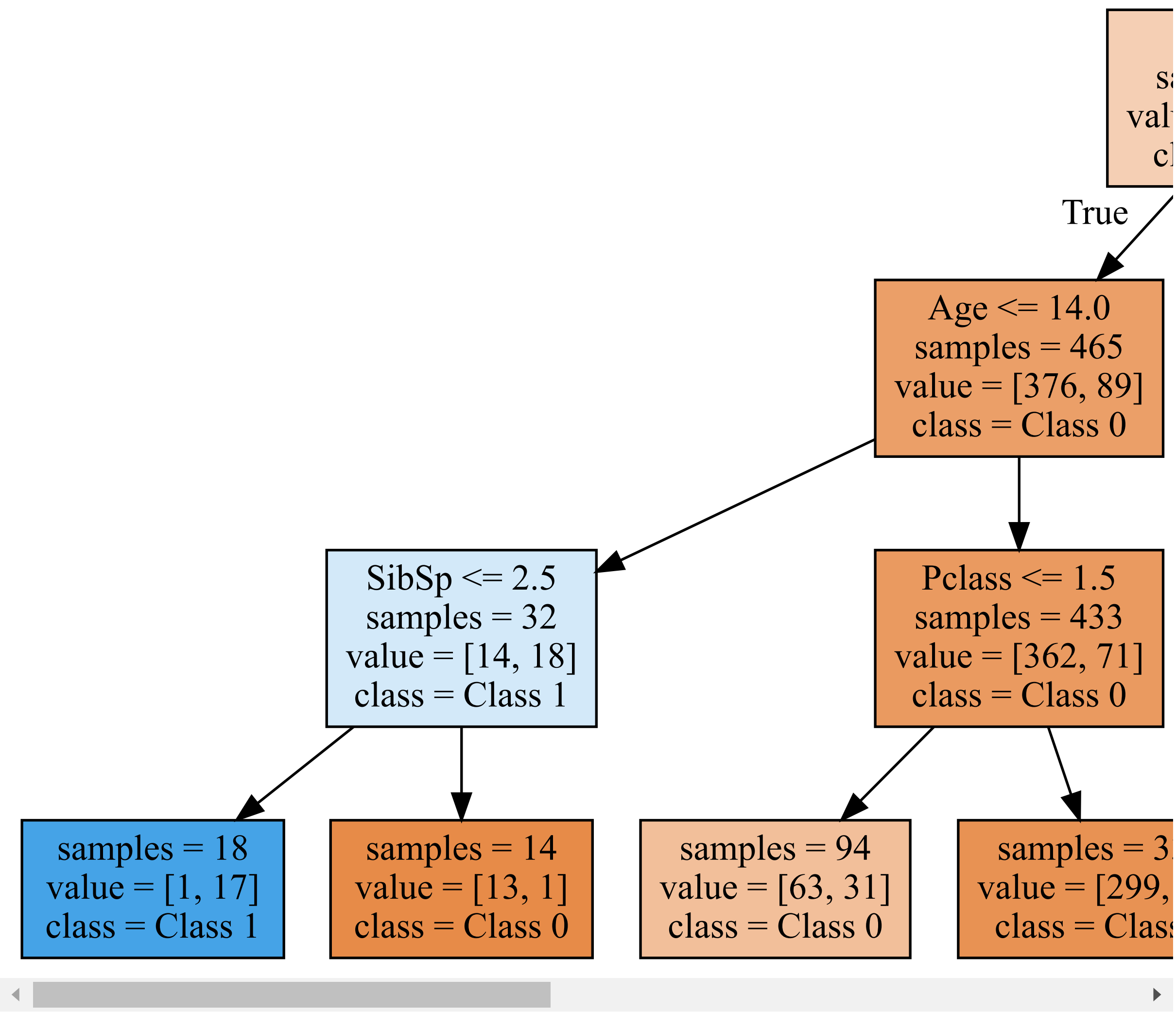
```
tree = DecisionTreeClassifier(max_depth = 6, random_state=0)
tree.fit(X_train, y_train)

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: 0.872
Accuracy on test set: 0.827
```

In [14]:

```
tree = DecisionTreeClassifier(max_depth = 3, random_state=0)
tree.fit(X_train, y_train)

export_graphviz(tree, out_file="tree.dot", class_names=["Class 0", "Class 1"],
                feature_names=features, impurity=False, filled=True)

with open('tree.dot') as f:
    dot_graph = f.read()

graphviz.Source(dot_graph)
```

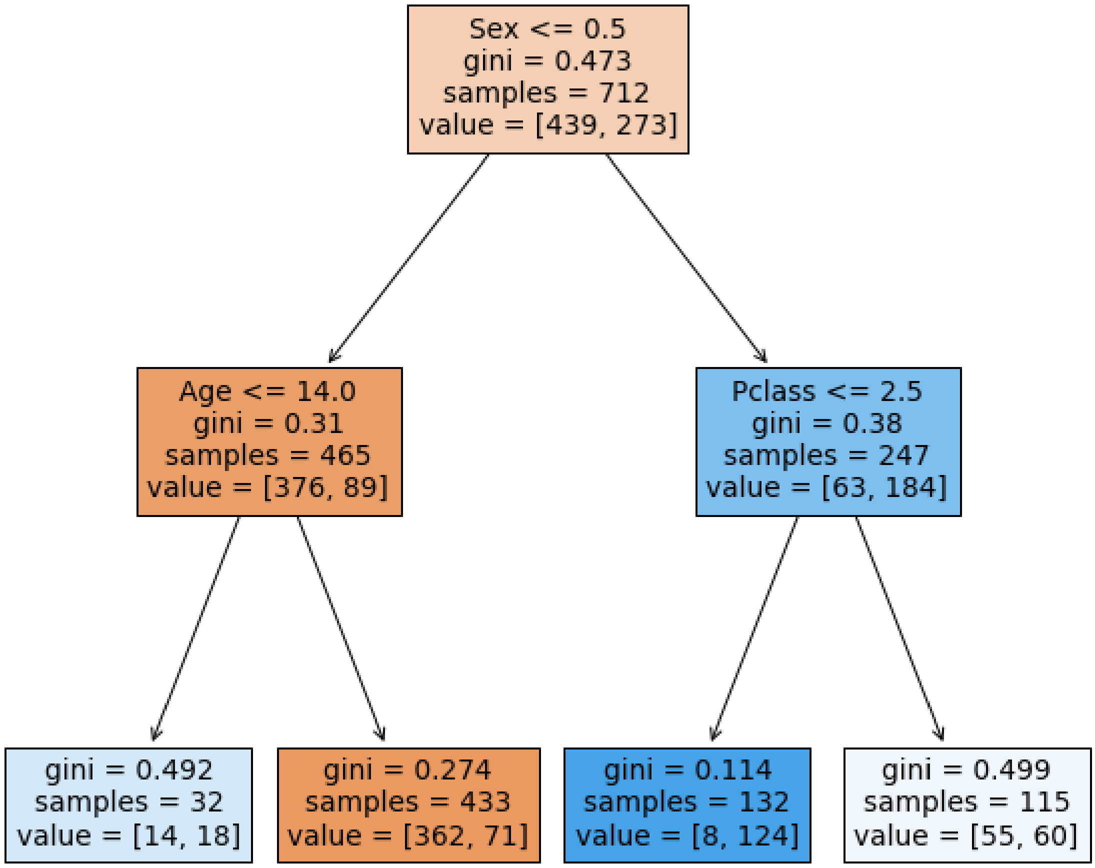
Out[14]:



graphvizはインストールとパスを通す必要があるため、そうでないプロット方法も示しておきます。

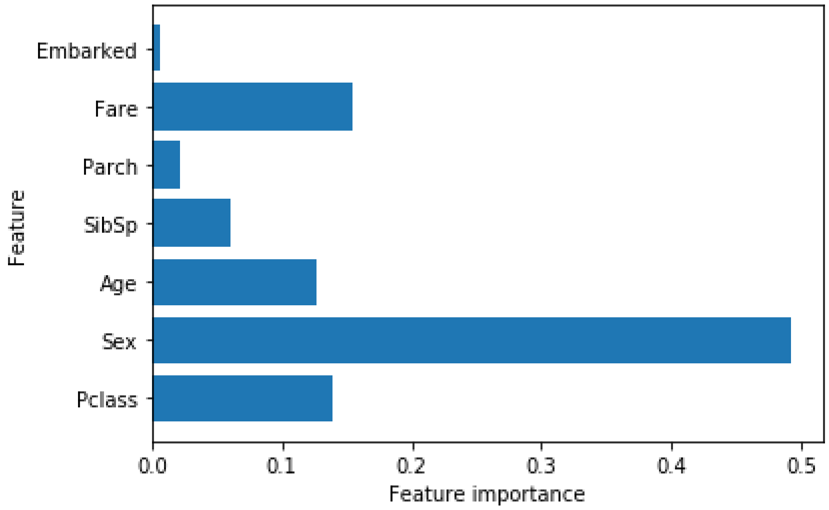
In [15]:

```
tree = DecisionTreeClassifier(max_depth = 2, random_state=0)
tree.fit(X_train, y_train)

fig, ax = plt.subplots(figsize=(10, 10))
plot_tree(tree, feature_names=features, filled=True)
plt.show()
```



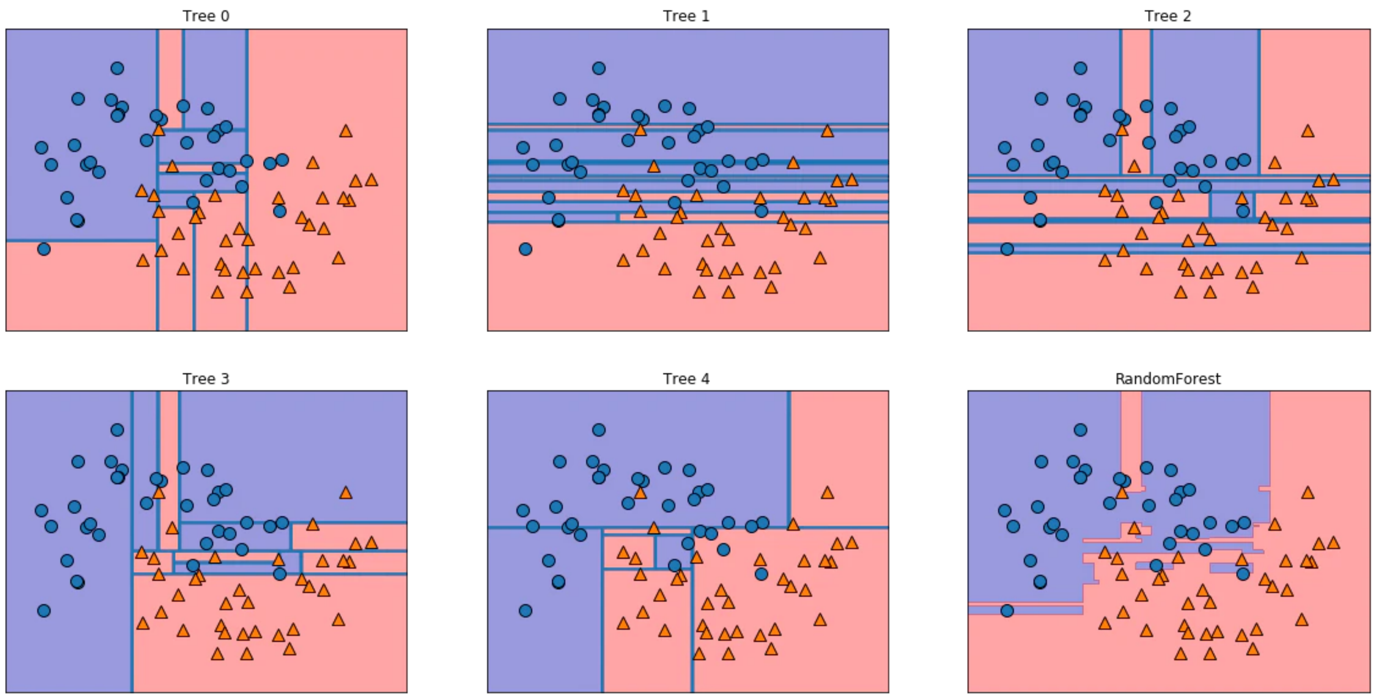
In [16]:

```
tree = DecisionTreeClassifier(max_depth = 6, random_state=0)
tree.fit(X_train, y_train)

def plot_feature_importances_cancer(model):
    n_features = len(features)
    plt.barh(range(n_features), model.feature_importances_, align='center')
    plt.yticks(np.arange(n_features), features)
    plt.xlabel('Feature importance')
    plt.ylabel('Feature')

plot_feature_importances_cancer(tree)
```



2. ランダムフォレスト

ランダムフォレストは、用意した決定木の分類予測確率（○：0.8、△：0.2　など）の平均を取る。



In [17]:

```
forest = RandomForestClassifier(n_estimators=5, random_state=0)
forest.fit(X_train, y_train)

print('Accuracy on training set: {:.3f}'.format(forest.score(X_train, y_train)))
print('Accuracy on test set: {:.3f}'.format(forest.score(X_test, y_test)))
```

```
Accuracy on training set: 0.961
Accuracy on test set: 0.821
```

In [18]:

```
forest = RandomForestClassifier(n_estimators=7, random_state=0)
forest.fit(X_train, y_train)

print('Accuracy on training set: {:.3f}'.format(forest.score(X_train, y_train)))
print('Accuracy on test set: {:.3f}'.format(forest.score(X_test, y_test)))
```

```
Accuracy on training set: 0.963
Accuracy on test set: 0.832
```

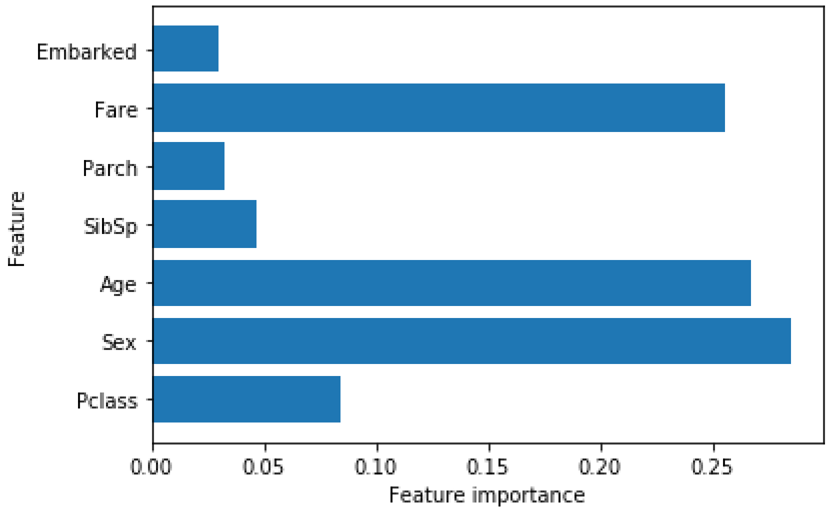
In [19]:

```
%%time

forest = RandomForestClassifier(n_estimators=10, random_state=0)
forest.fit(X_train, y_train)

print('Accuracy on training set: {:.3f}'.format(forest.score(X_train, y_train)))
print('Accuracy on test set: {:.3f}'.format(forest.score(X_test, y_test)))
```

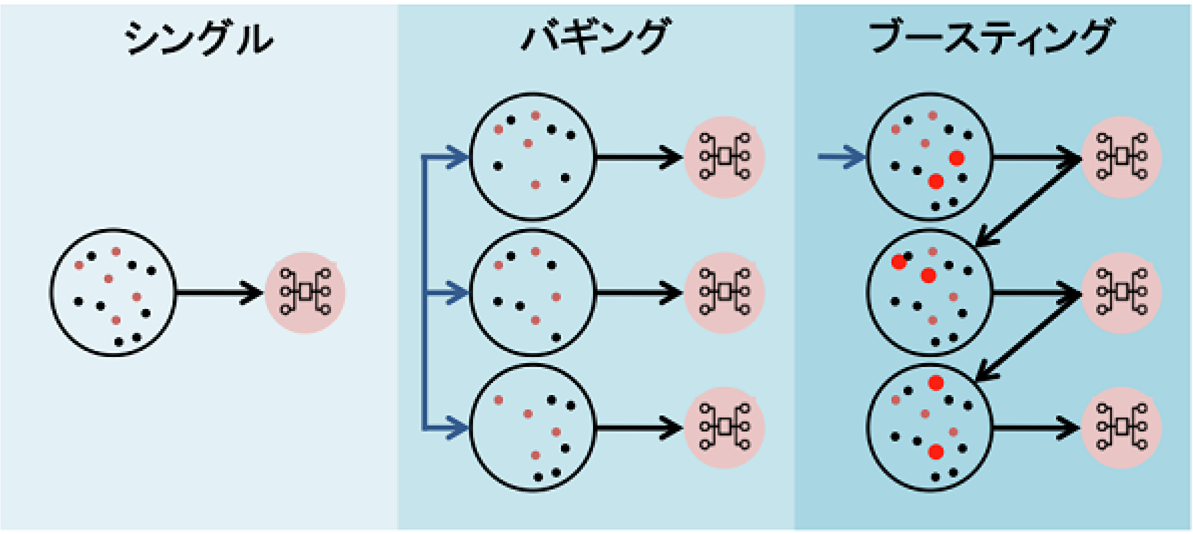
```
Accuracy on training set: 0.963
Accuracy on test set: 0.844
Wall time: 256 ms
```

In [20]:

```
plot_feature_importances_cancer(forest)
```



3. 勾配ブースティング（Gradient Boosting）



In [21]:

```
gbrt = GradientBoostingClassifier(random_state=0, max_depth=1, learning_rate=0.7)
gbrt.fit(X_train, y_train)

print('Training set score: {:.3f}'.format(gbrt.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(gbrt.score(X_test, y_test)))
```

```
Training set score: 0.853
Test set score: 0.832
```

In [22]:

```
gbrt = GradientBoostingClassifier(random_state=0, max_depth=1, learning_rate=0.1)
gbrt.fit(X_train, y_train)

print('Accuracy Training set score: {:.3f}'.format(gbrt.score(X_train, y_train)))
print('Accuracy Test set score: {:.3f}'.format(gbrt.score(X_test, y_test)))
```

```
Accuracy Training set score: 0.819
Accuracy Test set score: 0.804
```

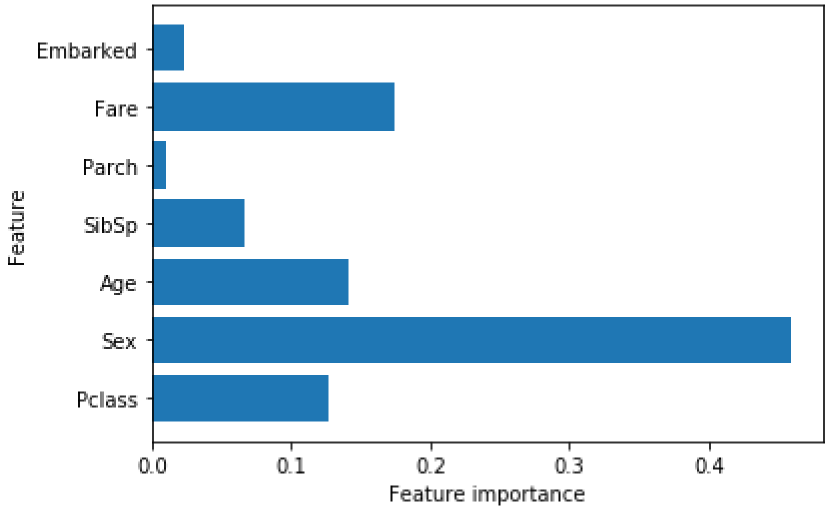
In [23]:

```
%%time

gbrt = GradientBoostingClassifier(random_state=0, max_depth=3, learning_rate=0.1)
gbrt.fit(X_train, y_train)

print('Accuracy Training set score: {:.3f}'.format(gbrt.score(X_train, y_train)))
print('Accuracy Test set score: {:.3f}'.format(gbrt.score(X_test, y_test)))
```

```
Accuracy Training set score: 0.900
Accuracy Test set score: 0.855
Wall time: 436 ms
```

In [24]:

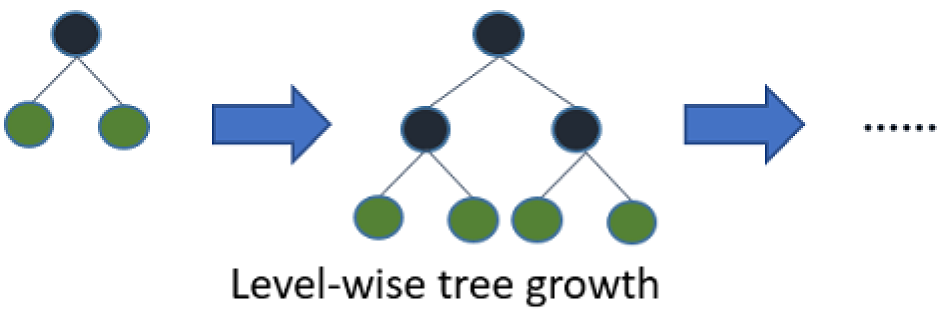
```
plot_feature_importances_cancer(gbrt)
```



実用的な勾配ブースティングモデルについても、いくつか見ておきます。（軽く触れる程度とします）

4. XGBoost（eXtreme Gradient Boosting）

・データとの相性が良ければ、精度が高くなりやすい
・計算に時間がかかる
・パラメータ調整が適切でないと、過学習が起こりやすい



In [25]:

```
# optuna
params = {'n_estimators': 187, 'max_depth': 6, 'learning_rate': 0.2}

cls = xgb.XGBClassifier(**params)
cls.fit(X_train, y_train)

print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.969
Test set score: 0.860
```

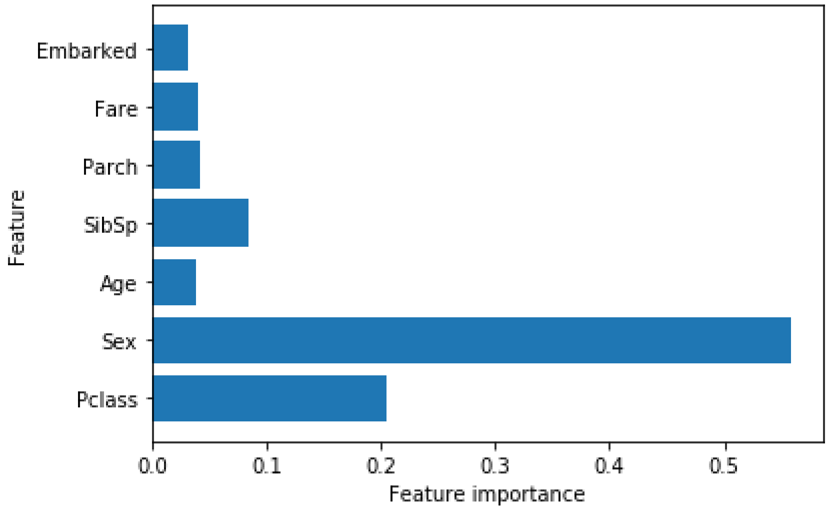
In [26]:

```
%%time

# optuna
params = {'max_bin': 427, 'n_estimators': 105}

cls = xgb.XGBClassifier(**params)
cls.fit(X_train, y_train)

print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.966
Test set score: 0.866
Wall time: 366 ms
```

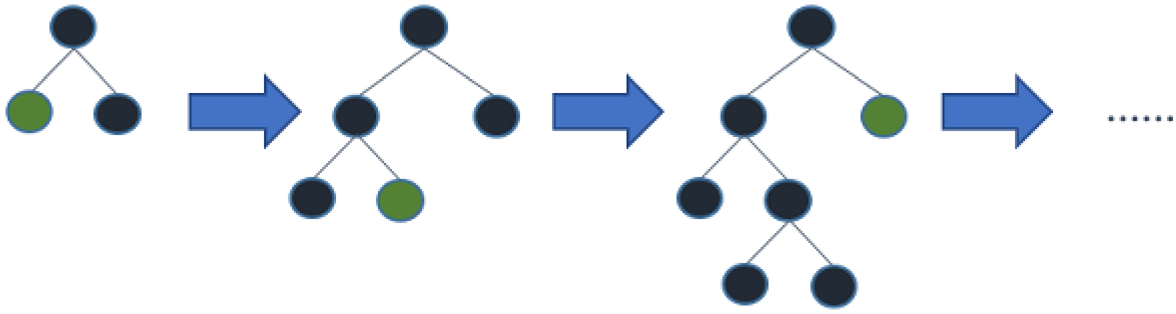
In [27]:

```
plot_feature_importances_cancer(cls)
```



5. LightGBM（Light Grandient Boosting Model）

・カテゴリカル変数をそのまま使用できる
・計算時間を短縮できる
・パラメータ調整が適切でないと、過学習が起こりやすい



Leaf-wise tree growth

In [28]:

```
# optuna
params = {'num_leaves': 10, 'n_estimators': 113, 'max_depth': 8, 'learning_rate': 0.05}

cls = lgb.LGBMClassifier(**params)
cls.fit(X_train, y_train)

print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.881
Test set score: 0.849
```

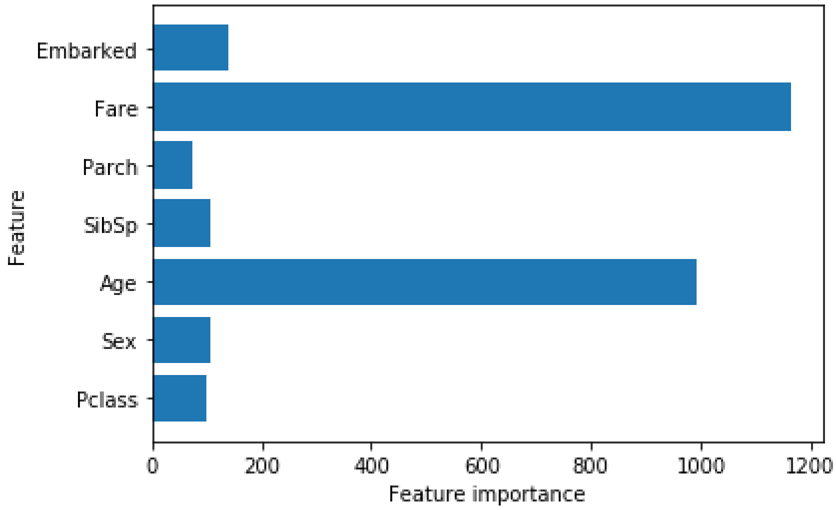
In [29]:

```
%%time

# optuna
params = {'max_bin': 427, 'num_leaves': 100}

cls = lgb.LGBMClassifier(**params)
cls.fit(X_train, y_train)

print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.944
Test set score: 0.855
Wall time: 231 ms
```

In [30]:

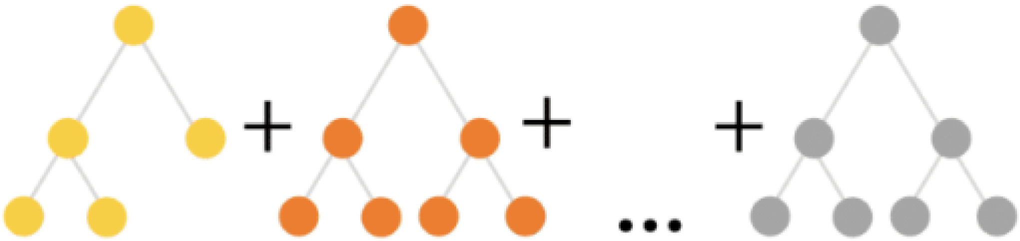
```
plot_feature_importances_cancer(cls)
```



※LightGBMは、今回のように数値変換してしまうより、カテゴリカル変数をそのまま使用した方が、精度が高くなる可能性がある。

6. CatBoost（Category Boosting）

・カテゴリカル変数を扱いやすい
・計算に時間がかかる
・パラメータ調整が適切でないと、過学習が起こりやすい



In [31]:

```
# optuna
params = {'n_estimators': 136, 'max_depth': 3, 'learning_rate': 0.62}

cls = CatBoostClassifier(**params)
cls.fit(X_train, y_train)
```

```
0:	learn: 0.5121904	total: 194ms	remaining: 26.2s
1:	learn: 0.4743104	total: 198ms	remaining: 13.2s
2:	learn: 0.4444765	total: 200ms	remaining: 8.85s
3:	learn: 0.4254633	total: 207ms	remaining: 6.83s
4:	learn: 0.4175372	total: 209ms	remaining: 5.47s
5:	learn: 0.4121246	total: 210ms	remaining: 4.56s
6:	learn: 0.4060387	total: 212ms	remaining: 3.9s
7:	learn: 0.4016509	total: 213ms	remaining: 3.41s
8:	learn: 0.4008569	total: 214ms	remaining: 3.02s
9:	learn: 0.3994919	total: 216ms	remaining: 2.72s
10:	learn: 0.3959648	total: 217ms	remaining: 2.47s
11:	learn: 0.3935381	total: 220ms	remaining: 2.27s
12:	learn: 0.3927453	total: 226ms	remaining: 2.13s
13:	learn: 0.3910029	total: 227ms	remaining: 1.98s
14:	learn: 0.3902787	total: 229ms	remaining: 1.84s
15:	learn: 0.3899352	total: 230ms	remaining: 1.73s
16:	learn: 0.3882807	total: 231ms	remaining: 1.62s
17:	learn: 0.3879221	total: 232ms	remaining: 1.52s
18:	learn: 0.3877781	total: 234ms	remaining: 1.44s
```

In [32]:

```
print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.910
Test set score: 0.838
```

In [33]:

```
%%time

# optuna
params = {'depth' : 6, 'learning_rate' : 0.16, 'early_stopping_rounds' : 10, 'iterations' : 200,}

cls = CatBoostClassifier(**params)
cls.fit(X_train, y_train)
```

```
0:	learn: 0.5995943	total: 5.6ms	remaining: 1.11s
1:	learn: 0.5313538	total: 11.5ms	remaining: 1.14s
2:	learn: 0.4912635	total: 16.6ms	remaining: 1.09s
3:	learn: 0.4623213	total: 27.5ms	remaining: 1.35s
4:	learn: 0.4526194	total: 29.4ms	remaining: 1.15s
5:	learn: 0.4459267	total: 32ms	remaining: 1.04s
6:	learn: 0.4411898	total: 34.8ms	remaining: 960ms
7:	learn: 0.4322463	total: 41.4ms	remaining: 993ms
8:	learn: 0.4257809	total: 44.7ms	remaining: 948ms
9:	learn: 0.4141261	total: 48.4ms	remaining: 920ms
10:	learn: 0.4074414	total: 50.9ms	remaining: 874ms
11:	learn: 0.4020056	total: 60ms	remaining: 941ms
12:	learn: 0.3993023	total: 65ms	remaining: 934ms
13:	learn: 0.3930204	total: 69.3ms	remaining: 921ms
14:	learn: 0.3888778	total: 73.4ms	remaining: 906ms
15:	learn: 0.3848247	total: 79.6ms	remaining: 915ms
16:	learn: 0.3818055	total: 87.2ms	remaining: 939ms
17:	learn: 0.3789712	total: 90.5ms	remaining: 915ms
18:	learn: 0.3736283	total: 93.9ms	remaining: 894ms
```

Wall time: 1.81 s

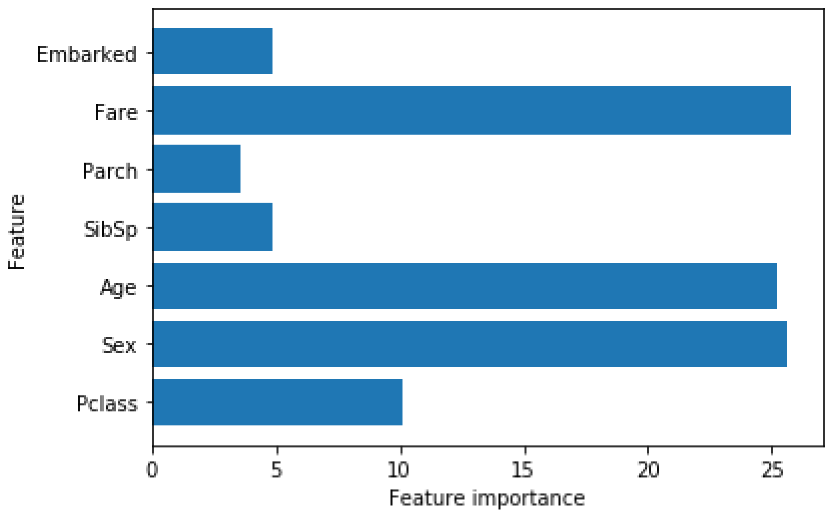
In [34]:

```
print('Training set score: {:.3f}'.format(cls.score(X_train, y_train)))
print('Test set score: {:.3f}'.format(cls.score(X_test, y_test)))
```

```
Training set score: 0.969
Test set score: 0.849
```

In [35]:

```
plot_feature_importances_cancer(cls)
```



考察

今回のTitanicデータにおいて、シングルやブースティングよりも
ランダムフォレストの方が、多くの特徴量を重要視していることが考えられる。

精度については、データとの相性や適切なパラメータの調整ができれば、勾配ブースティングの方が高くなりやすい。
ただし、ランダムフォレストでも、ある程度の精度は担保できており、時間も比較的かからないため、使いやすいというメリットがある。

また、カテゴリカル変数を含むデータや、Kaggleのように最後の1%のまで性能を絞り出す場合には、勾配ブースティングが向いている。

結論

決定木を用いたモデリングをする際は、まずランダムフォレストを試してから、勾配ブースティングを試してみると良い。

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