Elements Of Data Science - F2020

Week 6: Intro to Machine Learning Models Continued

10/18/2020

TODOs

- Readings:
  - Recommended: https://scikit-learn.org/stable/supervised_learning.html
  - Reference: PML Chapter Chap 3
- HW1, Due **Thurs Oct 22nd, 11:59pm ET**
- Answer and submit Quiz 6, **Sunday Oct 25th, 11:59pm ET**
- **Midterm**
  - Release Monday night 10/26
  - Due **Saturday Oct 31st, 11:59pm ET**
  - Have 24hrs after starting exam to finish
  - 30-40 questions (fill in the blank/multiple choice/short answer)
  - Online via Gradescope
  - Questions asked/answered **privately** via Piazza
  - Open-book, open-note, open-python

Today

- Finish Linear Models
- One Vs. Rest For Multiclass/Multilabel Classification
- Distance Based: kNN
- Tree Based: Decision Tree
- Ensembles: Bagging, Boosting, Stacking

Questions?

Linear Models

- Linear Regression
- Logistic Regression
- SVM

Wine as Multi-Class Classification

Wine as Multi-Class Classification

In [2]:
```
df_wine = pd.read_csv('../data/wine_dataset.csv',usecols=['alcohol','ash','proline','hue','class'])

X = df_wine[['proline','hue']]
y = df_wine['class']

zscore = lambda x: (x-x.mean()) / x.std()

X_zscore = X.apply(zscore,axis=0)
alcohol_zscore = zscore(df_wine.alcohol)

y.value_counts().sort_index()
```

Out[2]:
```
0    59
1    71
2    48
Name: class, dtype: int64
```

One Vs. Rest (OvR) Classification For Multiclass, Multilabel

One Vs. Rest (OvR) Classification For Multiclass, Multilabel

- Can use any binary classifier for Multiclass/Multilabel classification by training multiple models:
  - model 1 : class 1 vs (class 2 and class 3)
  - model 2 : class 2 vs (class 1 and class 3)
  - model 3 : class 3 vs (class 1 and class 2)

- For Multiclass
  - Predict $\hat{y}$ using the model with highest $P(y = \hat{y} \mid x)$, or distance from boundary, or ...

- For Multilabel
  - Predict $\hat{y}$ for any model that predicts a value above some threshold

See sklearn for more info and other methods

OvR For Logistic Regression

OvR For Logistic Regression

In [3]:
```
from sklearn.linear_model import LogisticRegression
logr = LogisticRegression(multi_class='ovr', # default
                          max_iter=1000      # to avoid errors
                         )
logr.fit(X_zscore,y)

print(logr.predict(X_zscore.iloc[[15,82,166]]))
print(logr.predict_proba(X_zscore.iloc[[15,82,166]]))
```

```
[0 1 2]
[[9.67392098e-01 3.14881014e-02 1.11980048e-03]
 [1.46331313e-01 8.53010324e-01 6.58362811e-04]
 [1.75637296e-01 3.44369368e-01 4.79993336e-01]]
```

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```
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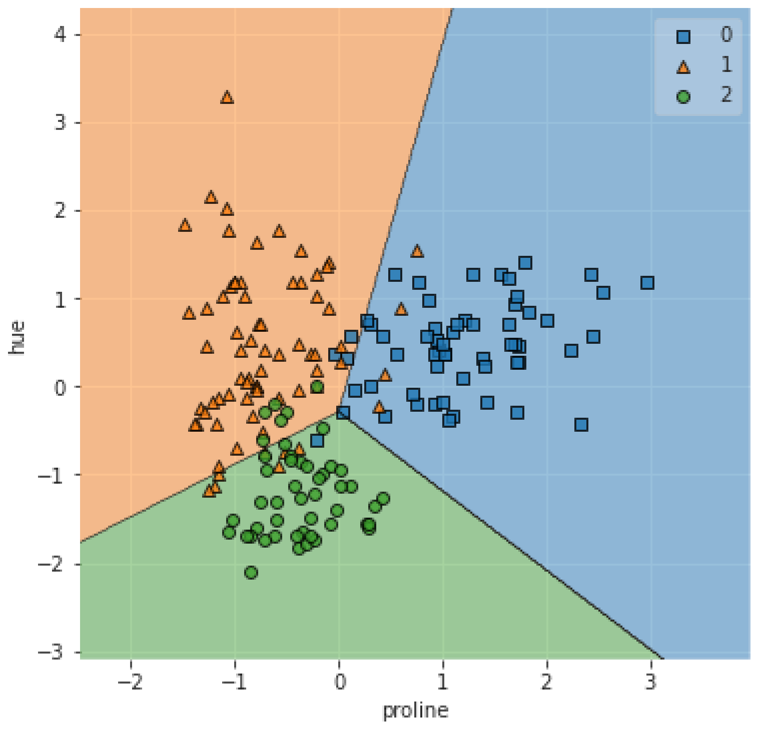
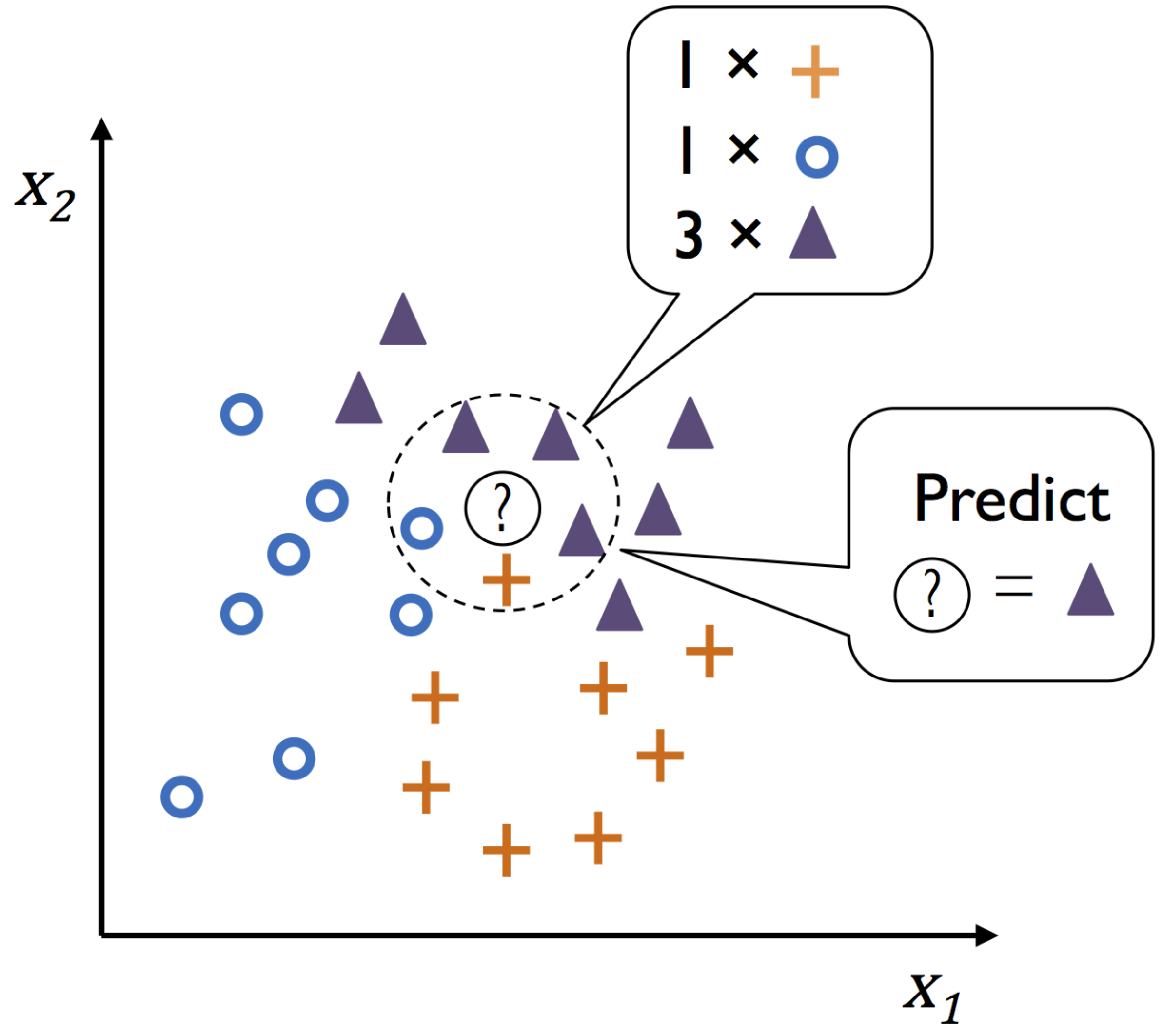
 [1.46331313e-01 8.53010324e-01 6.58362811e-04]
 [1.75637296e-01 3.44369368e-01 4.79993336e-01]]
```

In [4]:
```
fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values,y.values,logr)
ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
```



Distance Based: k-Nearest Neighbor (kNN)

- What category do most of the k nearest neighbors belong to?



From PML

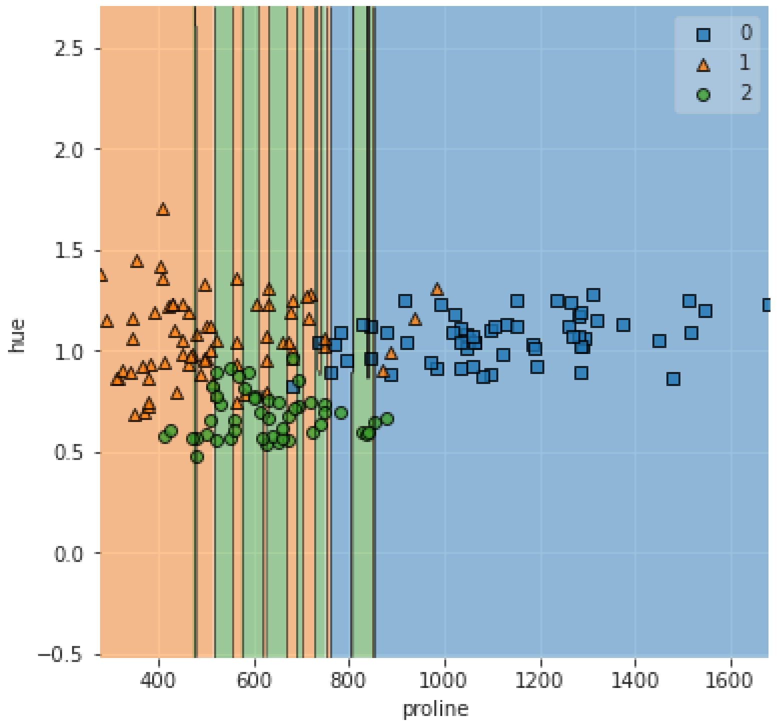
KNN in sklearn

KNN in sklearn

In [5]:
```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors=5)
knn.fit(X,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X.values, y.values, clf=knn);
ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
```

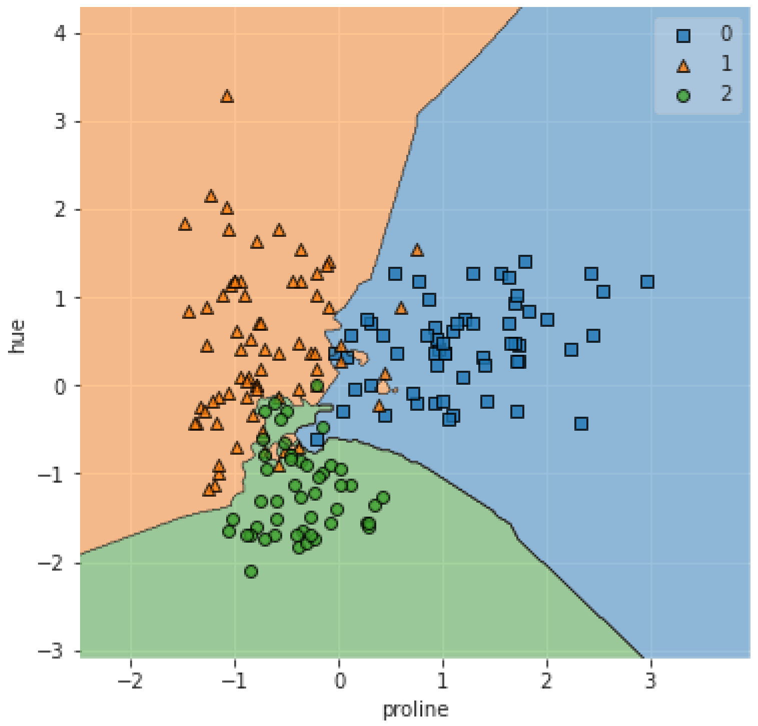


Effects of Standardization on Distance Based Methods

Effects of Standardization on Distance Based Methods

In [6]:
```
knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(X_zscore,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=knn);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



Curse of Dimensionality

The more dimensions, the further away things can be.

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In [7]:
```
x1 = np.array([0,0])
x2 = np.array([1,1])
(((x1 - x2)**2).sum())**.5
```

Out[7]:
```
1.4142135623730951
```

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```

Out[7]:
```
1.4142135623730951
```

In [8]:
```
x1 = np.array([0,0])
x2 = np.array([0,1])
(((x1 - x2)**2).sum())**.5
```

Out[8]:
```
1.0
```

Curse of Dimensionality

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(((x1 - x2)**2).sum())**.5
```

Out[8]: 1.0

In [9]:
```
x1,x2 = np.zeros(1000),np.ones(1000)
(((x1 - x2)**2).sum())**.5
```

Out[9]: 31.622776601683793

Curse of Dimensionality

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```
x1 = np.array([0,0])
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```

Out[7]: 1.4142135623730951

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```

Out[8]: 1.0

In [9]:
```
x1,x2 = np.zeros(1000),np.ones(1000)
(((x1 - x2)**2).sum())**.5
```

Out[9]: 31.622776601683793

In [10]:
```
x2[0] = 0
(((x1 - x2)**2).sum())**.5
```

Out[10]: 31.606961258558215

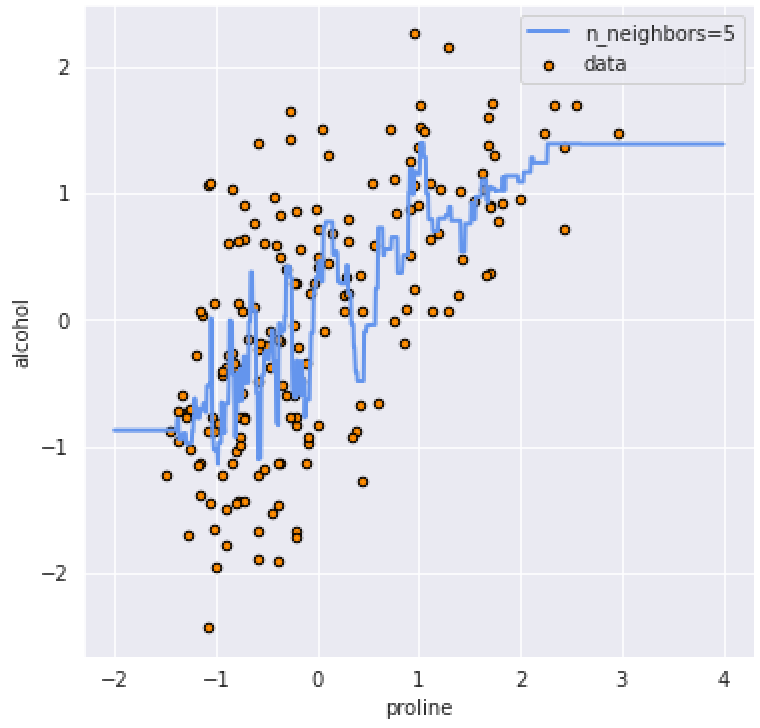
Regression with kNN

Regression with kNN

In [11]:
```
from sklearn.neighbors import KNeighborsRegressor, KNeighborsClassifier

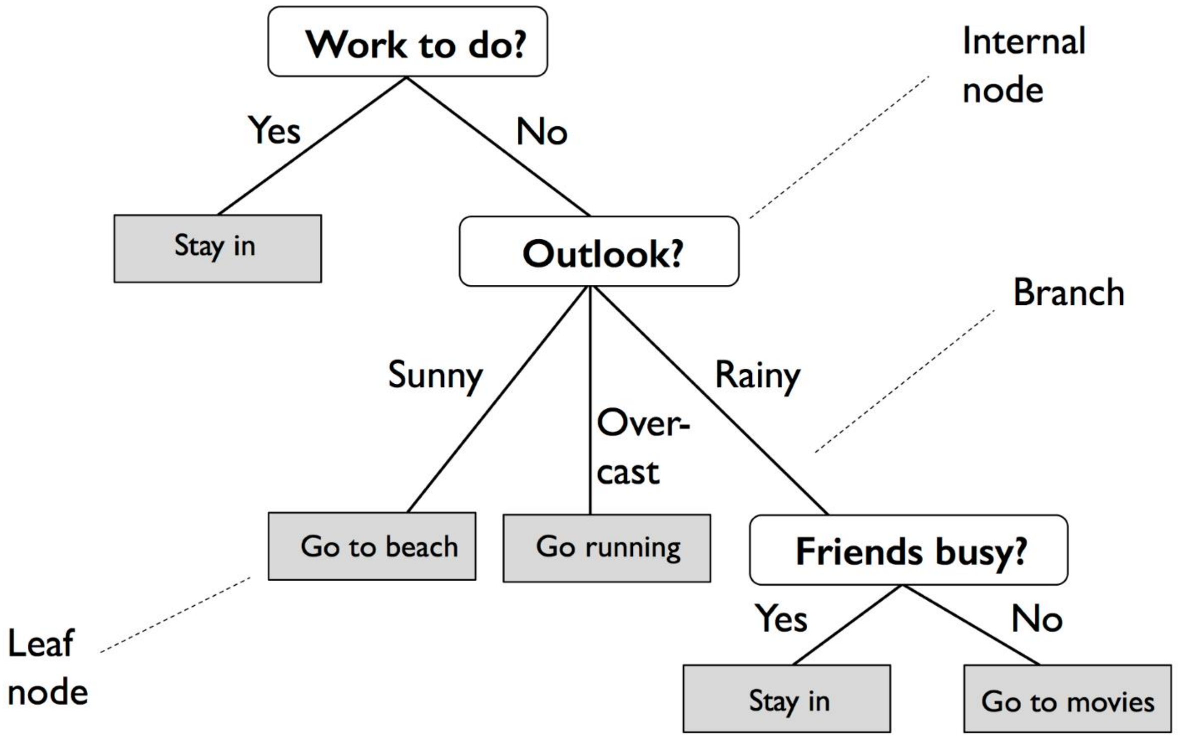
knnr = KNeighborsRegressor(n_neighbors=5)
knnr.fit(X_zscore.proline.values.reshape(-1,1),alcohol_zscore)
X_test = np.linspace(-2,4,1000).reshape(-1,1)
y_hat = knnr.predict(X_test)

fig,ax = plt.subplots(1,1,figsize=(6,6))
ax.scatter(X_zscore.proline, alcohol_zscore, s=20, edgecolor="black",
            c="darkorange", label="data")
ax.plot(X_test, y_hat, color="cornflowerblue",
         label="n_neighbors=5", linewidth=2)
ax.set_xlabel('proline'); ax.set_ylabel('alcohol'); ax.legend();
```



Decision Tree

- What answer does a series of yes/no questions lead us to?



From PML

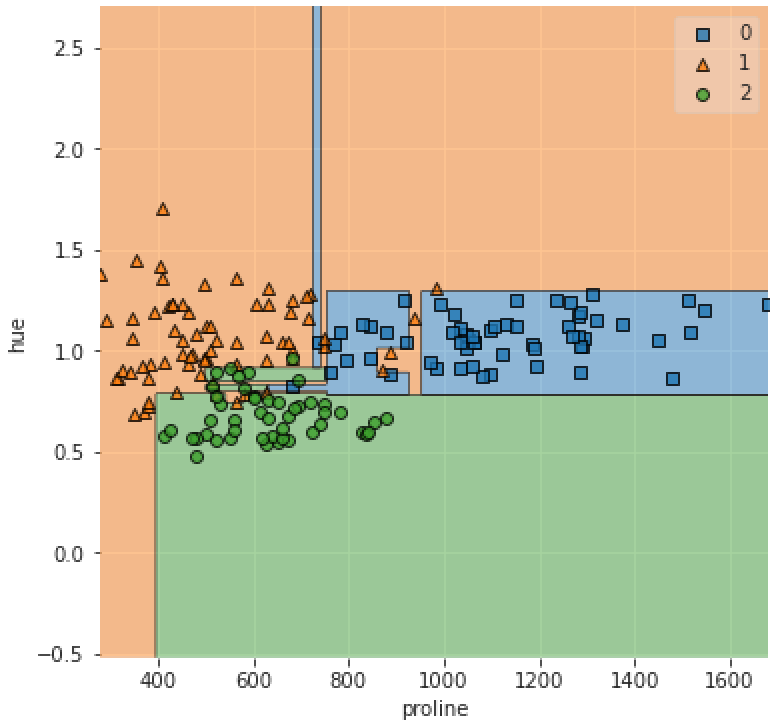
Decision Tree Classifier in sklearn

Decision Tree Classifier in sklearn

In [13]:
```
from sklearn.tree import DecisionTreeClassifier

dtc = DecisionTreeClassifier(max_depth=10)
dtc.fit(X,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X.values, y.values, clf=dtc);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```

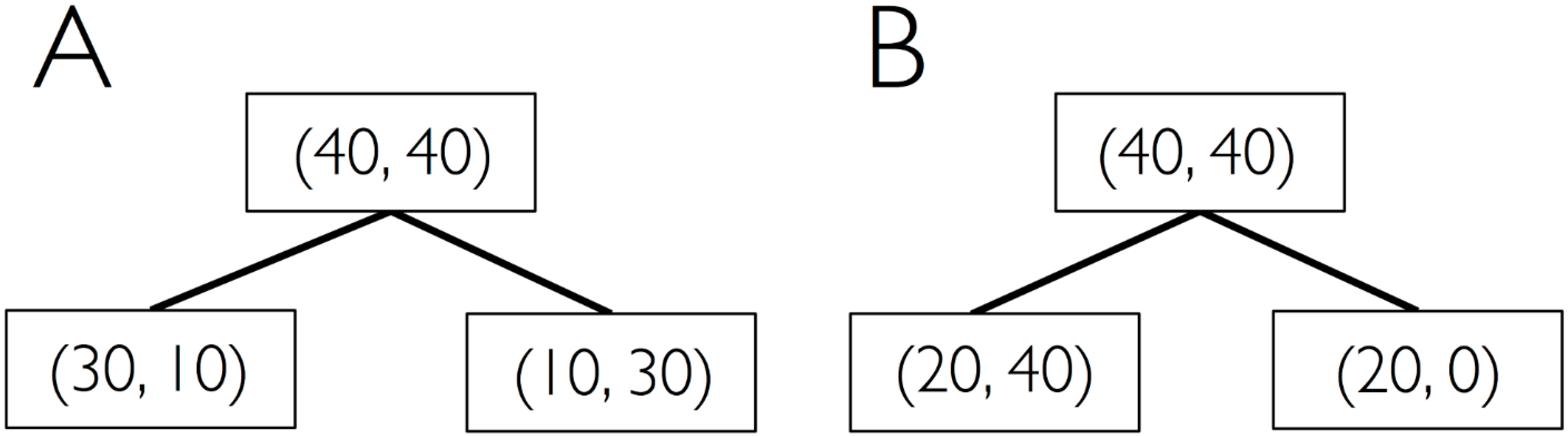


Building a Decision Tree

- How to decide which question to choose? **Reduce Impurity**

Building a Decision Tree

- How to decide which question to choose? **Reduce Impurity**



From PML

Plot Learned Decision Tree Using sklearn

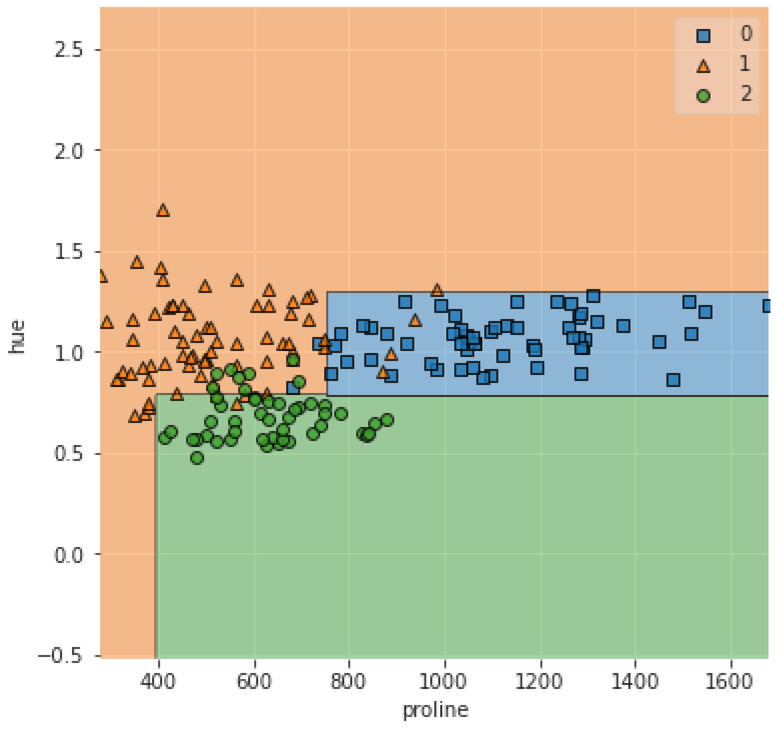
```
# Note: there is a conflict between plot_tree and seaborn.set_style in sklearn < .24
from sklearn.tree import plot_tree
# for tree with maxdepth=10
plot_tree(dtc,ax=ax,fontsize=8,feature_names=X.columns,filled=True);
```

Decision Tree: Limit Maximum Depth

Decision Tree: Limit Maximum Depth

In [15]:
```
dtc_md3 = DecisionTreeClassifier(max_depth=3)
dtc_md3.fit(X,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X.values, y.values, clf=dtc_md3);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



Plot Learned Decision Tree Using sklearn

- For tree with max_depth=3

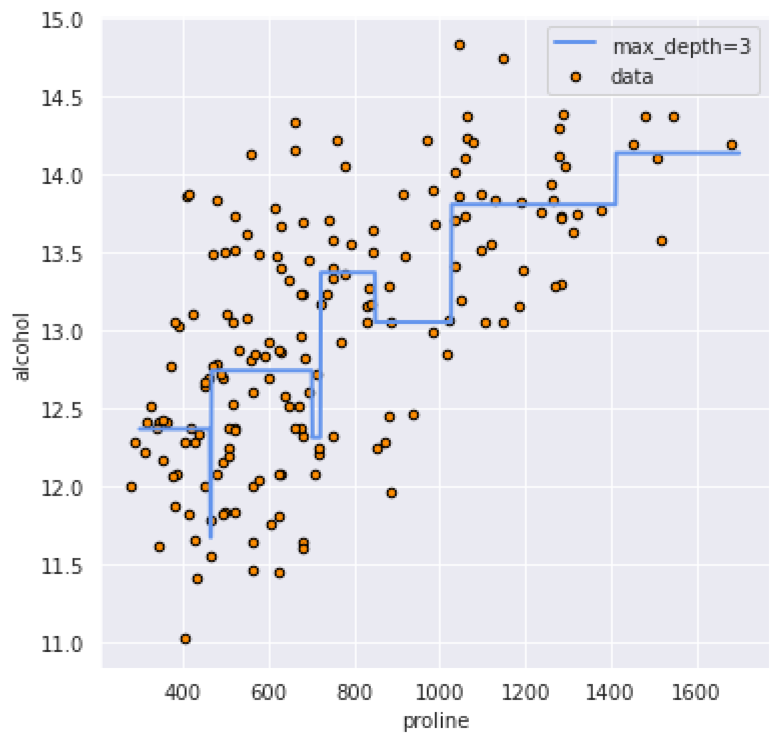
Regression with Decision Trees

Regression with Decision Trees

In [16]:
```
from sklearn.tree import DecisionTreeRegressor

dtr = DecisionTreeRegressor(max_depth=3)
dtr.fit(X.proline.values.reshape(-1,1),df_wine.alcohol)
X_test = np.linspace(300,1700,1000)[:,np.newaxis]
y_hat = dtr.predict(X_test)

fig,ax = plt.subplots(1,1,figsize=(6,6))
ax.scatter(X.proline, df_wine.alcohol, s=20, edgecolor="black",
            c="darkorange", label="data")
ax.plot(X_test, y_hat, color="cornflowerblue",
         label="max_depth=3", linewidth=2)
ax.set_xlabel('proline'); ax.set_ylabel('alcohol'); plt.legend();
```



Ensemble Methods

- "Wisdom of the crowd"
- Can often achieve better performance with collection of learners
- Often use shallow trees as base learners

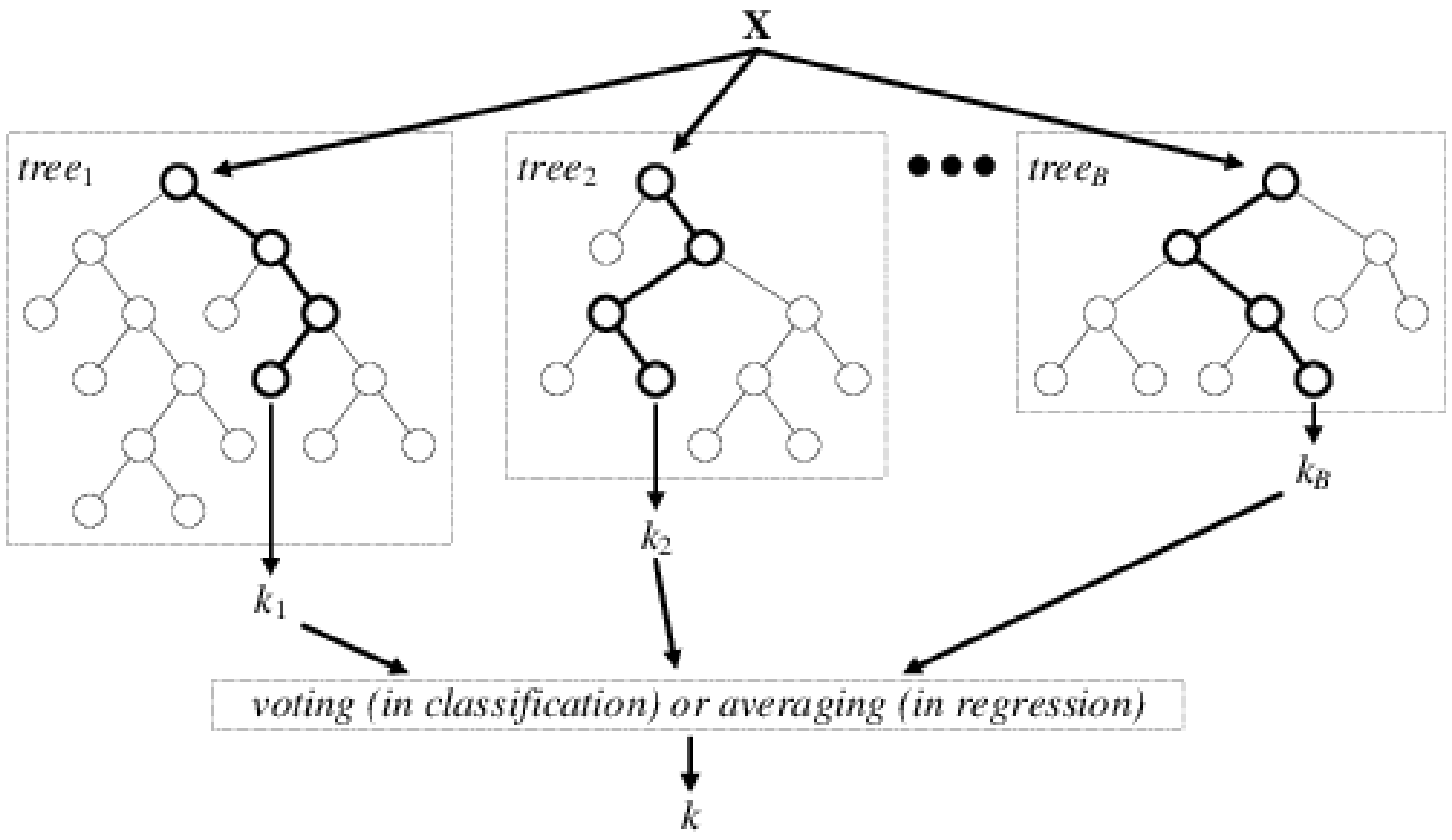
Ensemble Methods

- "Wisdom of the crowd"
- Can often achieve better performance with collection of learners
- Often use shallow trees as base learners

Common methods for generating ensembles:

- **Bagging** (Bootstrap Aggregation)
  - Random Forest
- **Boosting**
  - Gradient Boosting
- **Stacking**

Random Forest and Gradient Boosted Trees



From https://www.researchgate.net/publication/301638643_Electromyographic_Patterns_during_Golf_Swing_Activation_Sequence_Profiling_and_Prediction_of_Shot_Effectiveness

Bagging with Random Forests

- Trees built with bootstrap samples and subsets of features
- Achieve variation with random selection of observations and features

Sample indices	Bagging round 1	Bagging round 2	…
1	2	7	…
2	2	3	…
3	1	2	…
4	3	1	…
5	7	1	…
6	2	7	…
7	4	7	…

C_1 C_2 C_m

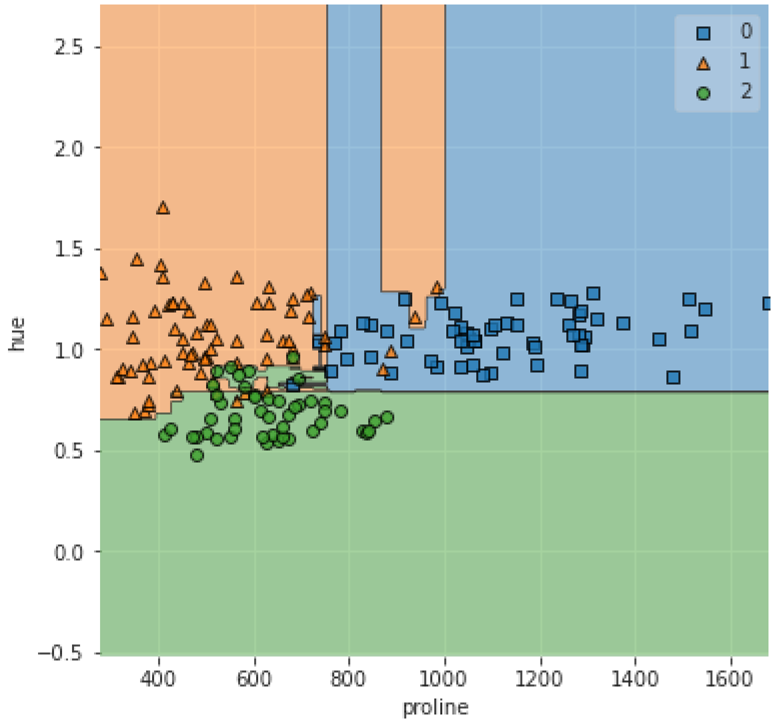
Random Forests with sklearn

Random Forests with sklearn

In [17]:
```
from sklearn.ensemble import RandomForestClassifier

rfc = RandomForestClassifier(n_estimators=10, # number of trees in ensemble
                             n_jobs=-1,       # parallelize using all available cores
                             random_state=0  # for demonstration only
                            )
rfc.fit(X,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X.values, y.values, clf=rfc);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



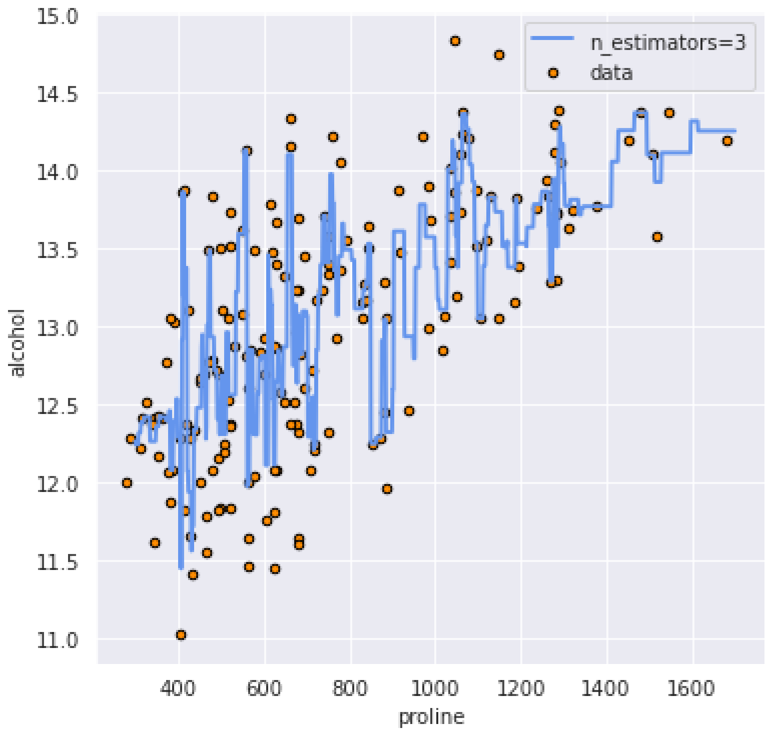
Regression with RandomForests

Regression with RandomForests

In [18]:
```
from sklearn.ensemble import RandomForestRegressor

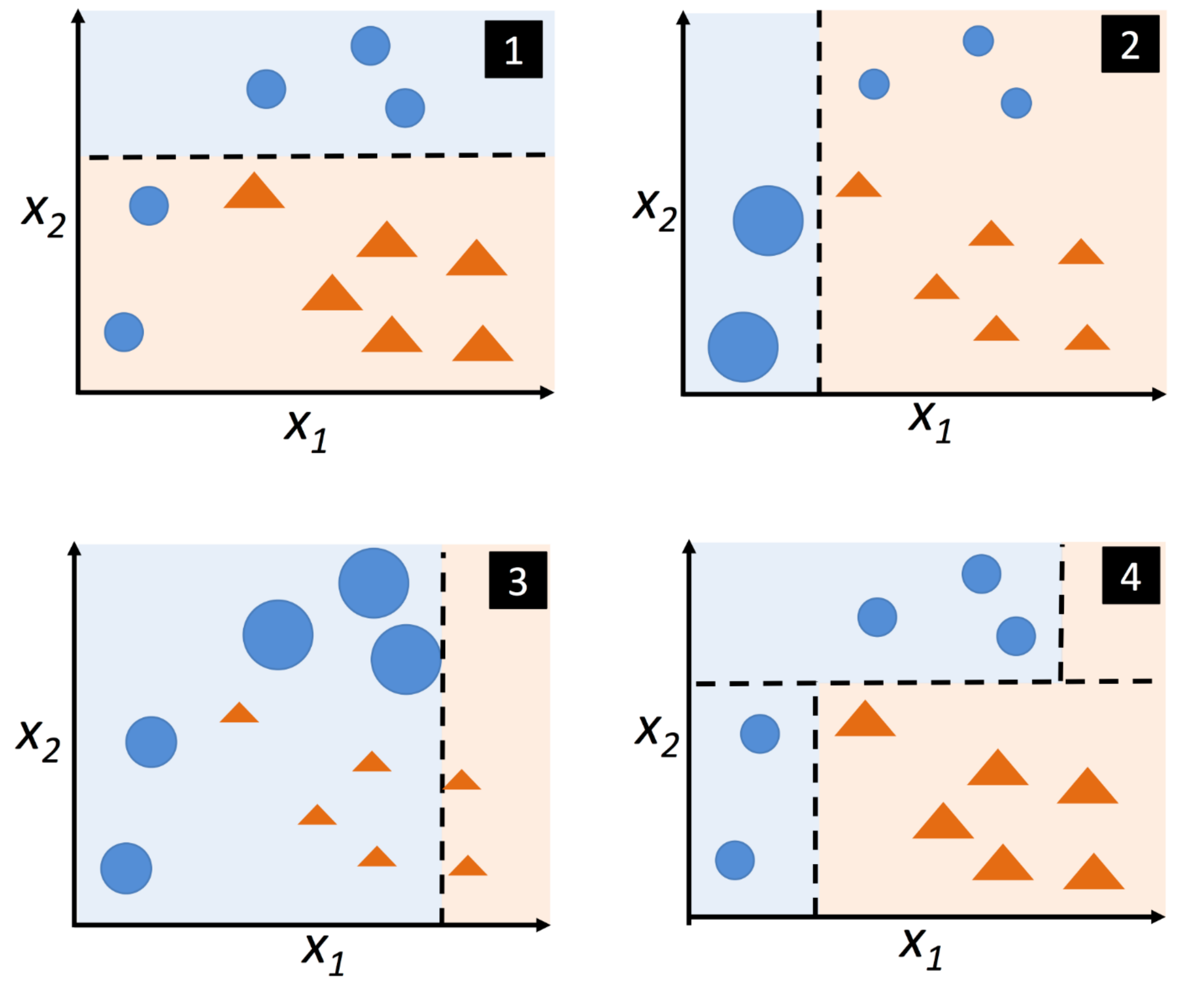
rfr = RandomForestRegressor(n_estimators=3, n_jobs=-1)
rfr.fit(df_wine.proline.values.reshape(-1,1),df_wine.alcohol)
X_test = np.linspace(300,1700,1000)[:,np.newaxis]
y_hat = rfr.predict(X_test)

fig,ax = plt.subplots(1,1,figsize=(6,6))
ax.scatter(df_wine.proline, df_wine.alcohol, s=20, edgecolor="black",
            c="darkorange", label="data")
ax.plot(X_test, y_hat, color="cornflowerblue",
         label="n_estimators=3", linewidth=2)
ax.set_xlabel('proline'); ax.set_ylabel('alcohol'); plt.legend();
```



Gradient Boosted Trees

- Trees built by adding weight to mis-classification
- Achieve variation due to changes in weights on observations



From PML

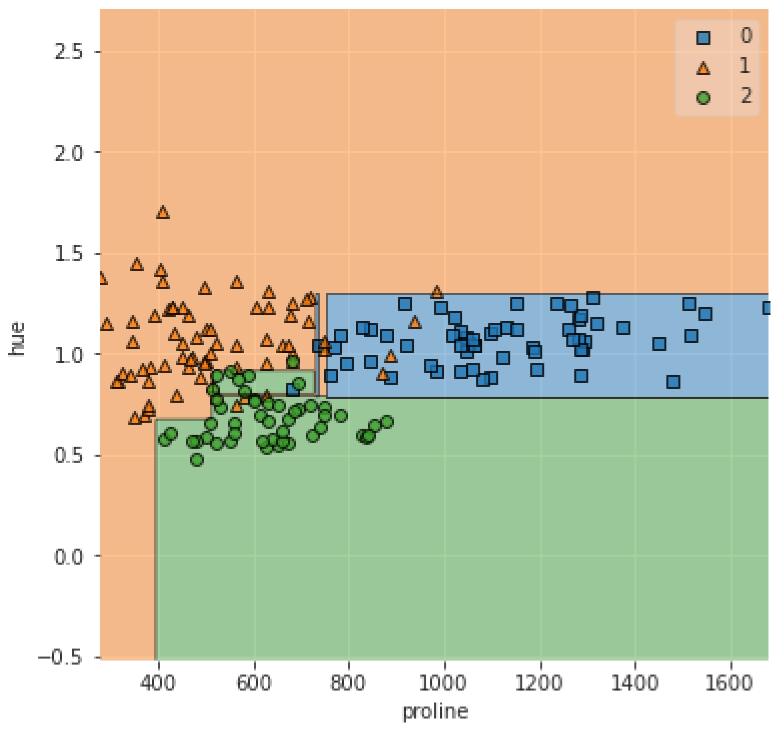
Gradient Boosted Trees in sklearn

Gradient Boosted Trees in sklearn

In [19]:
```
from sklearn.ensemble import GradientBoostingClassifier

gbc = GradientBoostingClassifier(n_estimators=10)
gbc.fit(X,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X.values, y.values, clf=gbc);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



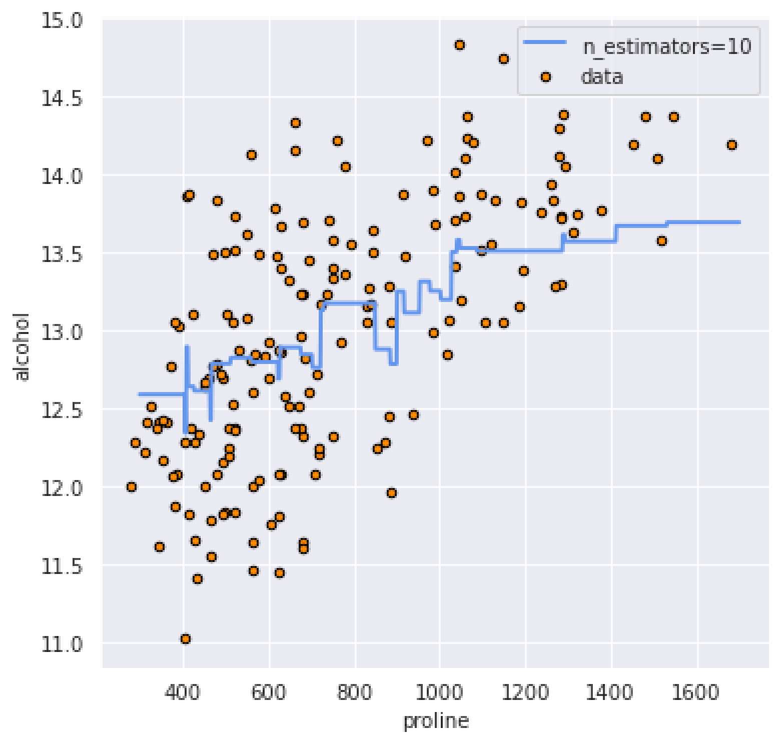
Regression with Gradient Boosted Trees

Regression with Gradient Boosted Trees

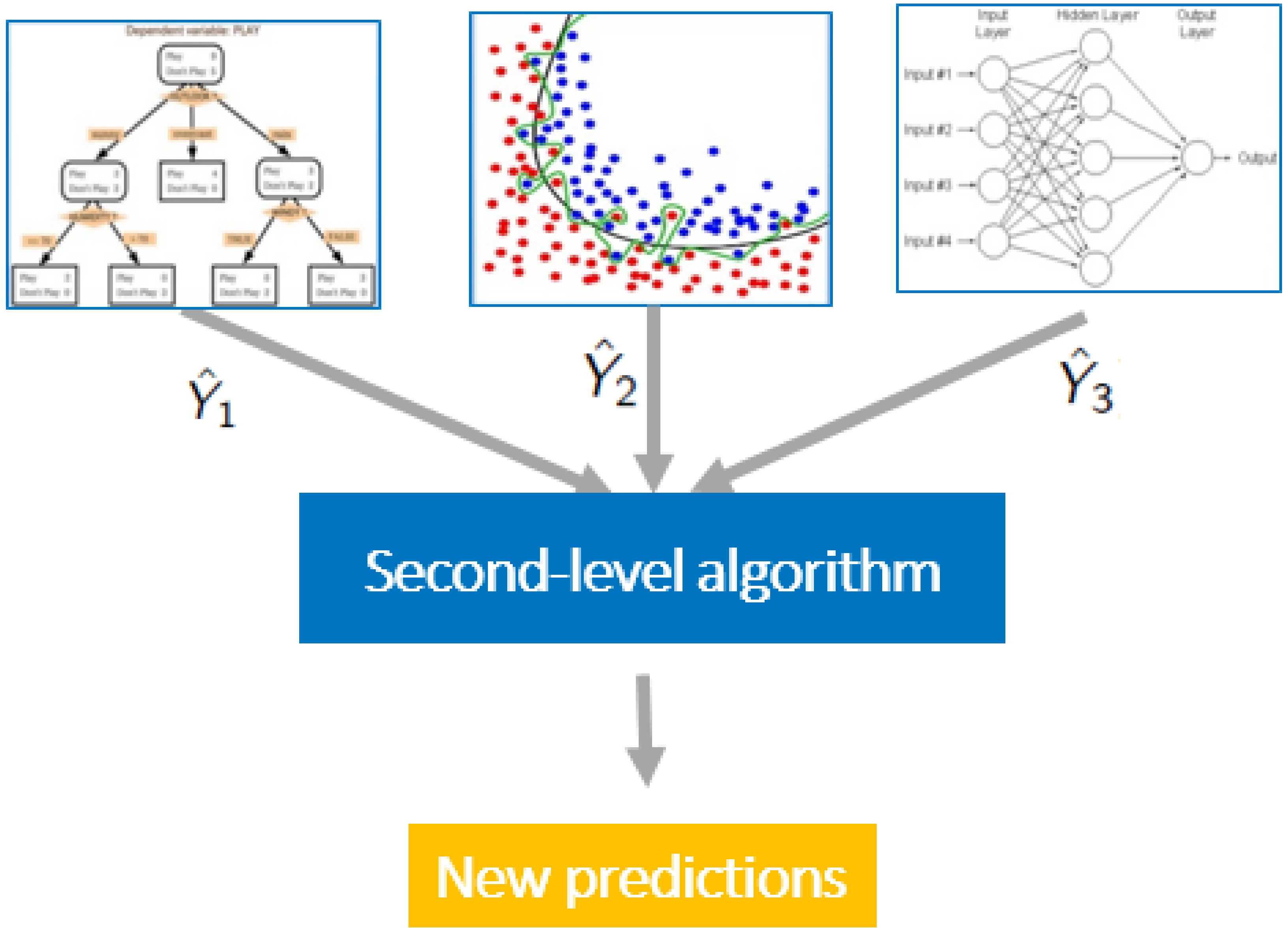
In [20]:
```
from sklearn.ensemble import GradientBoostingRegressor

gbr = GradientBoostingRegressor(n_estimators=10)
gbr.fit(df_wine.proline.values.reshape(-1,1),df_wine.alcohol)
X_test = np.linspace(300,1700,1000)[:,np.newaxis]
y_hat = gbr.predict(X_test)

fig,ax = plt.subplots(1,1,figsize=(6,6))
ax.scatter(df_wine.proline, df_wine.alcohol, s=20, edgecolor="black",
            c="darkorange", label="data")
ax.plot(X_test, y_hat, color="cornflowerblue",
         label="n_estimators=10", linewidth=2)
ax.set_xlabel('proline'); ax.set_ylabel('alcohol'); plt.legend();
```



Stacking



From https://blogs.sas.com/content/subconsciousmusings/2017/05/18/stacked-ensemble-models-win-data-science-competitions/

Stacking with mlxtend for Classification

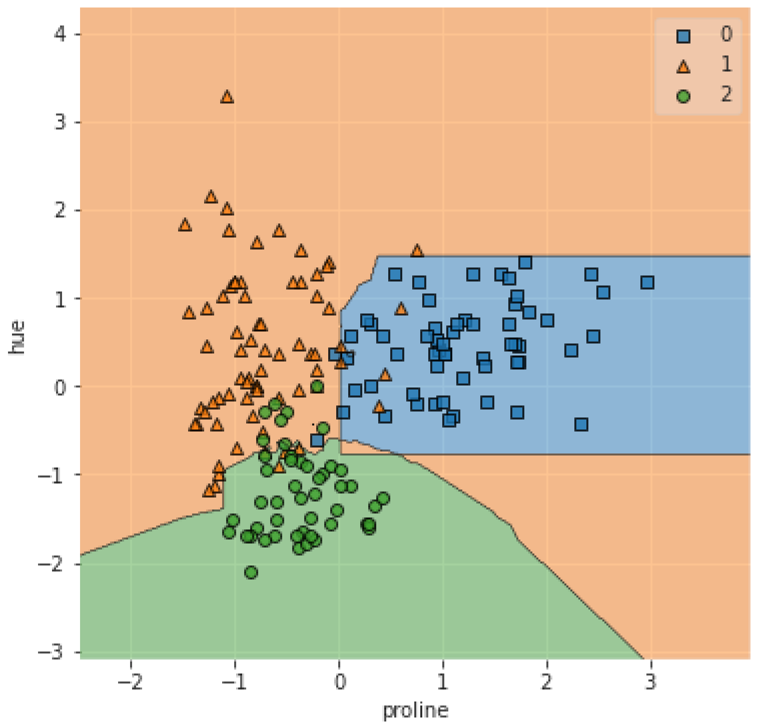
Stacking with mlxtend for Classification

In [21]:
```
from mlxtend.classifier import StackingClassifier

ensemble = [LogisticRegression(max_iter=1000),
            DecisionTreeClassifier(max_depth=3),
            KNeighborsClassifier(n_neighbors=3)]

stc = StackingClassifier(ensemble,LogisticRegression())
stc.fit(X_zscore,y)

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=stc);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



Stacking with mlxtend for Regression

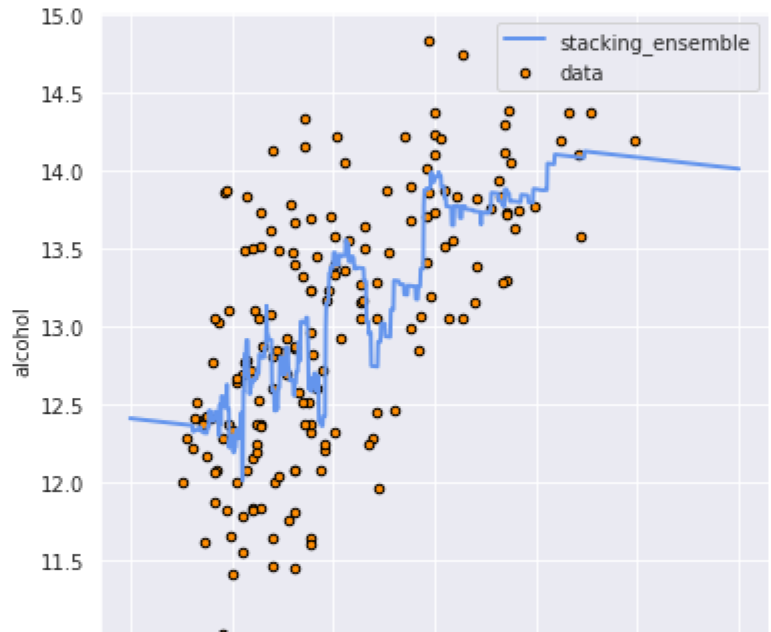
Stacking with mlxtend for Regression

In [22]:
```
from mlxtend.regressor import StackingRegressor

ensemble = [LinearRegression(),
            DecisionTreeRegressor(max_depth=3),
            KNeighborsRegressor(n_neighbors=6)]

stackr = StackingRegressor(ensemble,LinearRegression())
stackr.fit(X_zscore.proline.values.reshape(-1,1),df_wine.alcohol)
X_test = np.linspace(-2,4,1000)[:,np.newaxis]
y_hat = stackr.predict(X_test)

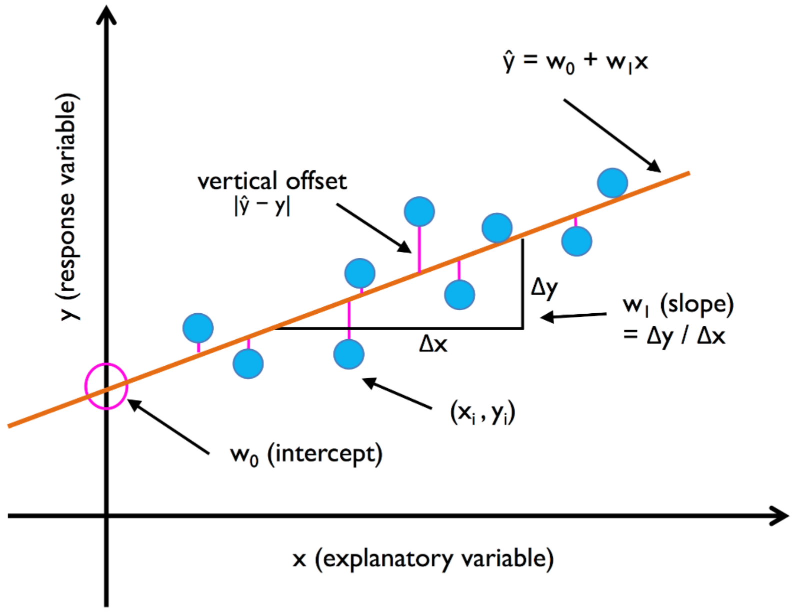
fig,ax = plt.subplots(1,1,figsize=(6,6))
ax.scatter(X_zscore.proline.values.reshape(-1,1), df_wine.alcohol, s=20, edgecolor="black",
            c="darkorange", label="data")
ax.plot(X_test, y_hat, color="cornflowerblue",
         label="stacking_ensemble", linewidth=2)
ax.set_xlabel('proline'); ax.set_ylabel('alcohol');
plt.legend();
```



Review of Models

Model Review: Simple/Multiple Linear Regression

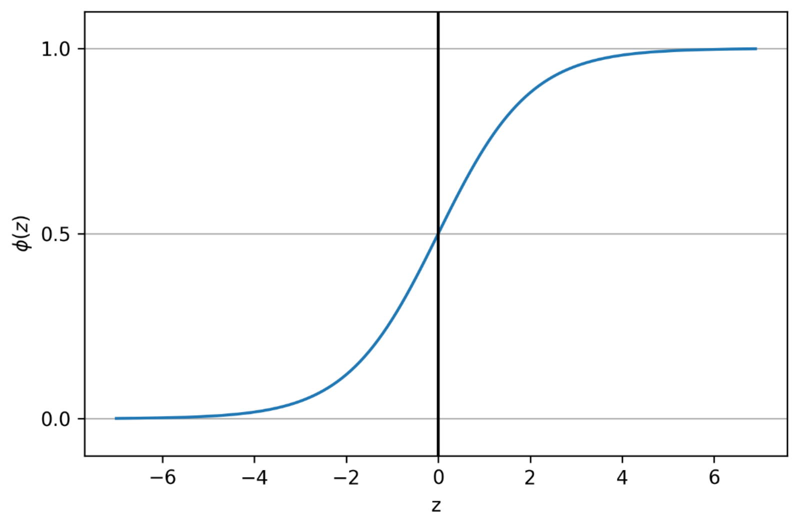
- Use for: Regression
- Pros:
    - fast to train
    - interpretable coefficients
- Cons:
    - assumes linear relationship
    - depends on removing colinear features



from PML

Model Review: Logistic Regression

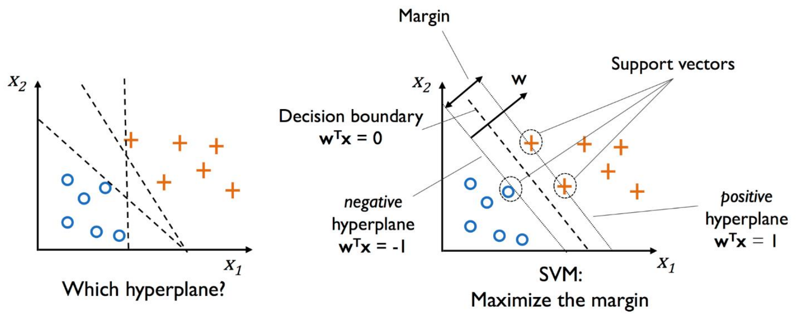
- Use for: Classification
- Pros:
  - fast to train
  - interpretable coefficients (log odds)
- Cons:
  - assumes linear boundary
  - depends on removing colinear features



from PML

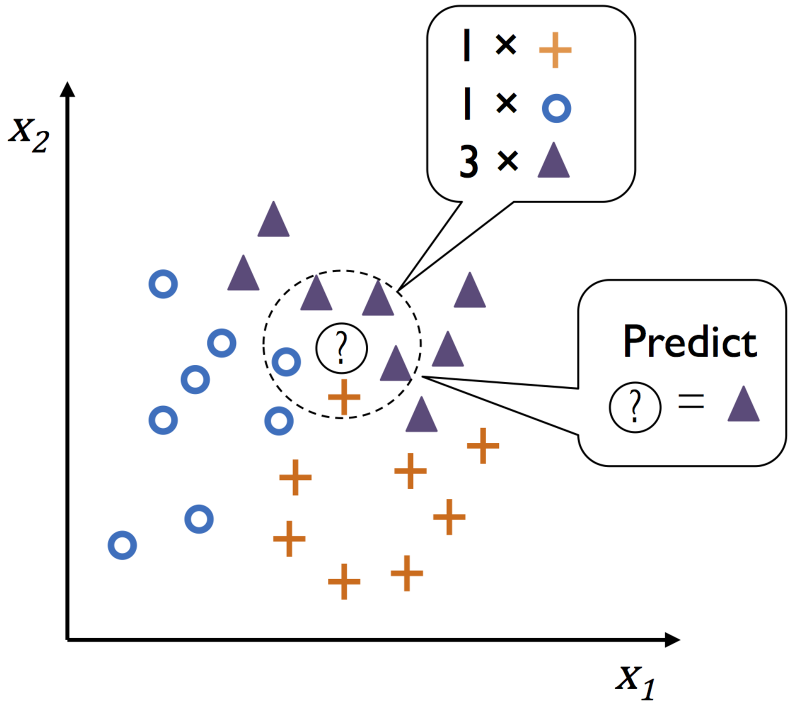
Model Review: Support Vector Machine (SVM)

- Use for: Classification and Regression
- Pros:
    - fast to evaluate
    - can use kernel trick to learn non-linear functions
- Cons:
    - slow to train
    - can fail to converge on very large datasets



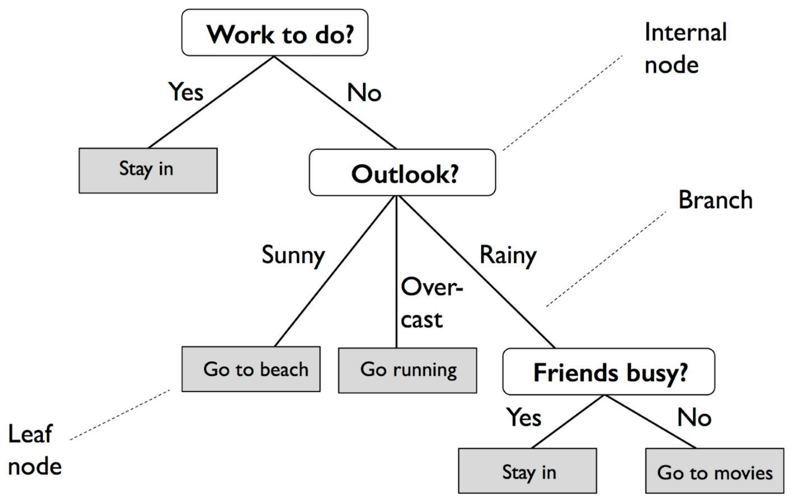
Model Review: k Nearest Neighbor (kNN)

- Use for: Classification or Regression
- Pros:
  - fast to train
  - non-linear boundary
- Cons:
  - potentially slow to predict
  - curse of dimensionality



Model Review: Decision Tree

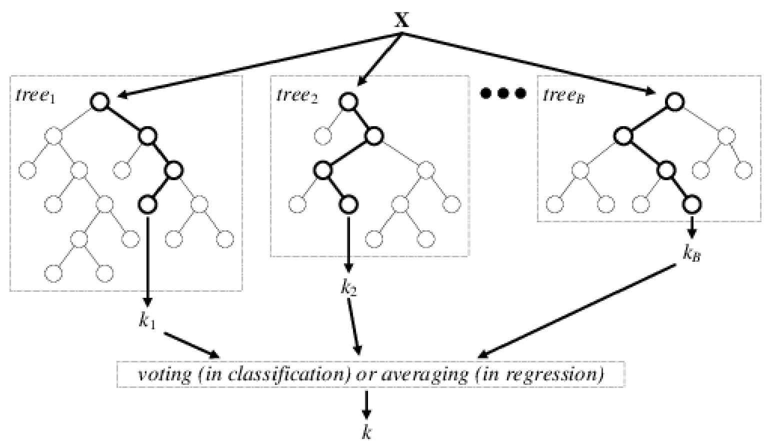
- Use for: Classification or Regression
- Pros:
  - very interpretable
  - quick to predict
  - can handle numeric and categorical variables without transformation
- Cons:
  - tendency to overfit (learn training set too well, more next class!)



From PML

Model Review: Random Forest (Ensemble via Bagging)

- Use for: Classification or Regression
- Pros:
  - less likely to overfit than decision tree
  - quick to train (through parallelization, quick to predict
- Cons:
  - less interpretible, though still possible



From https://www.researchgate.net/publication/301638643_Electromyographic_Patterns_during_Golf_Swing_Activation_Sequence_Profiling_and_Prediction_of_Shot_Effectiveness

Model Review: Gradient Boosted Trees (Ensemble via Boosting)

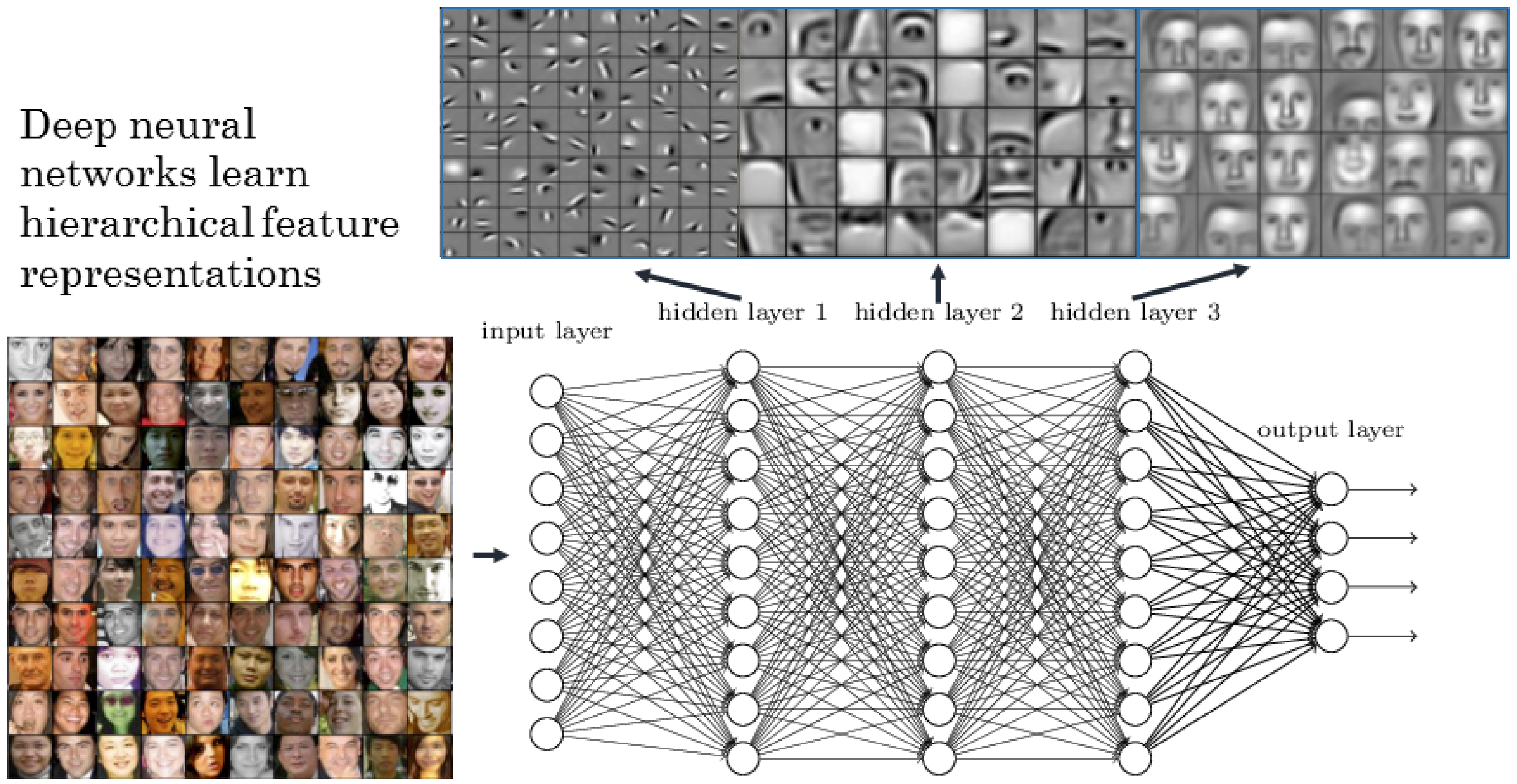
- Use for: Classification or Regression
- Pros:
    - pays more attention to difficult decision regions
    - quick to predict
    - tends to work well on difficult tasks
- Cons:
    - slow to train (parallelization not possible)
    - less interpretible, though still possible

Model Review: Ensemble via Stacking

- Use for: Classification (or Regression)
- Pros:
  - combines benefits of multiple learning types
  - easy to implement
  - tends to win competitions
- Cons:
  - difficult to interpret
  - training/prediction time depends on component models

Neural Networks (aka Deep Learning)

- Pros and Cons of Deep Learning
  - sensitive to initialization and structure
  - high complexity -> needs more data
  - low interpretability
  - can learn complex interactions
  - performs well on tasks involving complex signals (ex images, sound, etc)



Questions?