Elements Of Data Science - S2021

Week 5: Machine Learning Models

2/15/2021

TODOs

- Readings:
    - PDSH 05.03 Hyperparameters and Model Validation
    - Recommended: https://scikit-learn.org/stable/model_selection.html
    - Recommended: PML Chapter 6 (Except for Pipelines)
    - Reference: https://scikit-learn.org/stable/supervised_learning.html
    - Reference: PML Chapter Chap 3 and 7
- Answer and submit Quiz 5
- Quiz4, HW1, Due Tues Feb 16th, 11:59pm ET
- HW2 Out next week, due after spring break
- Midterm, after spring break

Today

- Intro to Machine Learning Models
- Linear models: Simple, Multi-Variable, Logistic
- One Vs. Rest For Multi-Class/Multi-Label Classification
- Distance Based: kNN
- Tree Based: Decision Tree
- Ensembles: Bagging, Boosting, Stacking

Questions?

Environment Setup

Environment Setup

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

sns.set_style('darkgrid')
%matplotlib inline
```

Modeling and ML

- What is a Model?
    - Specification of a mathematical (or probabilistic) relationship between different variables.

- What is Machine Learning?
    - Creating and using models that are learned from data.

Questions for Models

Questions for Models

In [2]:
```
df_wine = pd.read_csv('../data/wine_dataset.csv',usecols=['alcohol','ash','proline','hue','class'])
df_wine.sample(5,random_state=1)
```

Out[2]:

	alcohol	ash	hue	proline	class
161	13.69	2.54	0.96	680.0	2
117	12.42	2.19	1.06	345.0	1
19	13.64	2.56	0.96	845.0	0
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- Can we predict label "class" from the other columns? **(Classification)**
- Can we predict target "hue" from the other columns? **(Regression)**
- What are the important features when predicting "hue"? **(Feature Selection)**
- Can a model tell us about how the features and target interact? **(Interpretation)**
- Do the features group together at all? **(Clustering)**

Data Vocabulary for ML

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- X, features, attributes, independent/exogenous/explanatory variables
    - Ex: alcohol, trip_distance, company_industry
- y, target, label, outcome, dependent/endogenous/response variables
    - Ex: class, hue, tip_amount, stock_price
- $f(X) \rightarrow y$, Model that maps features X to target y

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    - generate predictions or understand interactions?

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    - generate predictions or understand interactions?
- Model Family
    - Linear, Tree, Distance, Probability, Neural Net, Ensemble, ...

Supervised vs Unsupervised vs Reinforcement Learning

Is there a target, y?

Other Learning Paradigms

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- Do we have a mix of labeled and unlabeled?
    - **Semi-Supervised Learning**
    - Can we use structure of unlabeled data along with labeled?

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- Do we have a mix of labeled and unlabeled?
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- Will we continue getting new data?
    - **Online Learning**
    - Is there an oracle (ground truth) we can consult?
    - Can we select which points to make predictions on?

Supervised Learning: Regression vs Classification

- **Regression** -> predict a numeric value
    - Ex: tip_amount, stock_price, wine_hue

Prediction vs Interpretation

- Do we care more about: accuracy when generating predictions?
    - Ex: For a given trip, what will the tip size likely be?
    - Ex: For a given loan, will there be a default?

- Do we care more about: understanding how X relates to y?
    - Ex: What happens to tip size as taxi trip length increases?
    - Ex: What is the relationship between debt and loan default?

Model Families for Supervised Learning

- Linear
    - Simple/Multiple Linear Regression
    - Logistic Regression (for Classification)
    - Support Vector Machines?
    - Perceptron?
- Distance Based
    - K-Nearest Neighbor
- Tree Based
    - Decision Tree

Model Families for Supervised Learning Continued

- Ensemble
    - Random Forest
    - Gradient Boosted Trees
    - Stacking
- Network
    - Multi-layer Perceptron?
    - Deep Neural-Networks
    - Convolutional Neural Nets
    - Recurrant Neural Nets
- Probability
    - Naive Bayes
    - Bayes Net

Example: Regression with a Linear Model

What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

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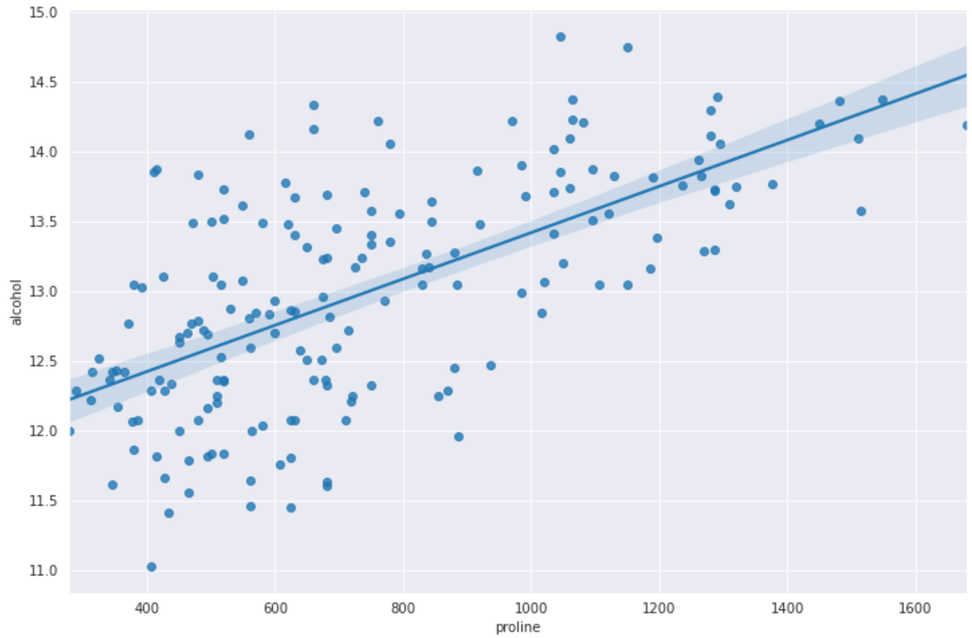
What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

In [4]:
```
fig,ax = plt.subplots(1,1,figsize=(12,8))
sns.regplot(x='proline', y='alcohol', data=df_wine);
```



Aside: Correlation

Question: are total_bill and tips correlated?

Aside: Correlation

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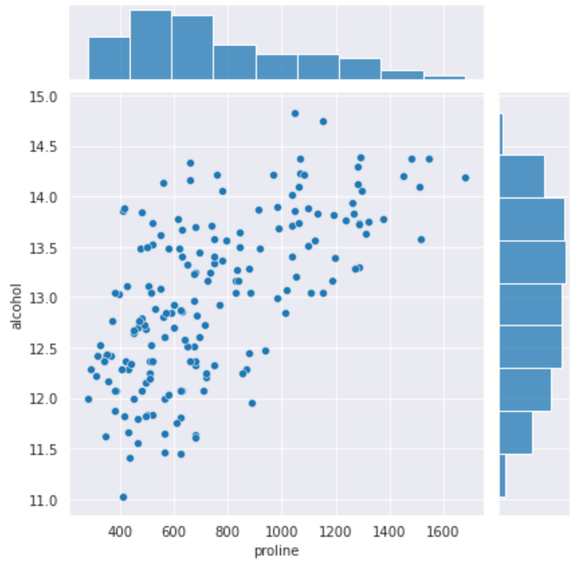
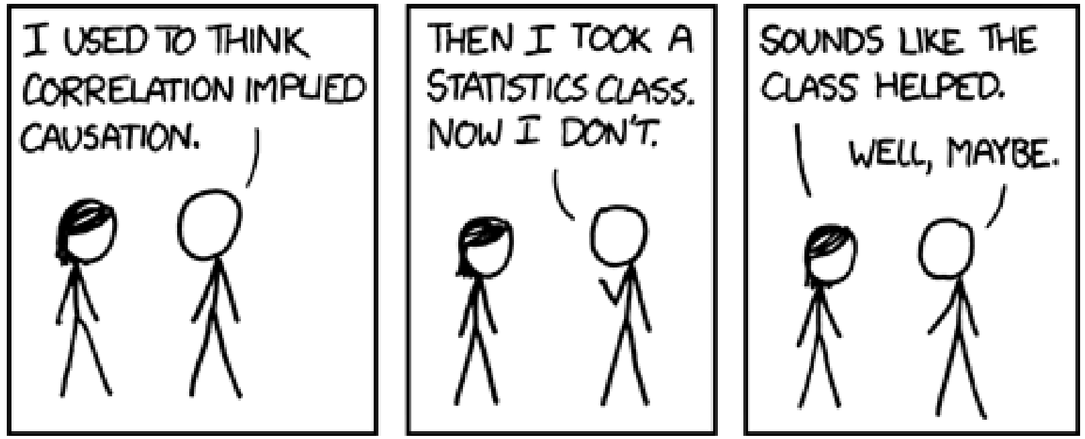
In [5]:
```
sns.jointplot(x='proline',y='alcohol',data=df_wine);
```



Obligitory Correlation vs. Causation



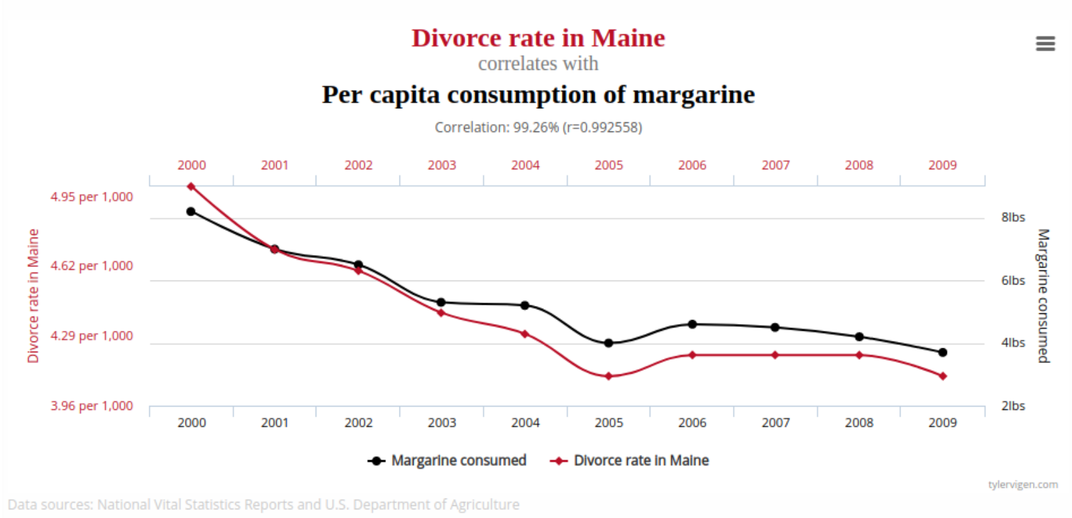
https://imgs.xkcd.com/comics/correlation.png

- Correlation does not mean causation!

- Causal Inference
    - controlled experiment
    - control for confounding variables

Spurious Correlation

- Also, look hard enough and you'll find correlation.
  - See spurious correlations for examples



Aside: Correlation

- Could calculate Pearson Correlation Coefficient
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    - On the Effects of Non-Normality on the Distribution of the Sample Product-Moment Correlation Coefficient

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In [6]:
```
from scipy.stats import pearsonr
r,p = pearsonr(df_wine.proline,df_wine.alcohol)
print(f'r: {r:.2f}, p: {p:.2f}')
```

```
r: 0.64, p: 0.00
```

Aside: Correlation

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```

- We know that as proline goes up alcohol goes up, but by how much?

Python Modeling Libraries

Prediction - scikit-learn

Interpretation - scikit-learn and statsmodels

Additional Tools - mlxtend

Aside: MLxtend and conda-forge

- **MLxtend:** (machine learning extensions) is a Python library of useful tools for the day-to-day data science tasks.

- **Conda-Forge:** A community-led collection of recipes, build infrastructure and distributions for the conda package manager.


```
$ conda install --name eods-s21 --channel conda-forge mlxtend
```

Simple Linear Regression

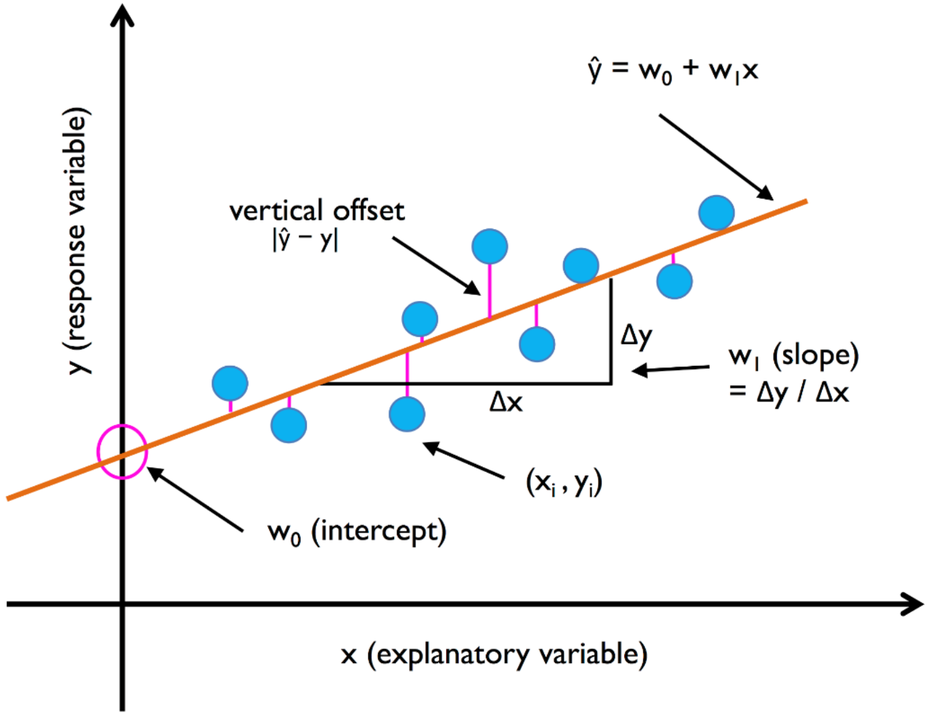
Simple Linear Regression

$$y = w_1 x + w_0 + \varepsilon_i$$

- y : dependent, endogenous, response, target, label (Ex: `alcohol`)
- x_i : independent, exogenous , explanatory, feature, attribute (Ex: `proline`)
- w_1 : coefficient, slope
- w_0 : bias term, intercept
- ε_i : error, hopefully small, often assumed $\mathcal{N}(0, 1)$

- Want to find values for w_1 and w_0 that best fit the data.
- Find a line as close to our observations as possible

Simple Linear Regression

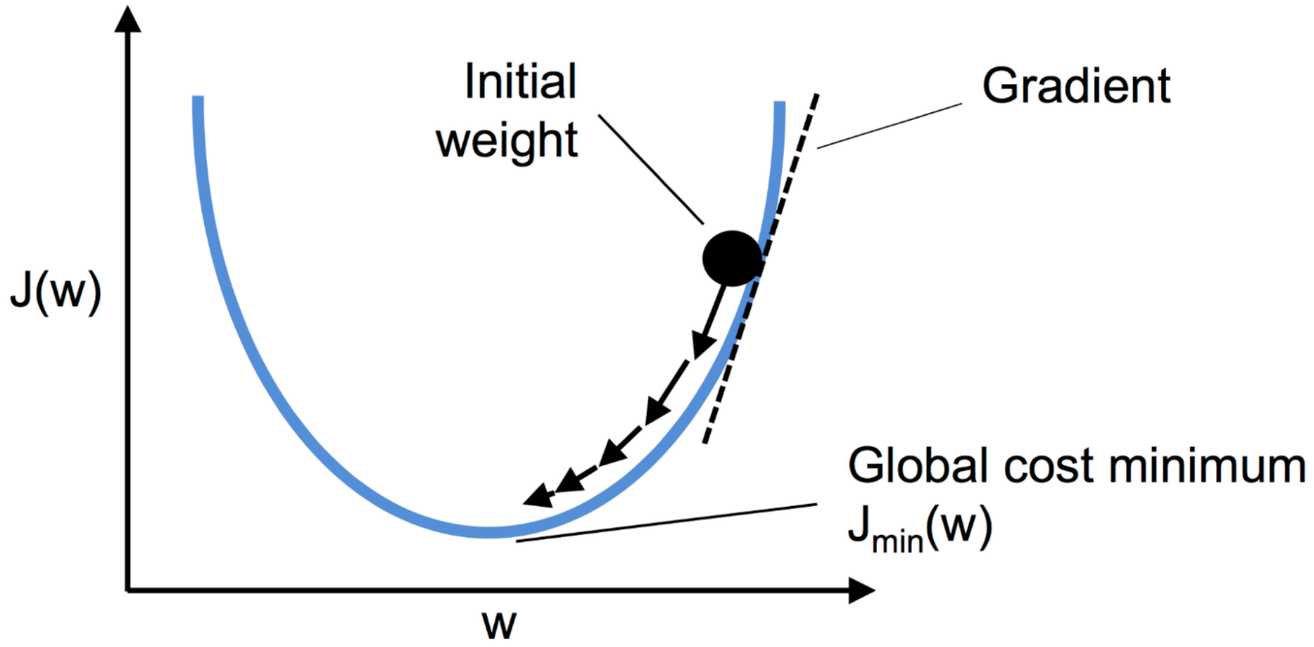


from PML

Finding w_1 and w_0 with Ordinary Least Squares

- **prediction**: $\hat{y}_i = f(x_i) = w_1 x_i + w_0$
- **error**: $error(y_i, \hat{y}_i) = y_i - \hat{y}_i$
- **sum of squared errors**: $\sum_{i=1:n} \left(y_i - \hat{y}_i\right)^2$
- **least squares**: make the sum of squared errors as small as possible
- **gradient descent**: minimize error by following the gradient wrt w_1, w_0
    - can sometime be optimized in closed form
    - often done iteratively

Aside: Gradient Descent Cont.



Aside: Gradient Descent

- Want to maximize or minimize something (Ex: squared error)

- **Gradient** : direction, vector of partial derivatives
    - can get complicated, often estimated

- **Gradient Descent** : take steps wrt the direction of the gradient
    - **maximize** : in the direction of the gradient
    - **minimize** : in the opposite direction of the gradient

- **Global Maximum/Minimum** : the single best solution
- **Local Maximum/Minimum** : the best solution in the neighborhood

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In [10]:
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# display learned coefficients (trailing underscore indicates learned values)
print(lr.coef_)
print(lr.intercept_)
```

```
[0.0016595]
11.761148483143147
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11.761148483143147
```

In [11]:
```
# predict given new values for proline
X = np.array([1000,2000]).reshape(-1,1)
lr.predict(X)
```

Out[11]:
```
array([13.42064866, 15.08014884])
```

Why .reshape(-1,1)?

scikit-learn models expect the input features to be 2 dimensional

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```
In [12]: df_wine.proline.values[:5]

Out[12]: array([1065., 1050., 1185., 1480.,  735.])
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In [13]:
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df_wine.proline.values.shape
```

Out[13]:
```
(178,)
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In [14]:
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df_wine.proline.values.reshape(-1,1).shape # -1 means "infer from the data"
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Alternatives:

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In [14]: df_wine.proline.values.reshape(-1,1).shape # -1 means "infer from the data"
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Alternatives:

```
In [15]: df_wine.loc[:,['proline']].shape
```

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```

Alternatives:

```
In [15]: df_wine.loc[:,['proline']].shape

Out[15]: (178, 1)

In [16]: df_wine[['proline']].shape

Out[16]: (178, 1)
```

Interpreting Coefficients

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In [17]:
```
print(f'beta={lr.coef_[0]:0.3f}, alpha={lr.intercept_:0.3f}')
```

```
beta=0.002, alpha=11.761
```

Interpreting Coefficients

In [17]:
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print(f'beta={lr.coef_[0]:0.3f}, alpha={lr.intercept_:0.3f}')
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beta=0.002, alpha=11.761
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In [18]:
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print(f'alchohol = {lr.coef_[0]:0.3f}*proline + {lr.intercept_:0.3f}')
```

```
alchohol = 0.002*proline + 11.761
```

Interpreting Coefficients

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```

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alchohol = 0.002*proline + 11.761
```

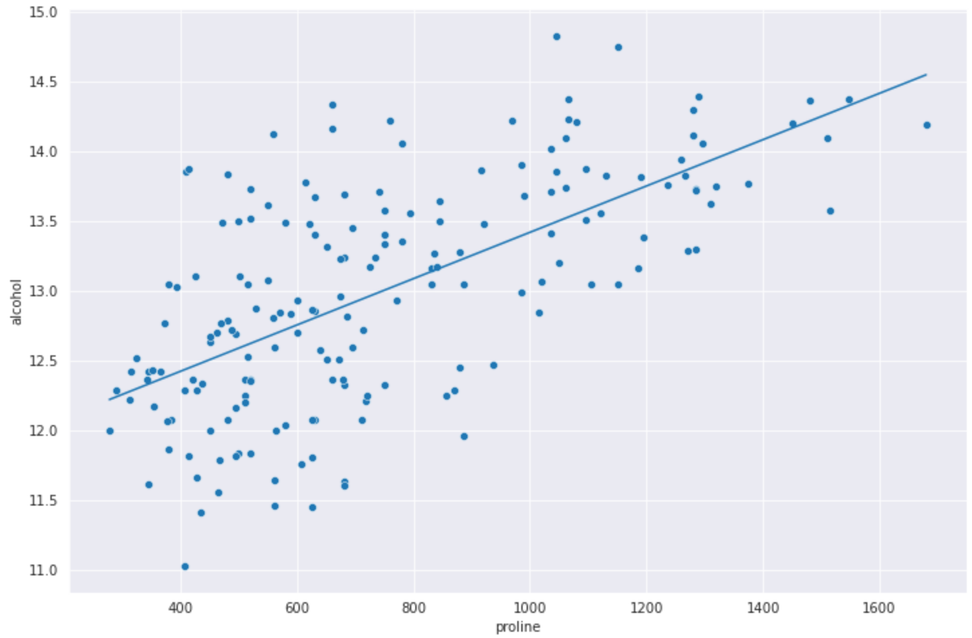
- When proline goes up by 1, alcohol goes up by .002
- When proline is 0, alcohol is 11.761

Plotting The Model

Plotting The Model

In [19]:
```
x_predict = [df_wine.proline.min(),df_wine.proline.max()]
y_hat = lr.predict(np.array(x_predict).reshape(-1,1))

fig,ax = plt.subplots(1,1,figsize=(12,8))
ax = sns.scatterplot(x=df_wine.proline,y=df_wine.alcohol);
ax.plot(x_predict,y_hat);
```



Multiple Linear Regression

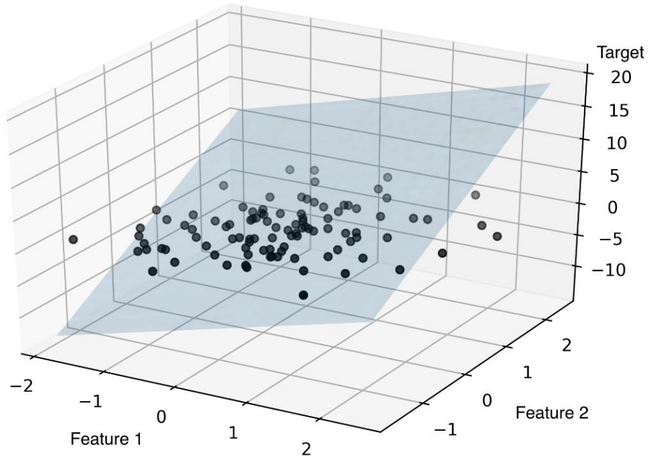
- Including multiple independent variables

$$y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + \ldots + w_m x_{im} + \varepsilon_i$$

Ex:

alcohol = w_0 + w_1*proline + w_2*hue

Objective: Find a plane that falls as close to our points as possible



Multiple Linear Regression in scikit-learn

Multiple Linear Regression in scikit-learn

In [20]:
```
mlr = LinearRegression()
mlr.fit(df_wine[['proline','hue']],y=df_wine.alcohol);

for idx,feature in enumerate(['proline','hue']):
    print(f'{feature:10s} : {mlr.coef_[idx]: 0.3f}')
print(f'{"intercept":10s} : {mlr.intercept_:0.3f}')
```

```
proline    :  0.002
hue        : -0.842
intercept  : 12.459
```

- If we hold everything else constant, what effect does the variable have
- If hue is held constant, a rise of 1 proline -> rise of .002 in alcohol
- If proline is held constant, a rise of 1 hue -> decrease of .842 in alcohol
- Can add interaction terms to allow both to move
    - Ex: hue * proline
    - more complicated to interpret

Multiple Linear Regression in statsmodels

Multiple Linear Regression in statsmodels

In [21]:
```
import statsmodels.api as sm

X = df_wine[['proline','hue']]
X = sm.add_constant(X)
y = df_wine.alcohol
sm_mlr = sm.OLS(y,X).fit() # Note: X,y passed as parameters to object, not fit
sm_mlr.summary()
```

Out[21]:

OLS Regression Results

Dep. Variable:	alcohol	**R-squared:**	0.467
Model:	OLS	**Adj. R-squared:**	0.461
Method:	Least Squares	**F-statistic:**	76.79
Date:	Mon, 15 Feb 2021	**Prob (F-statistic):**	1.15e-24
Time:	17:48:39	**Log-Likelihood:**	-158.89
No. Observations:	178	**AIC:**	323.8
Df Residuals:	175	**BIC:**	333.3
Df Model:	2		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
const	12.4593	0.203	61.347	0.000	12.058	12.860
proline	0.0018	0.000	12.325	0.000	0.002	0.002
hue	-0.8418	0.202	-4.175	0.000	-1.240	-0.444

Omnibus:	0.751	**Durbin-Watson:**	1.734
Prob(Omnibus):	0.687	**Jarque-Bera (JB):**	0.606
Skew:	0.142	**Prob(JB):**	0.739
Kurtosis:	3.028	**Cond. No.**	4.96e+03

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Dealing With the Intercept/Bias

- Two ways of keeping track of the bias term

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1. Keep it as a separate parameter:

  - $y = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_m x_m$
  - $y = w_0 + \sum_{i=1}^{m} w_i x_i$

Dealing With the Intercept/Bias

- Two ways of keeping track of the bias term

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  - $y = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_m x_m$
  - $y = w_0 + \sum_{i=1}^{m} w_i x_i$

2. Append a constant of $x_0 = 1$ so x and w are the same length

  - $y = w_0 x_0 + w_1 x_1 + w_2 x_2 + \ldots + w_m x_m$
  - $y = \sum_{i=0}^{m} w_i x_i$

Standardizing/Normalizing Features for Interpretation

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In [22]:
```
for (name,coef) in zip(['proline','hue'],mlr.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    :  0.002
hue        : -0.842
```

Standardizing/Normalizing Features for Interpretation

In [22]:
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for (name,coef) in zip(['proline','hue'],mlr.coef_):
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```
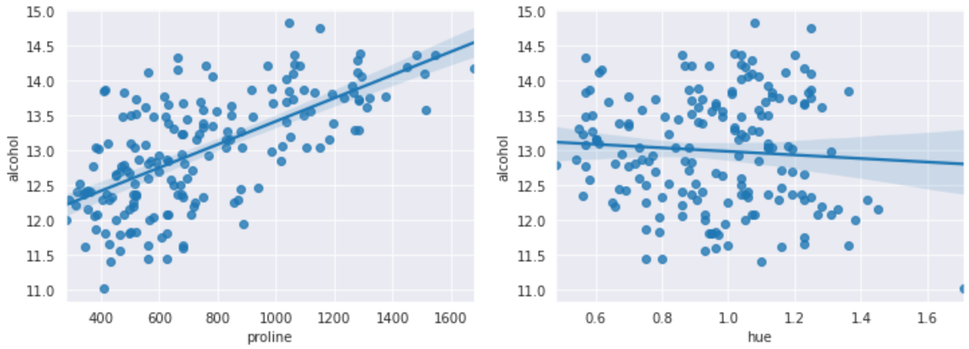

```
proline    :  0.002
hue        : -0.842
```

In [23]:
```
fig,ax = plt.subplots(1,2,figsize=(12,4))
sns.regplot(x='proline',y='alcohol',data=df_wine,ax=ax[0])
sns.regplot(x='hue',y='alcohol',data=df_wine,ax=ax[1]);
```



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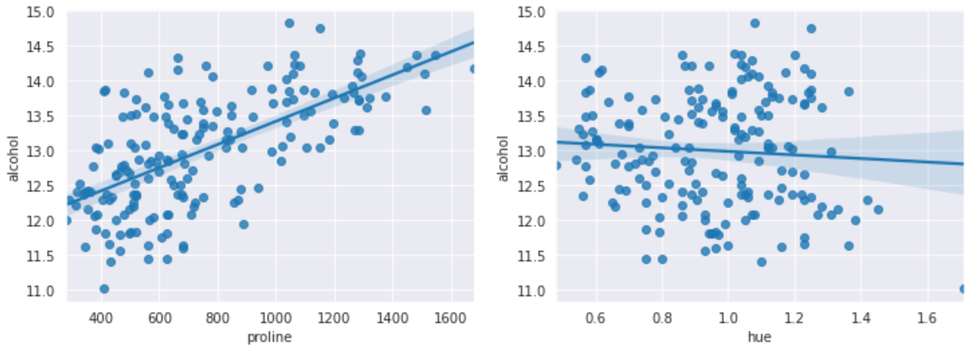

What would the coefficents look like if the features were on the same scale?

Standardizing/Normalizing Features for Gradient Descent

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$$z = \frac{x - \bar{x}}{s}$$

Standardizing/Normalizing Features for Gradient Descent

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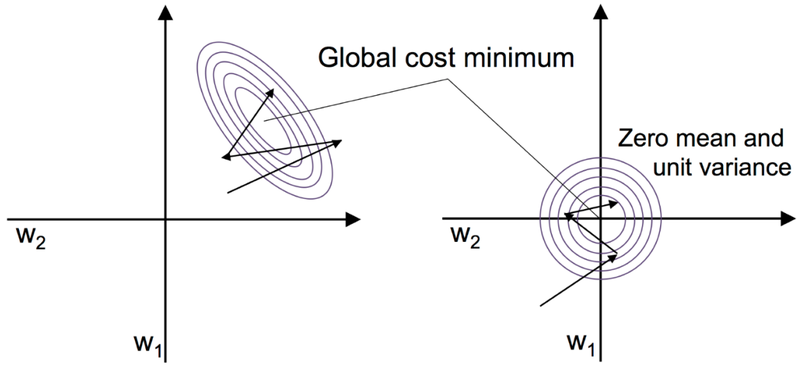

From PML

Multiple Linear Regression with Standardization/Normalization

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- `DataFrame.apply()`: apply a function to each column (axis=0) or each row (axis=1)

Multiple Linear Regression with Standardization/Normalization

- `DataFrame.apply()`: apply a function to each column (axis=0) or each row (axis=1)

In [24]:
```
X_zscore = df_wine[['proline','hue']].apply(lambda x: (x-x.mean())/x.std(),axis=0)

mlr_n = LinearRegression()
mlr_n.fit(X_zscore, df_wine.alcohol)
for (name,coef) in zip(X_zscore.columns,mlr_n.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    :  0.568
hue        : -0.192
```

Multiple Linear Regression with Standardization/Normalization

- `DataFrame.apply()`: apply a function to each column (axis=0) or each row (axis=1)

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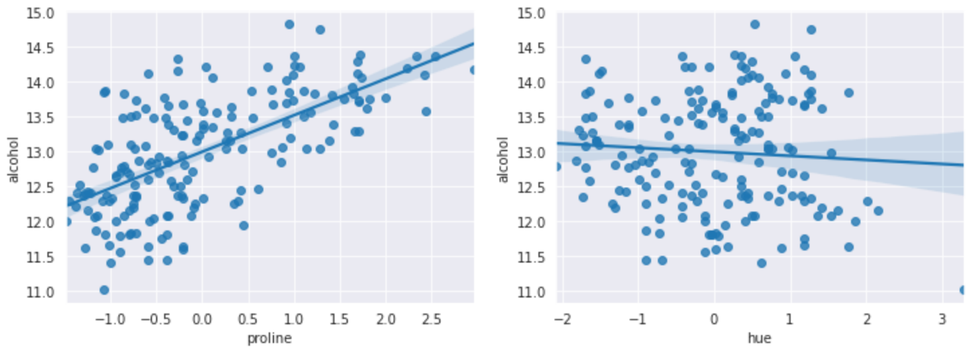
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    :  0.568
hue        : -0.192
```

In [25]:
```
fig,ax = plt.subplots(1,2,figsize=(12,4))
sns.regplot(x=X_zscore.proline,y=df_wine.alcohol,ax=ax[0]);
sns.regplot(x=X_zscore.hue,y=df_wine.alcohol,ax=ax[1]);
```



Colinarity

- MLR assumes features are linearly independent
    - eg: Can't rewrite one column as a weighted sum of the others
    - Ex: in tips dataset: number of entrees ordered will likely be linearly related to table size
- Issue: Model won't know how to estimate w
    - If we add to one w_i and subtract from another, there will be no change in error
- Try to remove obvious colinearity
    - can use correlation and linear regression to detect
    - Important to consider when constructing categorical features (feature engineering)

Aside: Interpretation Vs. Prediction

- Interpretation: Explain how observed features relate to observed target
- Prediction: Given new features, can we generate a prediction

- Often asked to do one or the other, be clear which is most important
- In prediction, may not worry about interpreting the model!

- There is increased attention on interpretability

Questions re Regression with Linear Models?

Classification

- **Regression** -> predict a numeric value
- **Classification** -> predict a discrete class, category

- **Binary classification** : two categories
    - pos/neg, cat/dog, win/lose
- **Multiclass classification** : more than two categories
    - red/green/blue, flower type, integer 0-10
- **Multilabel classification** : can assign more than one label to an instance
    - paper topics, entities in image

Wine as Binary Classification

Wine as Binary Classification

In [26]:
```
df_wine['class'].value_counts()
```

Out[26]:
```
1    71
0    59
2    48
Name: class, dtype: int64
```

Wine as Binary Classification

In [26]:
```
df_wine['class'].value_counts()
```

Out[26]:
```
1    71
0    59
2    48
Name: class, dtype: int64
```

In [27]:
```
# only keep classes 0 and 1
df_wine_2class = df_wine[df_wine['class'] < 2]

# rename 'class' as 'target', since class is a reserved python word
df_wine_2class = df_wine_2class.rename({'class':'target'},axis=1)

df_wine_2class.target.value_counts()
```

Out[27]:
```
1    71
0    59
Name: target, dtype: int64
```

Classifying Wine with a Linear Model

Classifying Wine with a Linear Model

- Can't use our linear regression model directly

Classifying Wine with a Linear Model

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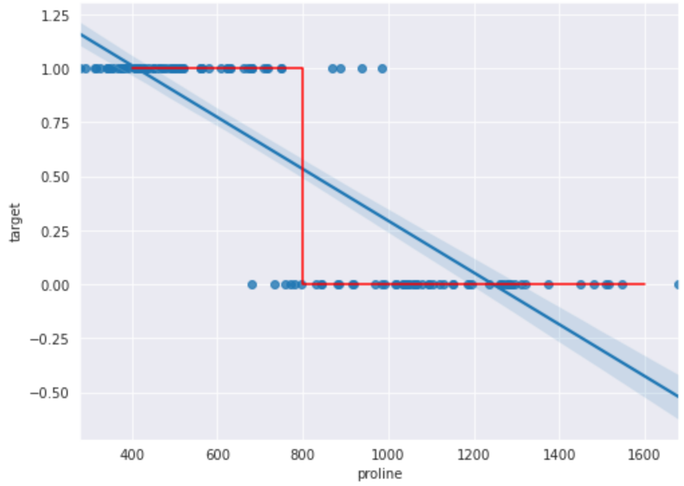
In [28]:
```
fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.regplot(x=df_wine_2class.proline,y=df_wine_2class.target);
ax.plot([400,800,800,1600],[1,1,0,0],c='r');
```



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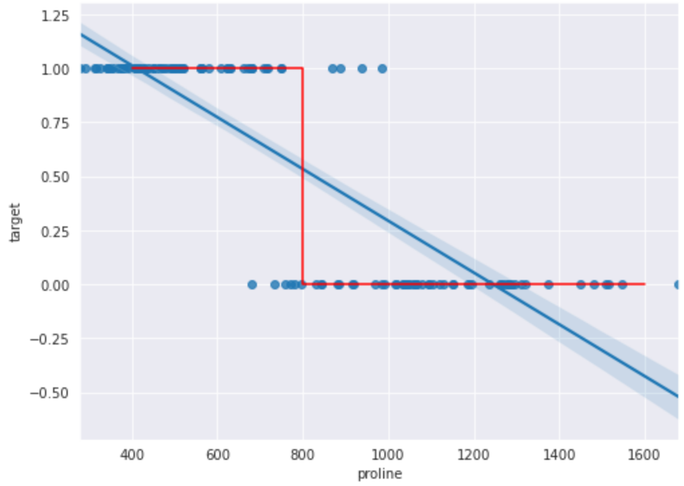

- Want something with that looks like a threshold
- Would like a prediction between 0 and 1

Logistic Regression

Logistic Regression

$$logistic(x) = \frac{1}{1+e^{(-x)}}$$

Logistic Regression

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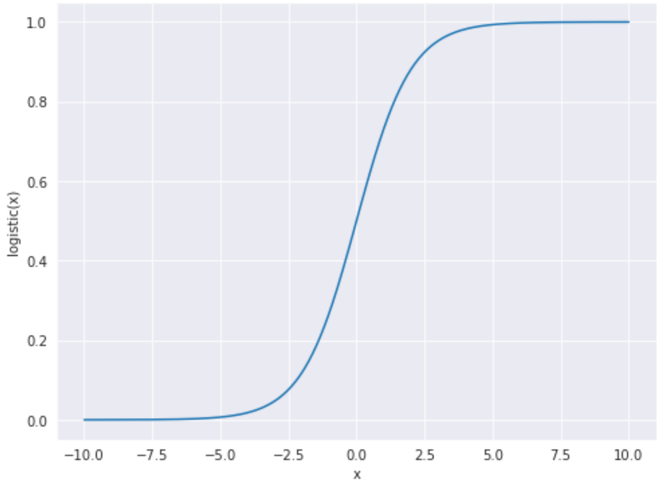
In [29]:
```
def logistic(x,w1=1,w0=0):
    return 1 / (1+np.exp(-(w0+w1*x)))

x = np.linspace(-10,10,1000) # generate 1000 numbers evenly spaced between -10 and 10
fig,ax = plt.subplots(1,1,figsize=(8,6))
ax.plot(x,logistic(x));
ax.set_xlabel('x');ax.set_ylabel('logistic(x)');
```



Logistic Regression with sklearn

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- Our problem becomes: $P(y_i = 1|x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

Logistic Regression with sklearn

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In [30]:
```
from sklearn.linear_model import LogisticRegression

X = df_wine_2class.proline.values.reshape(-1,1)
y = df_wine_2class.target

logr = LogisticRegression(fit_intercept=True).fit(X,y)
print(f'w_0 = {logr.intercept_[0]:0.2f}')
print(f'w_1 = {logr.coef_[0][0]:0.2f}')
```

```
w_0 = 11.97
w_1 = -0.01
```

Logistic Regression with sklearn

- Our problem becomes: $P(y_i = 1|x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

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logr = LogisticRegression(fit_intercept=True).fit(X,y)
print(f'w_0 = {logr.intercept_[0]:0.2f}')
print(f'w_1 = {logr.coef_[0][0]:0.2f}')
```
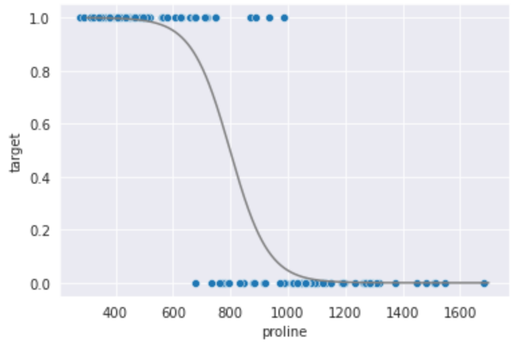

```
w_0 = 11.97
w_1 = -0.01
```

In [31]:
```
fig,ax = plt.subplots(1,1,figsize=(6,4))
x = np.linspace(300,1700,1000)
logistic_x = logistic(x,logr.coef_[0],logr.intercept_)
ax.plot(x,logistic_x,c='gray');
sns.scatterplot(x=df_wine_2class.proline,y=df_wine_2class.target, ax=ax);
```



Adding the Threshold

Adding the Threshold

- Can treat the output of the logistic function as $P(y = 1|x)$
- Threshold at .5 (50%) to get class prediction

Adding the Threshold

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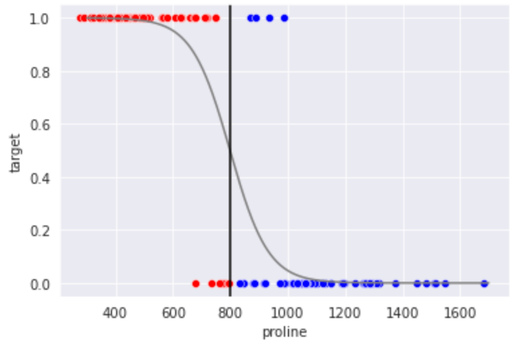
- Threshold at .5 (50%) to get class prediction

In [32]:
```
threshold = x[np.argmin(np.abs(logistic_x - .5))]

predicted_0 = df_wine_2class[df_wine_2class.proline <= threshold]
predicted_1 = df_wine_2class[df_wine_2class.proline > threshold]

fig,ax = plt.subplots(1,1,figsize=(6,4))
sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
ax.plot(x,logistic_x,c='gray');
ax.axvline(threshold,c='k');
```



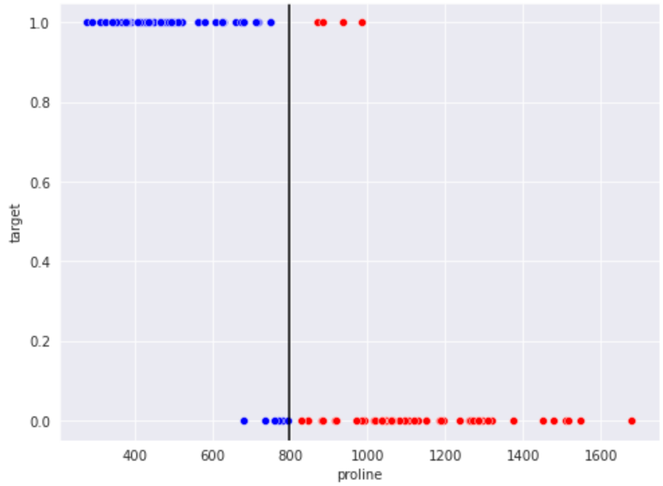
Getting Predictions from sklearn

Getting Predictions from sklearn

In [33]:
```
yhat = logr.predict(X)

predicted_0 = df_wine_2class[yhat==0]
predicted_1 = df_wine_2class[yhat==1]

fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
ax.axvline(threshold,c='k');
```



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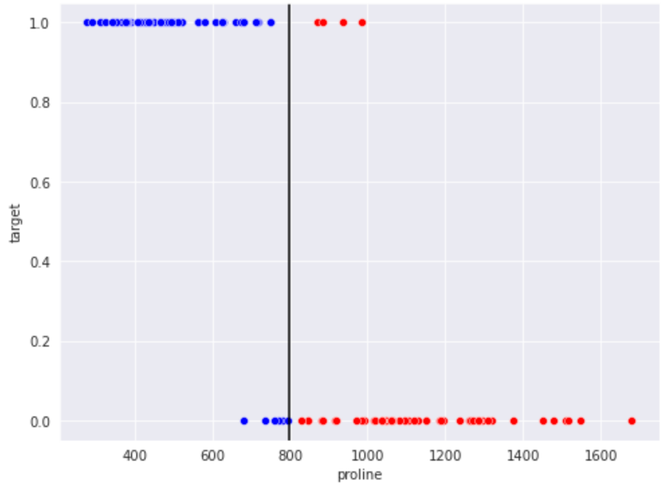

Note we have some errors!

Getting Probabilities from sklearn

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- said we could use output of logistic as $P(y = 1|x)$

Getting Probabilities from sklearn

- said we could use output of logistic as $P(y = 1|x)$

In [34]:
```
p_y = logr.predict_proba(X)
p_y[:5] # p(y=0|x), p(y=1|x)
```

Out[34]:
```
array([[9.81833759e-01, 1.81662409e-02],
       [9.77356984e-01, 2.26430157e-02],
       [9.96947414e-01, 3.05258552e-03],
       [9.99963234e-01, 3.67664871e-05],
       [2.77482032e-01, 7.22517968e-01]])
```

Getting Probabilities from sklearn

- said we could use output of logistic as $P(y = 1|x)$

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```
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p_y[:5] # p(y=0|x), p(y=1|x)
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Out[34]:
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       [9.99963234e-01, 3.67664871e-05],
       [2.77482032e-01, 7.22517968e-01]])
```
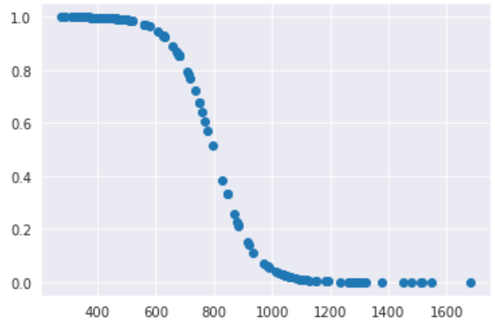

In [35]:
```
plt.scatter(df_wine_2class.proline,p_y[:,1]);
```



Interpreting Logistic Regression Coefficients

- After some math

$$\log\left(\frac{y_i}{1-y_i}\right) = w_0 + w_1 x_{i1}$$

- this is the **log odds ratio** of p(y=1)/p(y=0)
- odds range from 0 to positive infinity
- odds(.2) -> 1/5 -> 1 out of 6 times -> .16
- odds(5) -> 5/1 -> 5 out of 6 times -> .83

See here for a good explanation

Logistic Regression with Multiple Features

Logistic Regression with Multiple Features

In [36]:
```
X = df_wine_2class[['proline','hue']]
X_zscore = X.apply(lambda x: (x-x.mean())/x.std())

logrm = LogisticRegression().fit(X_zscore,y)
for (name,coef) in zip(X.columns,logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    : -3.464
hue        :  0.488
```

Logistic Regression with Multiple Features

In [36]:
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X = df_wine_2class[['proline','hue']]
X_zscore = X.apply(lambda x: (x-x.mean())/x.std())

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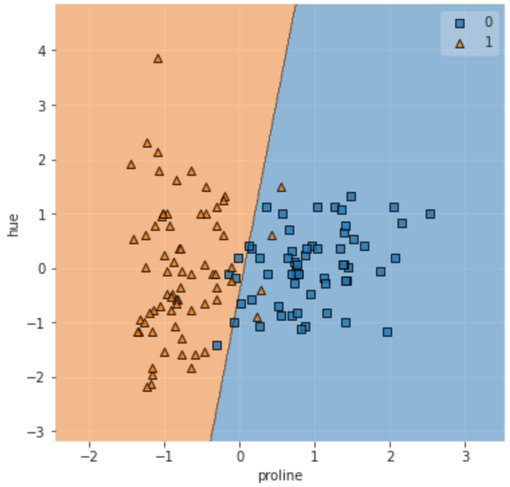
for (name,coef) in zip(X.columns,logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    : -3.464
hue        :  0.488
```

In [37]:
```
# need to have run: conda install -n eods-f20 -c conda-forge mlxtend
from mlxtend.plotting import plot_decision_regions

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



Reminder: Multi-Class and Multi-Label Classification

- **Multi-Class**: More than 2 classes (Binary Classifiction)
    - Ex: color is one of 'red', 'green' or 'blue'
- **Multi-Label**: Each item can belong to more than one class
    - Ex: picture contains ['car','bus','motorcycle']

Wine as Multi-Class Classification

Wine as Multi-Class Classification

In [38]:
```
df_wine = pd.read_csv('../data/wine_dataset.csv',usecols=['alcohol','ash','proline','hue','class'])

X = df_wine[['proline','hue']]
y = df_wine['class'] # 3 classes: [0,1,2]

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[38]:
```
0    59
1    71
2    48
Name: class, dtype: int64
```

One Vs. Rest (OvR) Classification For Multi-Class, Multi-Label

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

- For Multi-Label
    - 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 [39]:
```
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]]
```

OvR For Logistic Regression

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 [1.75637296e-01 3.44369368e-01 4.79993336e-01]]
```
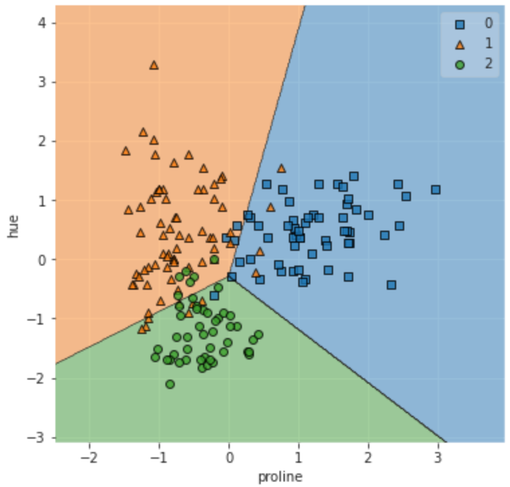
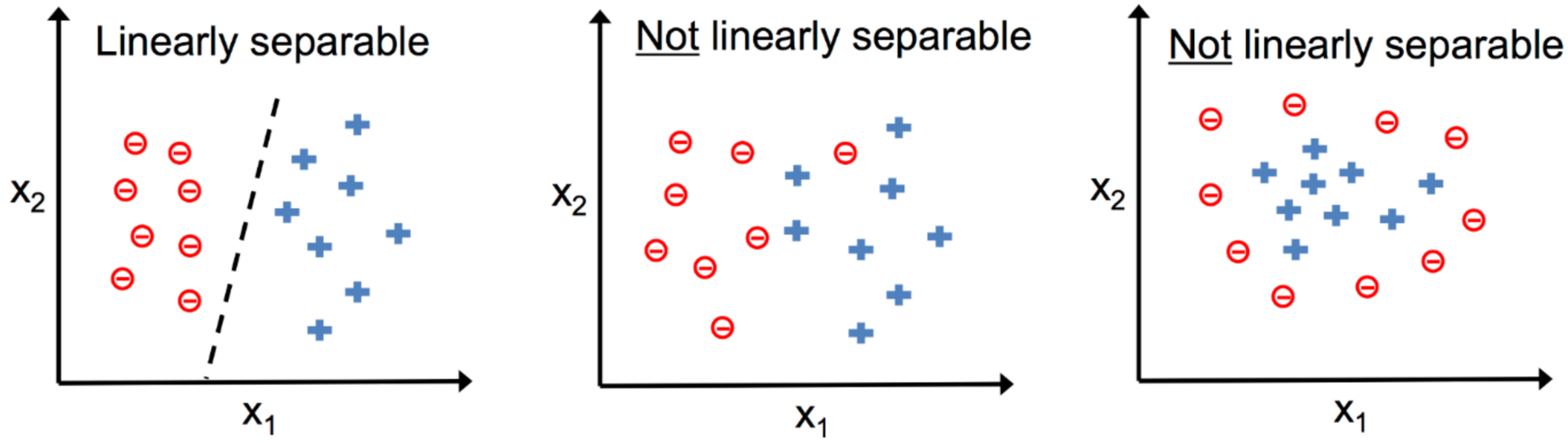

In [40]:
```
fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values,y.values,logr)
ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
```



Questions re Classification with Linear Models?

Linearly Seperable Data

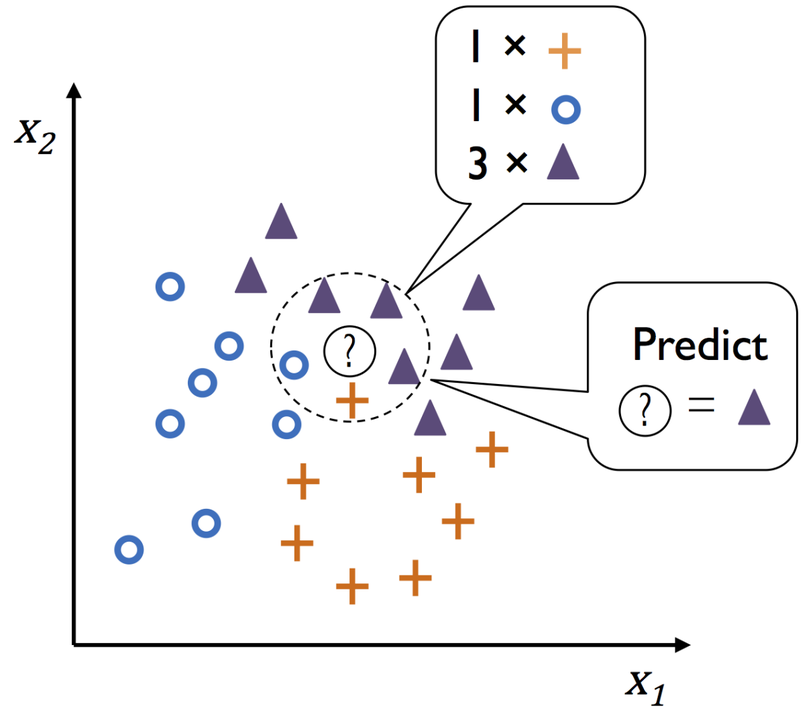
- Logistic Regression depends on data being linearly seperable



From PML

Distance Based: k-Nearest Neighbor (kNN)

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

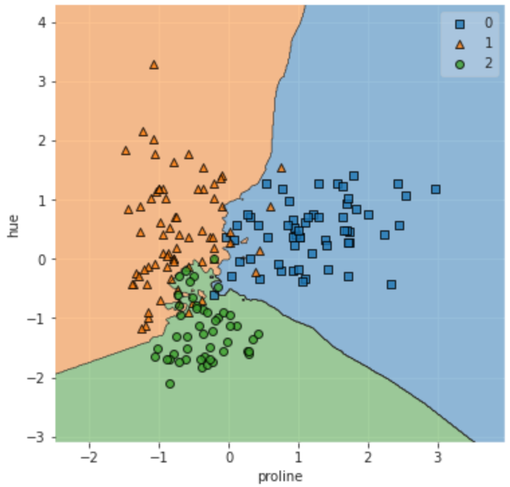


From PML

KNN in sklearn

KNN in sklearn

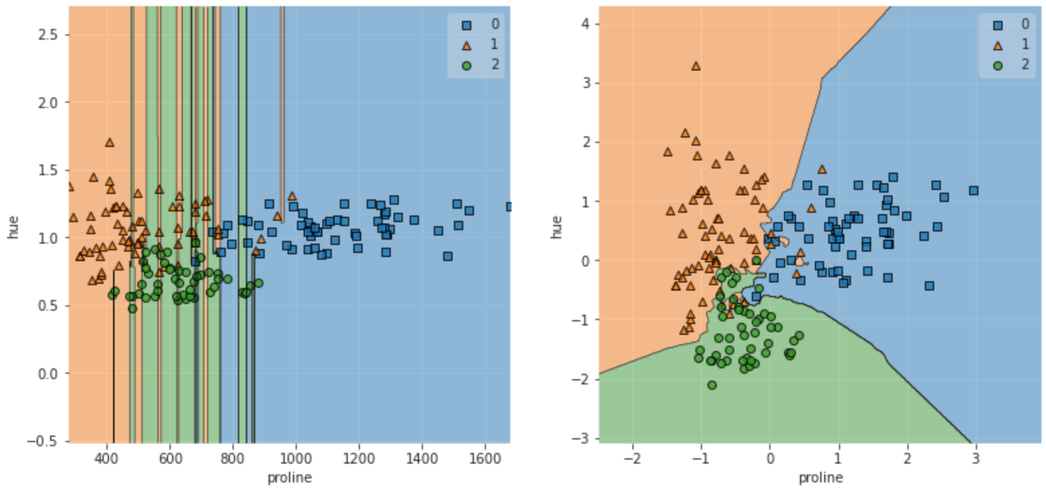
In [41]:
```
from sklearn.neighbors import KNeighborsClassifier

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

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.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

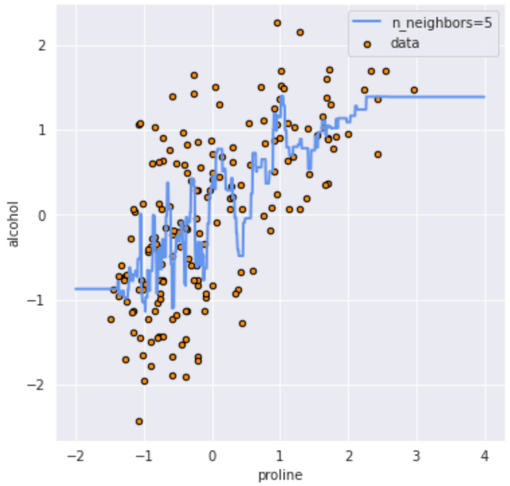
In [42]:
```
knn        = KNeighborsClassifier(n_neighbors=3).fit(X,y)
knn_zscore = KNeighborsClassifier(n_neighbors=3).fit(X_zscore,y)

fig,ax = plt.subplots(1,2,figsize=(13,6))
plot_decision_regions(X.values, y.values, clf=knn, ax=ax[0]);
ax[0].set_xlabel(X.columns[0]); ax[0].set_ylabel(X.columns[1]);

plot_decision_regions(X_zscore.values, y.values, clf=knn_zscore, ax=ax[1]);
ax[1].set_xlabel(X.columns[0]); ax[1].set_ylabel(X.columns[1]);
```



Regression with kNN

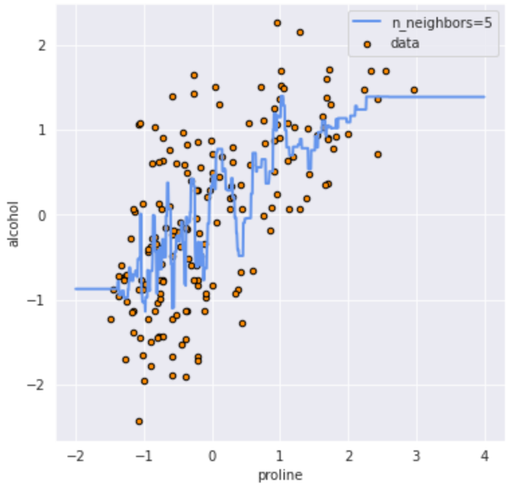
Regression with kNN

In [43]:
```
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();
```



Regression with kNN

In [43]:
```
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();
```

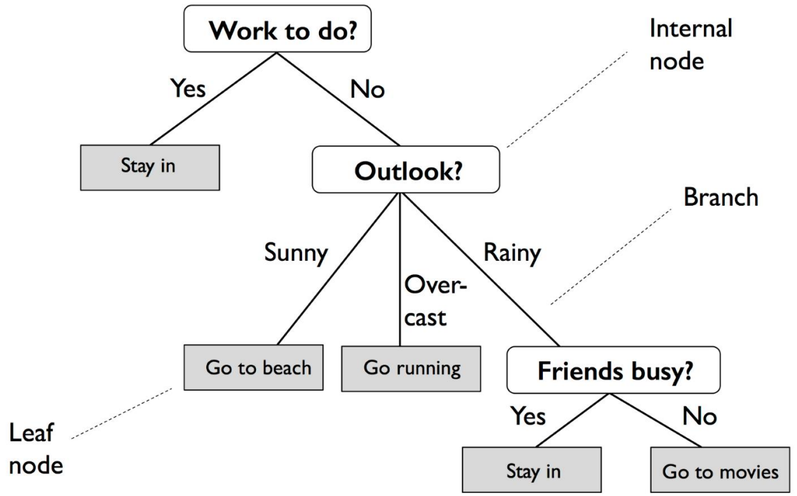


In [44]:
```
print(f'{X_zscore.iloc[1].proline:0.2f} : {knnr.predict(X_zscore.iloc[1].proline.reshape(-1,1))}')
```

```
0.96 : [1.16451234]
```

Decision Tree

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

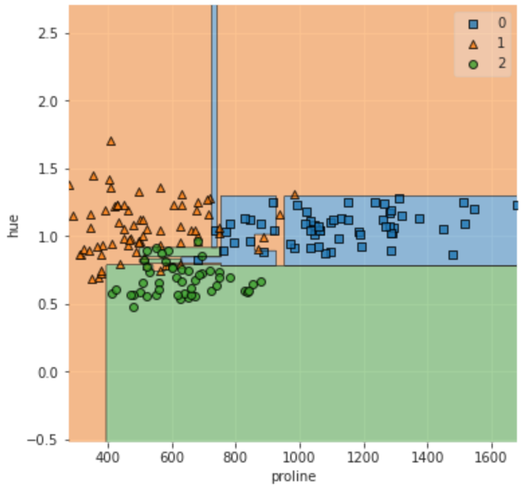


From PML

Decision Tree Classifier in sklearn

Decision Tree Classifier in sklearn

In [45]:
```
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]);
```

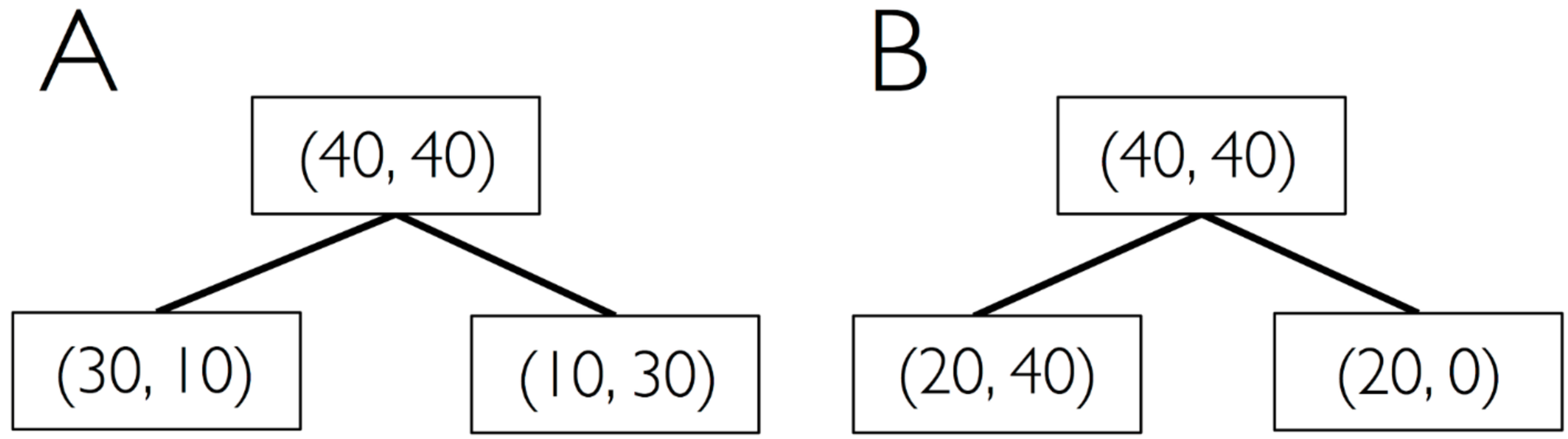


Building a Decision Tree

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

Building a Decision Tree

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



From PML

Choosing Questions To Minimize Impurity

Choosing Questions To Minimize Impurity

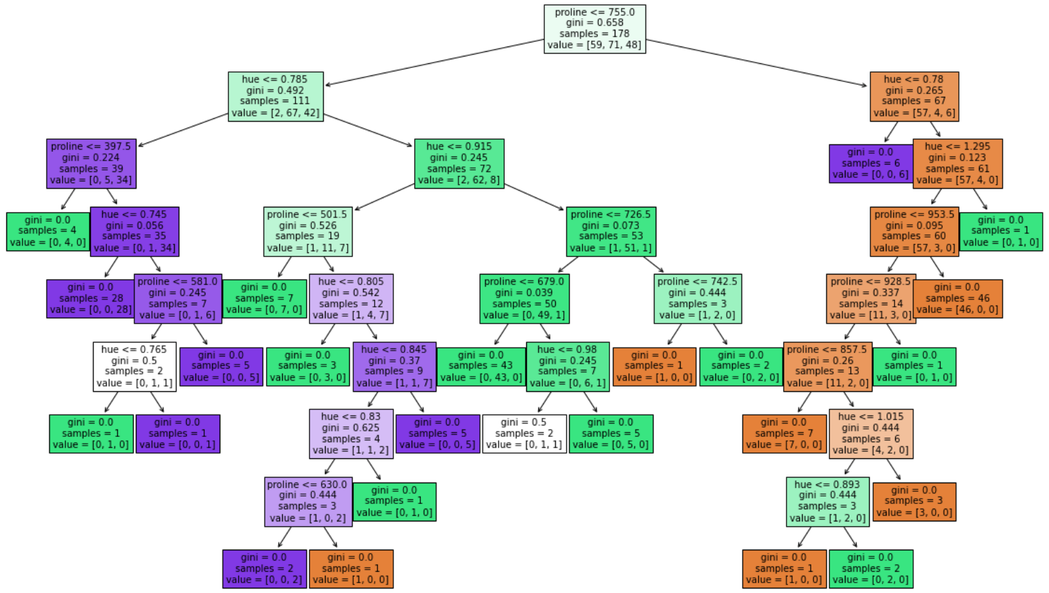
In [46]:
```
df = pd.DataFrame([[0,.2,0],[0,.7,0],[1,.7,1]],columns=['feature1','feature2','target'])
display(df)

# Is feature1 equal to 0?
print(df[df.feature1 == 0].target.values)
print(df[df.feature1 != 0].target.values)
print()

# Is feature2 <= .2?
print(df[df.feature2 <= .2].target.values)
print(df[df.feature2 >  .2].target.values)
```

	feature1	feature2	target
0	0	0.2	0
1	0	0.7	0
2	1	0.7	1

```
[0 0]
[1]

[0]
[0 1]
```

Plot Learned Decision Tree Using sklearn

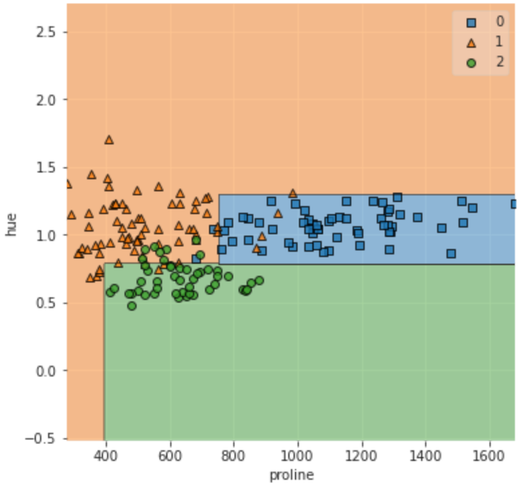
```
# Note: there is a conflict between plot_tree and seaborn.set_style in sklearn < .24
from sklearn.tree import plot_tree
# for tree with maxdepth=10
plot_tree(dtc,ax=ax,fontsize=8,feature_names=X.columns,filled=True);
```



Decision Tree: Limit Maximum Depth

Decision Tree: Limit Maximum Depth

In [47]:
```
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]);
```



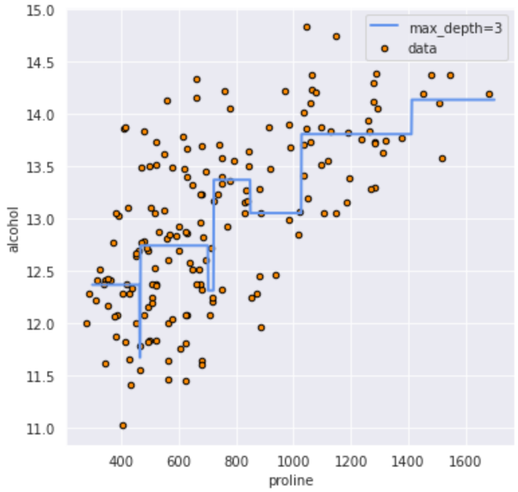
Plot Learned Decision Tree Using sklearn

- For tree with max_depth=3

Regression with Decision Trees

Regression with Decision Trees

In [48]:
```
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

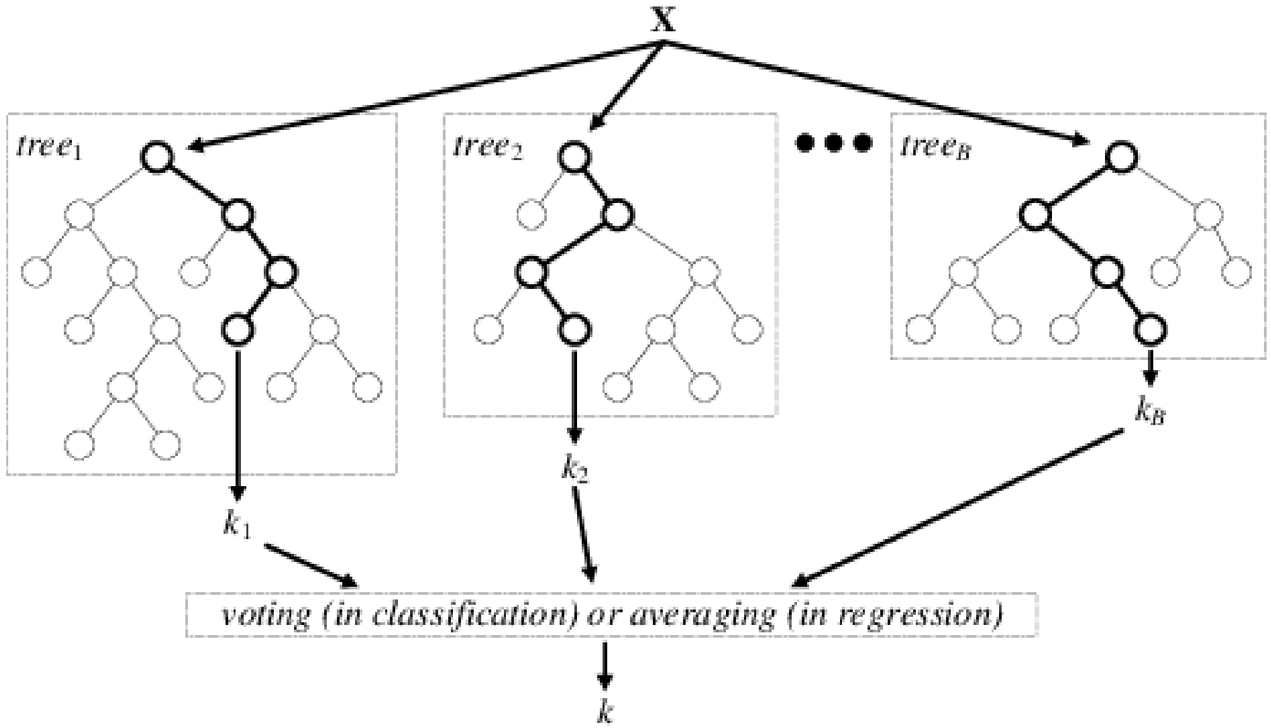
Ensemble Methods

- "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

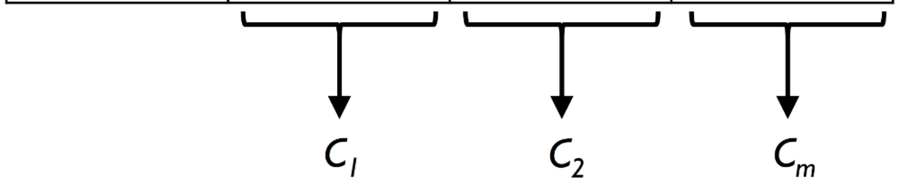


From https://www.researchgate.net/publication/301638643_Electromyographic_Patterns_during_Golf_Swing_Activation_Sequence_Profiling_and_Prediction_of_Shot_Effectiveness

Bagging with Random Forests

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

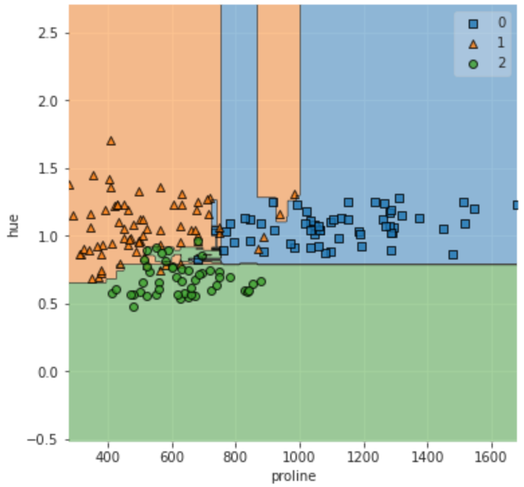
Sample indices	Bagging round 1	Bagging round 2	…
1	2	7	…
2	2	3	…
3	1	2	…
4	3	1	…
5	7	1	…
6	2	7	…
7	4	7	…



Random Forests with sklearn

Random Forests with sklearn

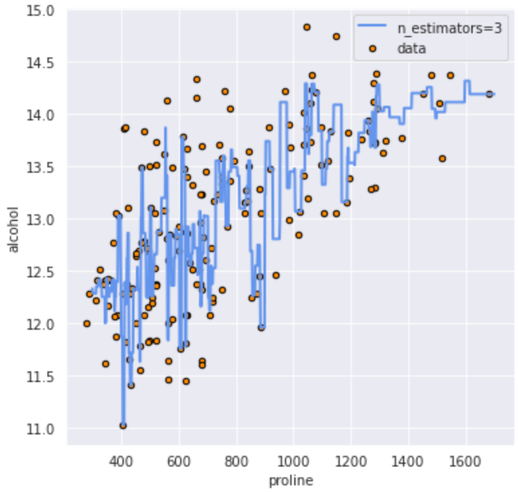
In [49]:
```
from sklearn.ensemble import RandomForestClassifier

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

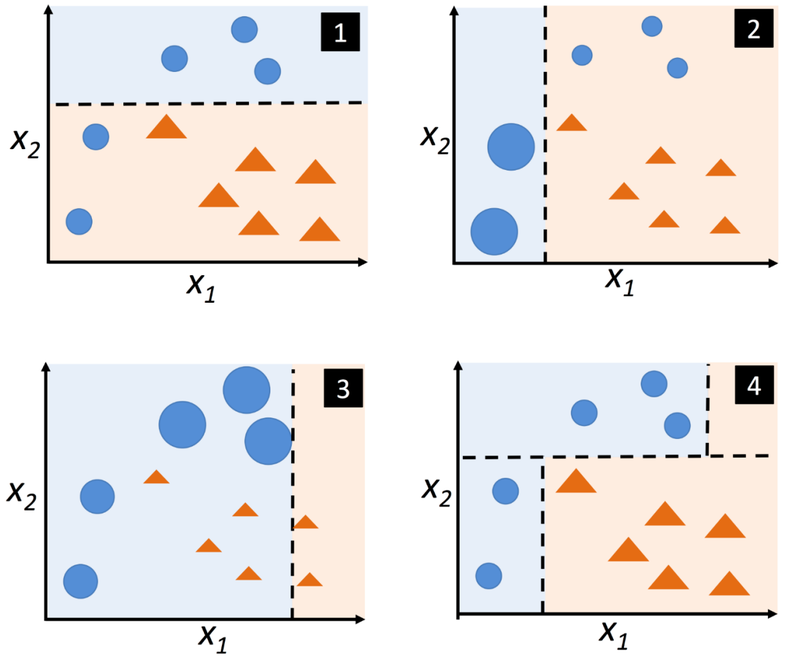
Regression with RandomForests

In [50]:
```
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

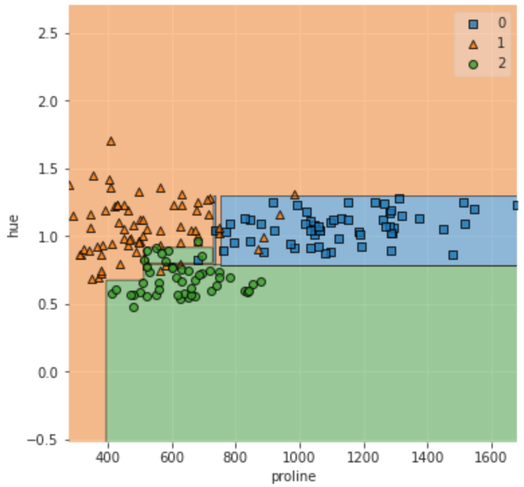


From PML

Gradient Boosted Trees in sklearn

Gradient Boosted Trees in sklearn

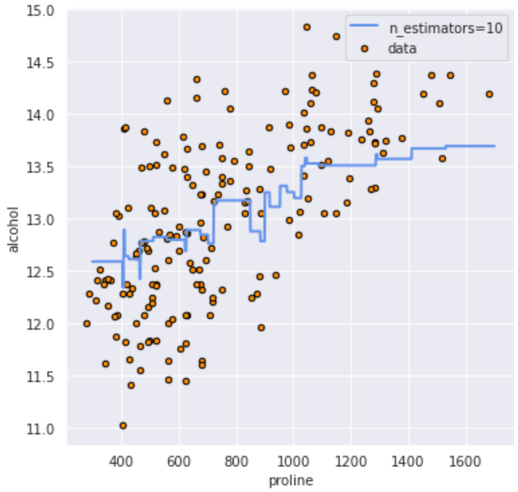
In [51]:
```
from sklearn.ensemble import GradientBoostingClassifier

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]);
```



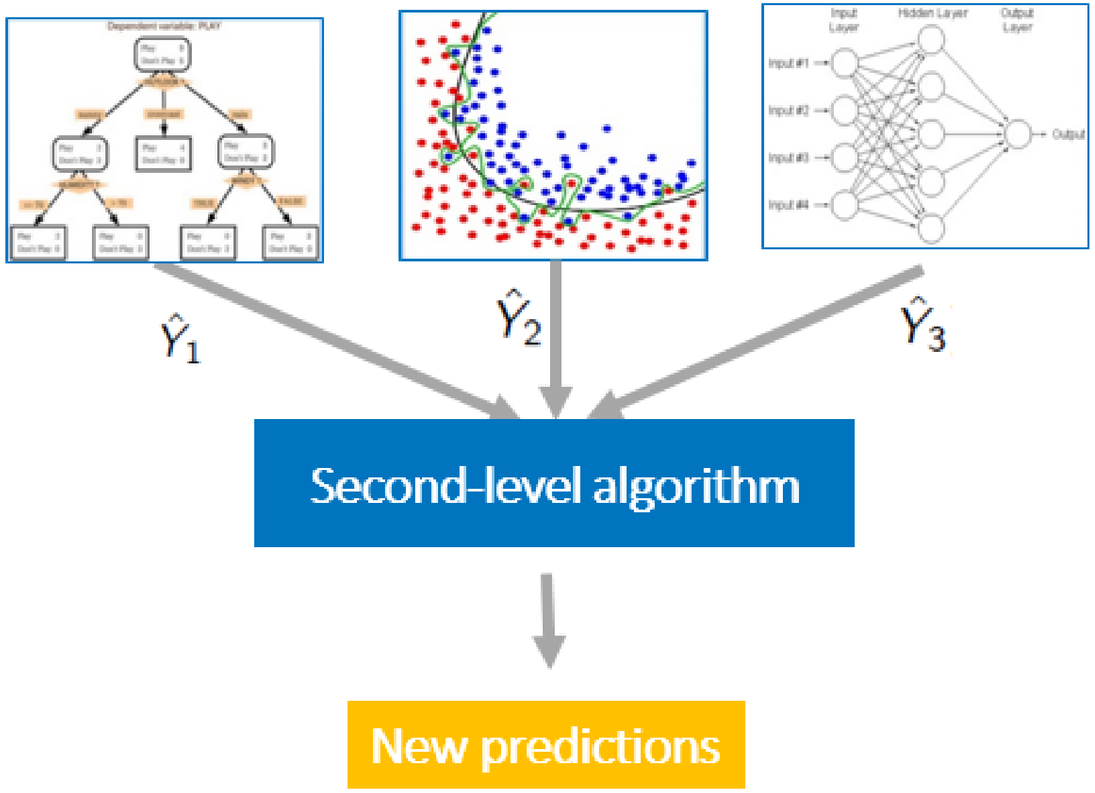
Regression with Gradient Boosted Trees

Regression with Gradient Boosted Trees

In [52]:
```
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

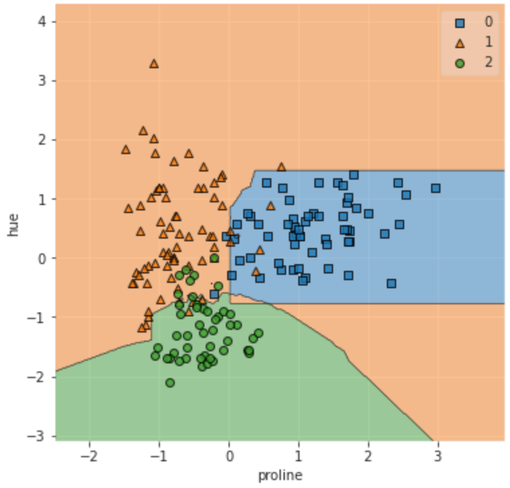


From https://blogs.sas.com/content/subconsciousmusings/2017/05/18/stacked-ensemble-models-win-data-science-competitions/

Stacking with mlxtend for Classification

Stacking with mlxtend for Classification

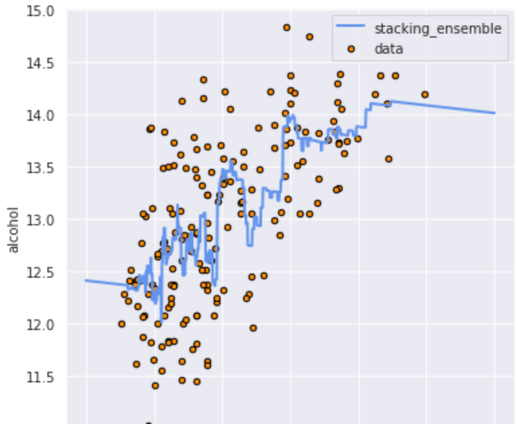
In [53]:
```
from mlxtend.classifier import StackingClassifier

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

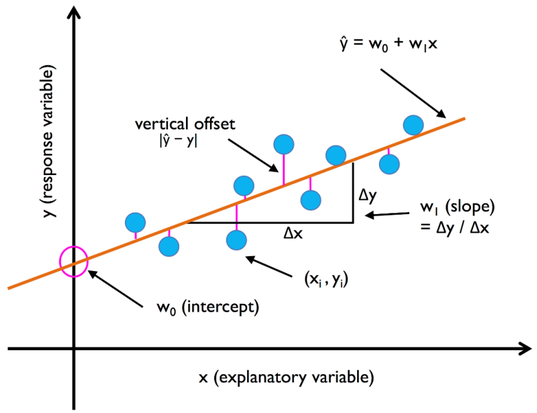
In [54]:
```
from mlxtend.regressor import StackingRegressor

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

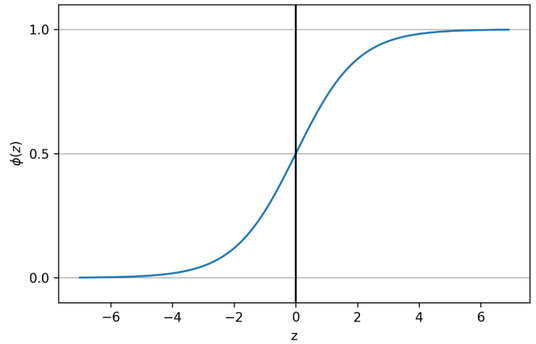
- Use for: Regression
- Pros:
    - fast to train
    - interpretable coefficients
- Cons:
    - assumes linear relationship
    - depends on removing colinear features



from PML

Model Review: Logistic Regression

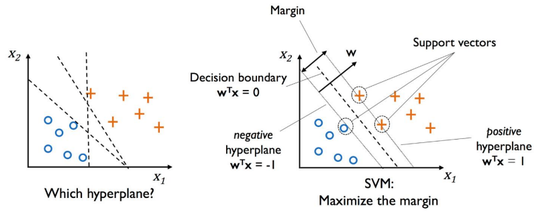
- Use for: Classification
- Pros:
    - fast to train
    - interpretable coefficients (log odds)
- Cons:
    - assumes linear boundary
    - depends on removing colinear features



from PML

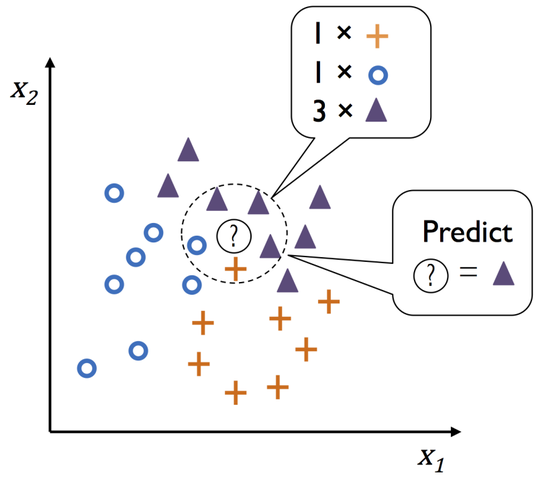
Model Review: Support Vector Machine (SVM)

- 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



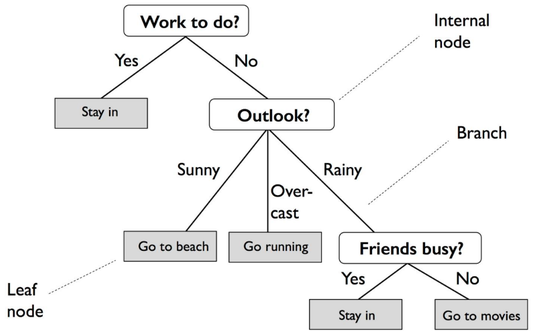
Model Review: k Nearest Neighbor (kNN)

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



Model Review: Decision Tree

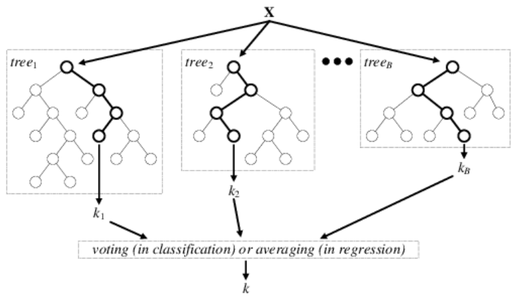
- Use for: Classification or Regression
- Pros:
    - very interpretable
    - quick to predict
    - can handle numeric and categorical variables without transformation
- Cons:
    - tendency to overfit (learn training set too well, more next class!)



From PML

Model Review: Random Forest (Ensemble via Bagging)

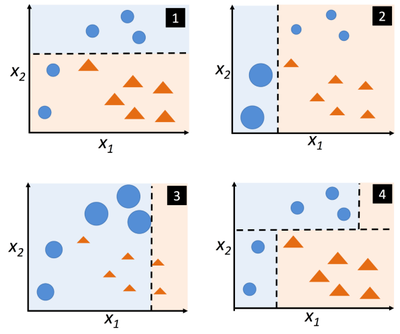
- Use for: Classification or Regression
- Pros:
    - less likely to overfit than decision tree
    - quick to train (through parallelization, quick to predict
- Cons:
    - less interpretible, though still possible



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



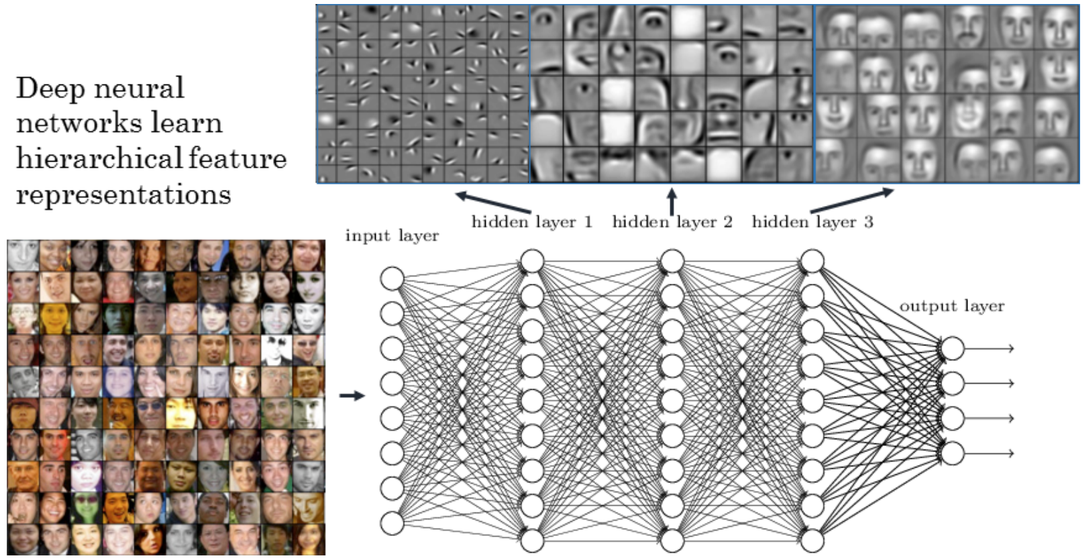
Model Review: Ensemble via Stacking

- 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

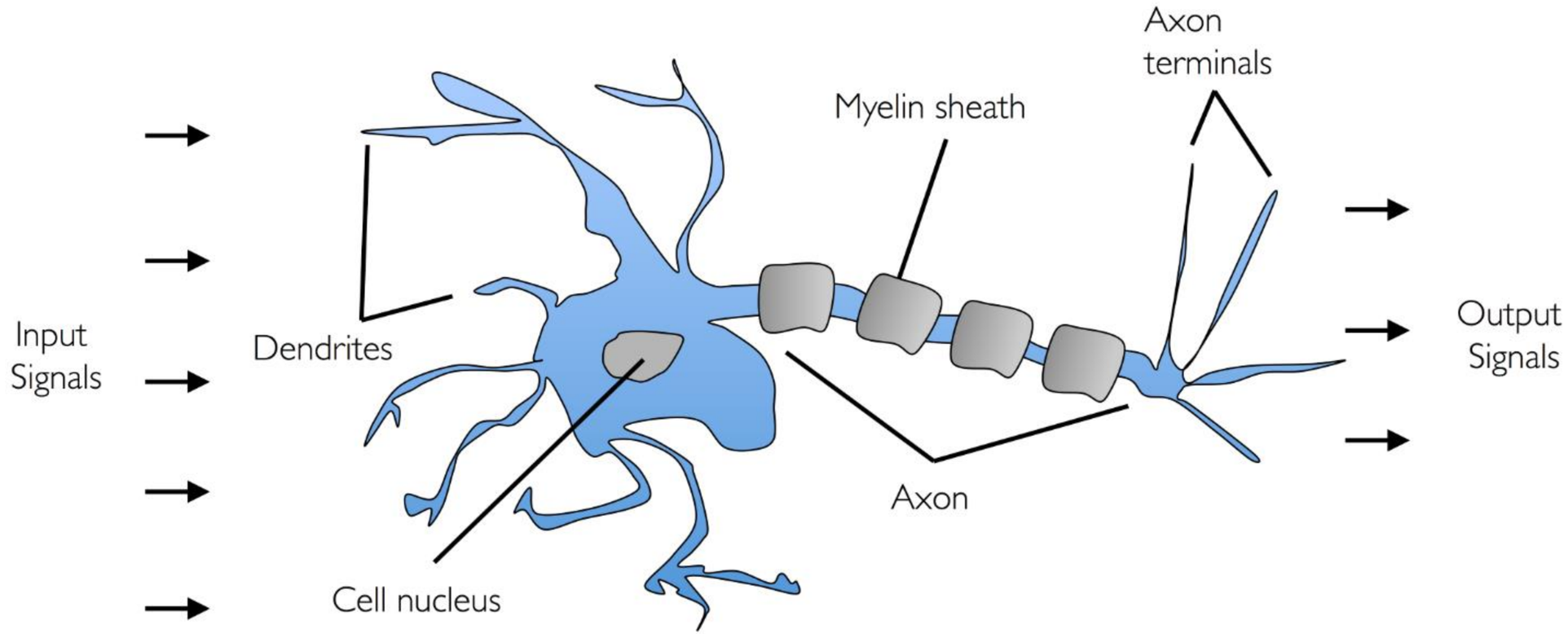
If we have time...

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)

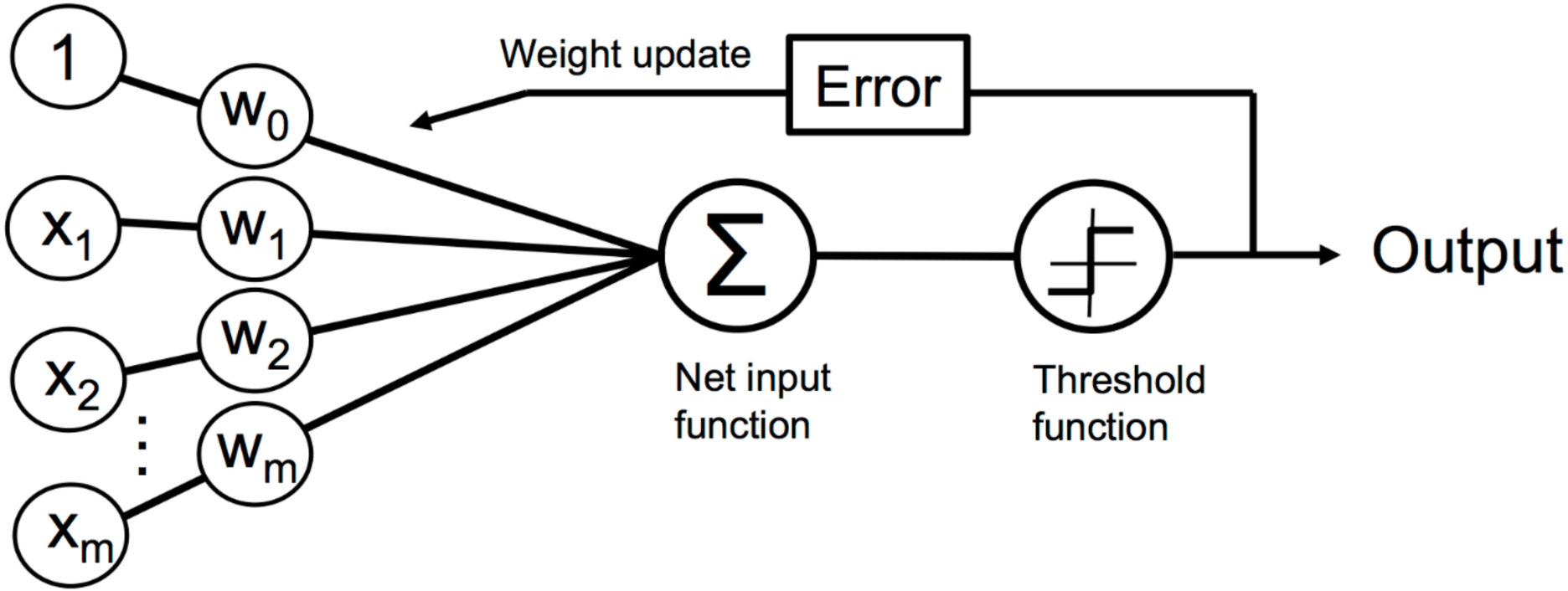


From Perceptron to Artificial Neural Network



From PML

Perceptron: Early Neuron Model

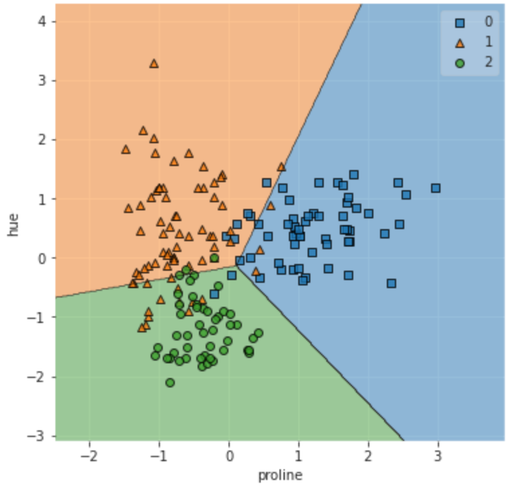


From PML

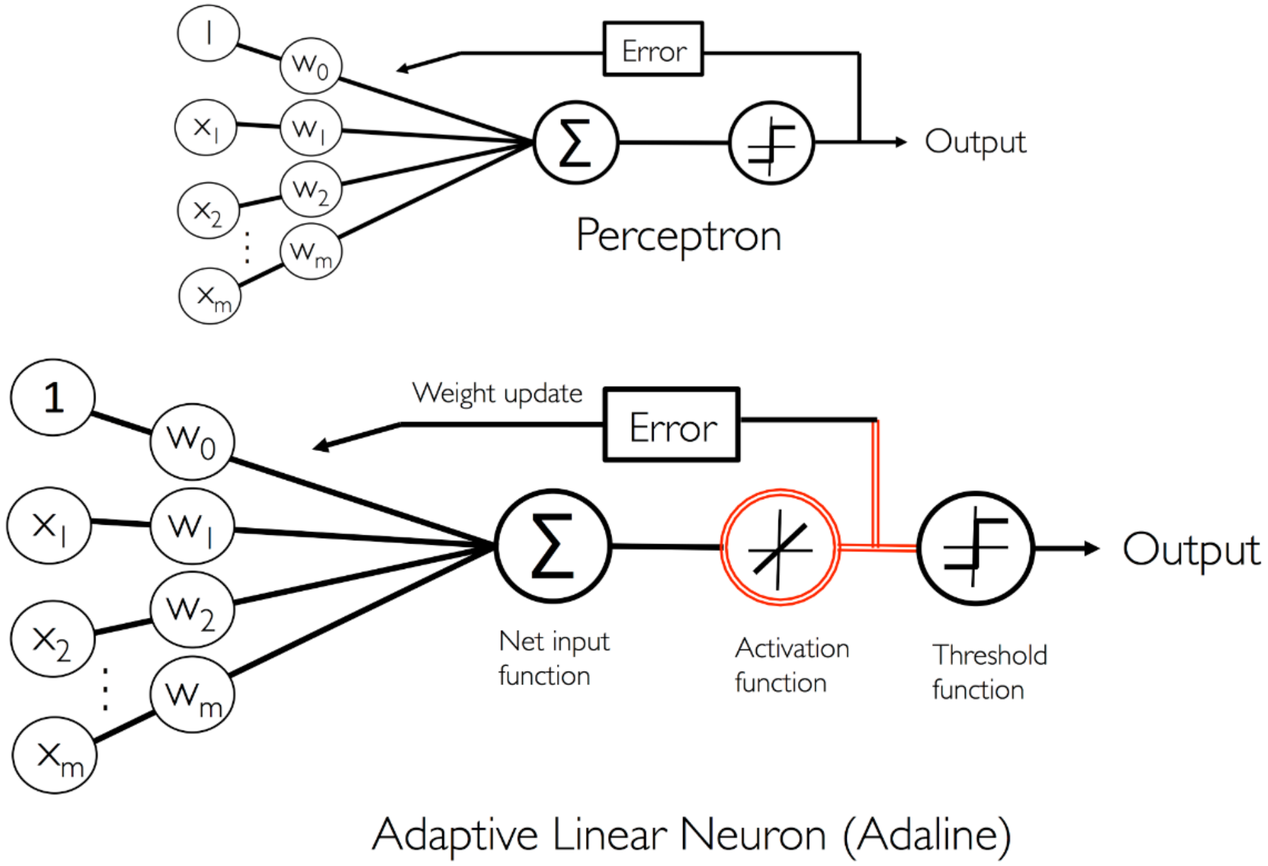
Perceptron in sklearn

Perceptron in sklearn

In [55]:
```
from sklearn.linear_model import Perceptron
perceptron = Perceptron()
perceptron.fit(X_zscore,y);

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

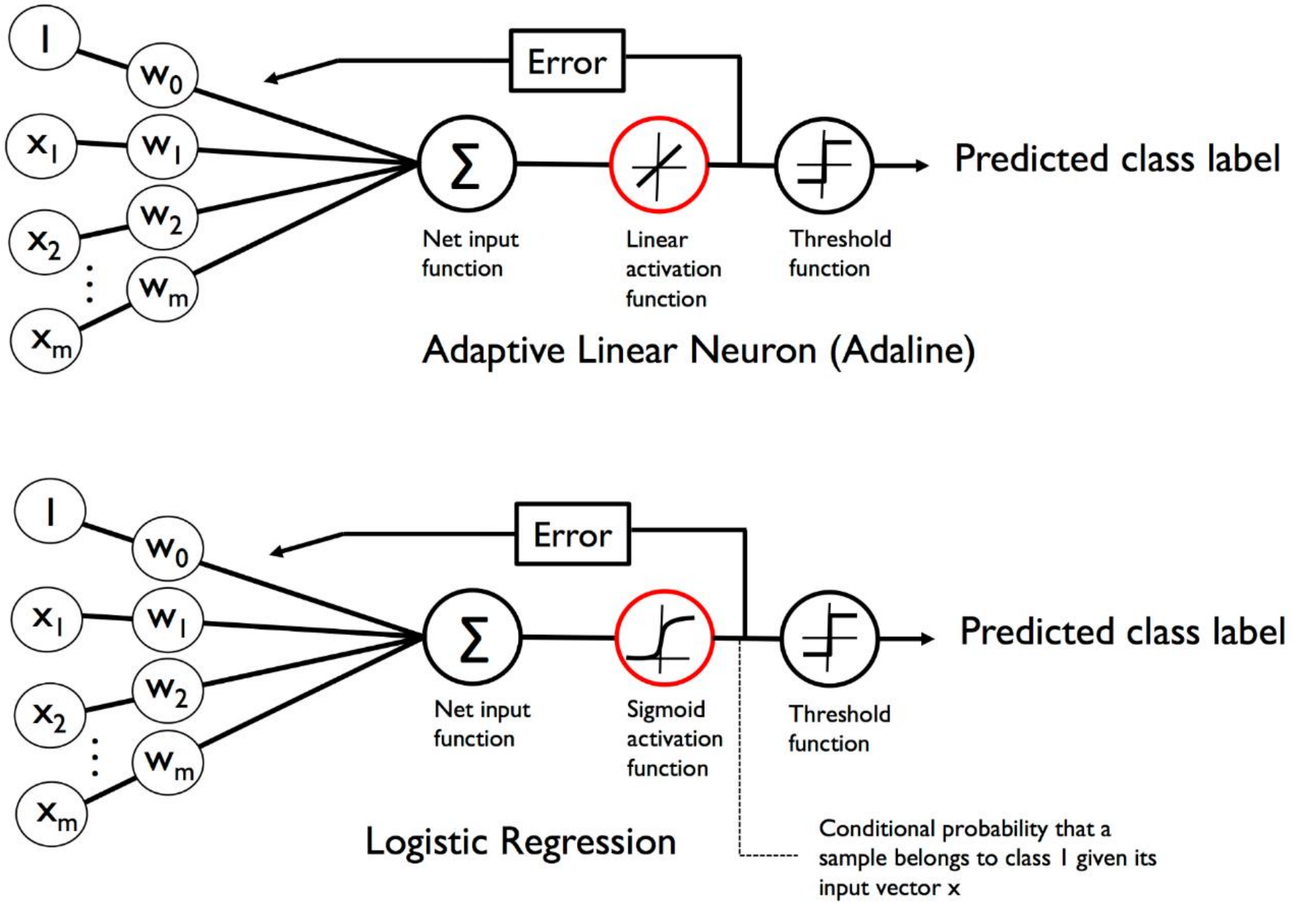


Perceptron to Adaline



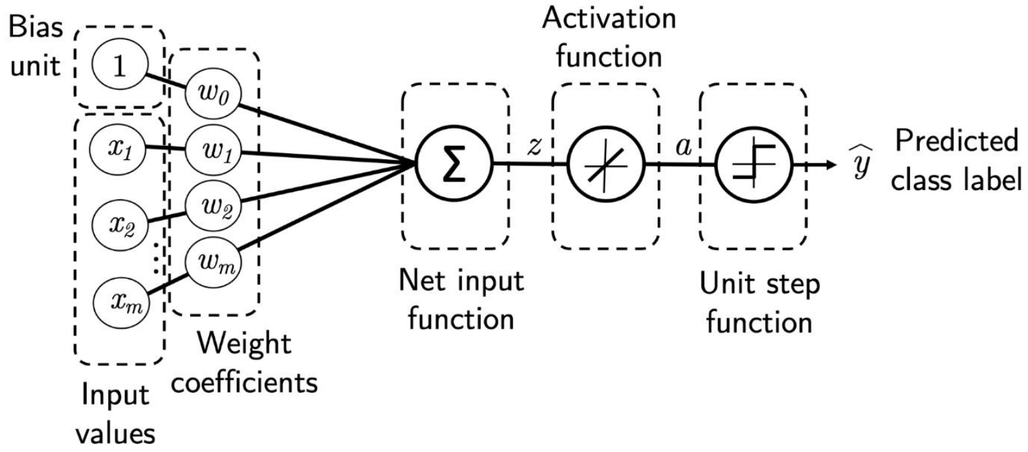
From PML

Adaline to Logistic Regression



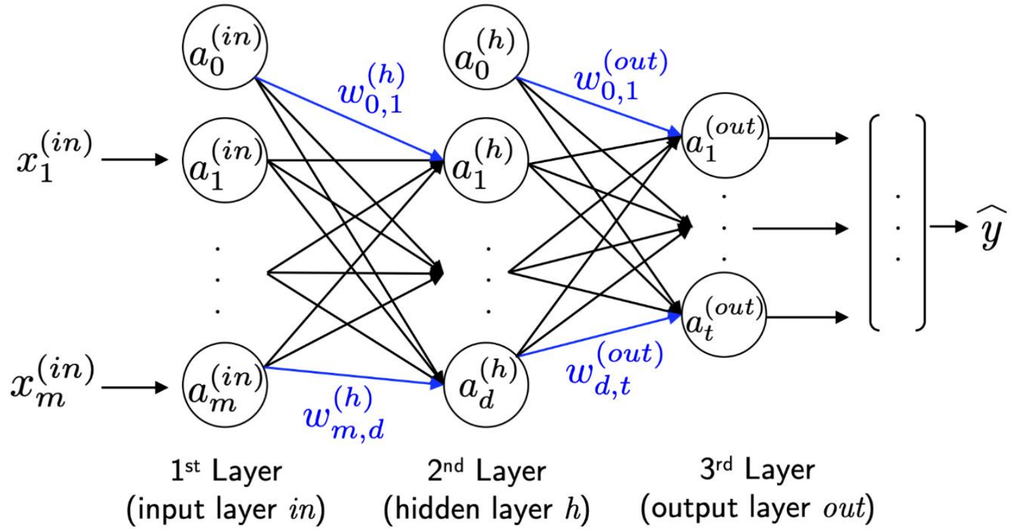
From PML

Components of Single Layer Neural Net



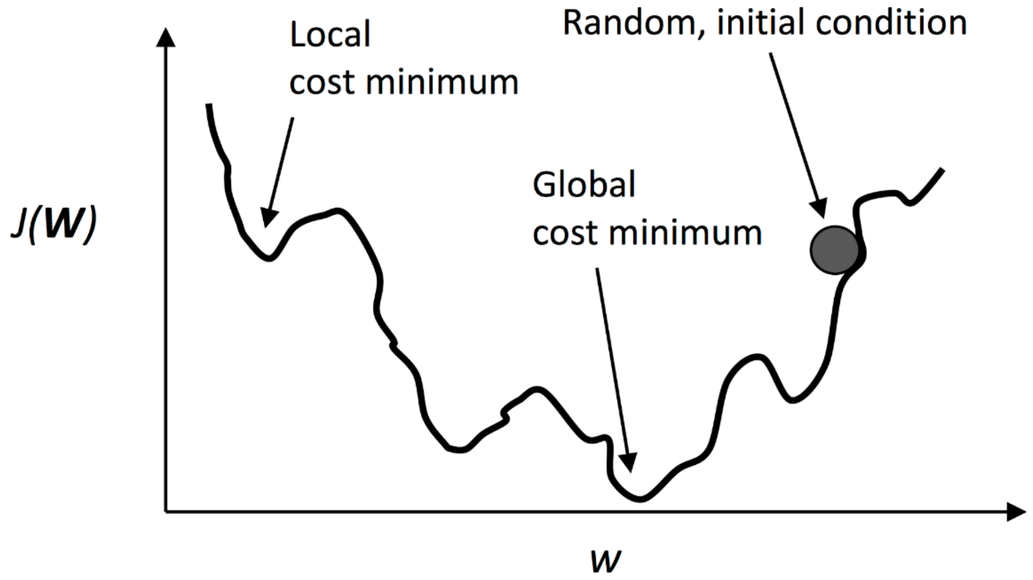
From PML

Multi-Layer Neural Network



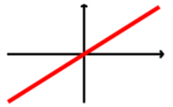
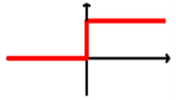
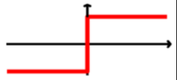
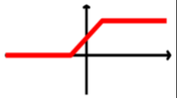
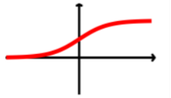
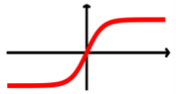
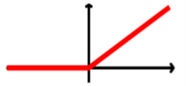
From PML

Complex Optimization Space



From PML

Activation Functions

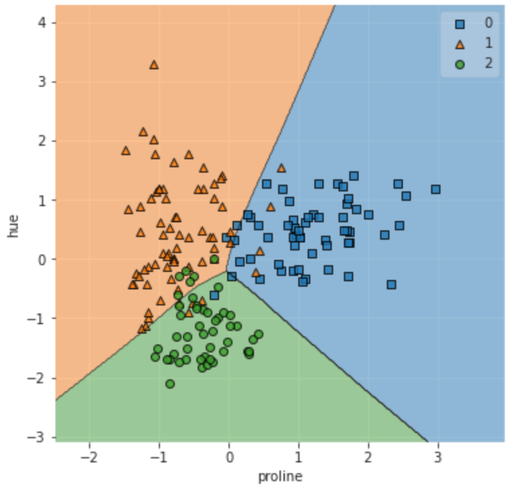
Activation function	Equation	Example	1D graph
Linear	$\phi(z) = z$	Adaline, linear regression	
Unit step (Heaviside function)	$\phi(z) = \begin{cases} 0 & z < 0 \\ 0.5 & z = 0 \\ 1 & z > 0 \end{cases}$	Perceptron variant	
Sign (signum)	$\phi(z) = \begin{cases} -1 & z < 0 \\ 0 & z = 0 \\ 1 & z > 0 \end{cases}$	Perceptron variant	
Piece-wise linear	$\phi(z) = \begin{cases} 0 & z \leq -½ \\ z + ½ & -½ \leq z \leq ½ \\ 1 & z \geq ½ \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, multilayer NN	
Hyperbolic tangent (tanh)	$\phi(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$	Multilayer NN, RNNs	
ReLU	$\phi(z) = \begin{cases} 0 & z < 0 \\ z & z > 0 \end{cases}$	Multilayer NN, CNNs	

From PML

Multi-Layer Perceptron with sklearn

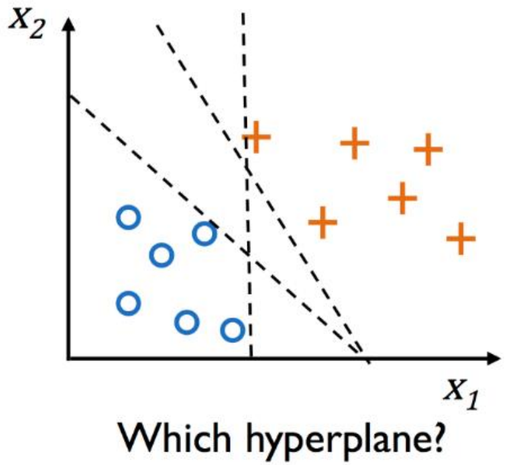
Multi-Layer Perceptron with sklearn

In [56]:
```
from sklearn.neural_network import MLPClassifier, MLPRegressor
mlp = MLPClassifier(hidden_layer_sizes=(100,),
                    max_iter=1000)
mlp.fit(X_zscore,y);

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

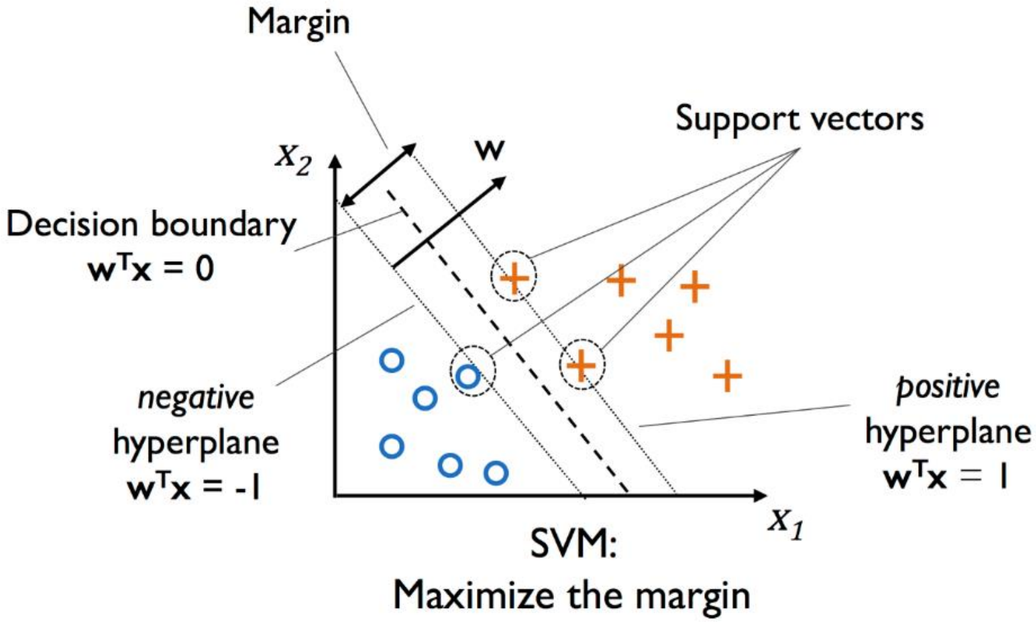


Which boundary should we use? Support Vector Machines (SVMs)

- For a linearly seperable dataset, where should we place the decision boundary?
- Support Vector Machine (SVM) tries to "maximize the margin" between classes



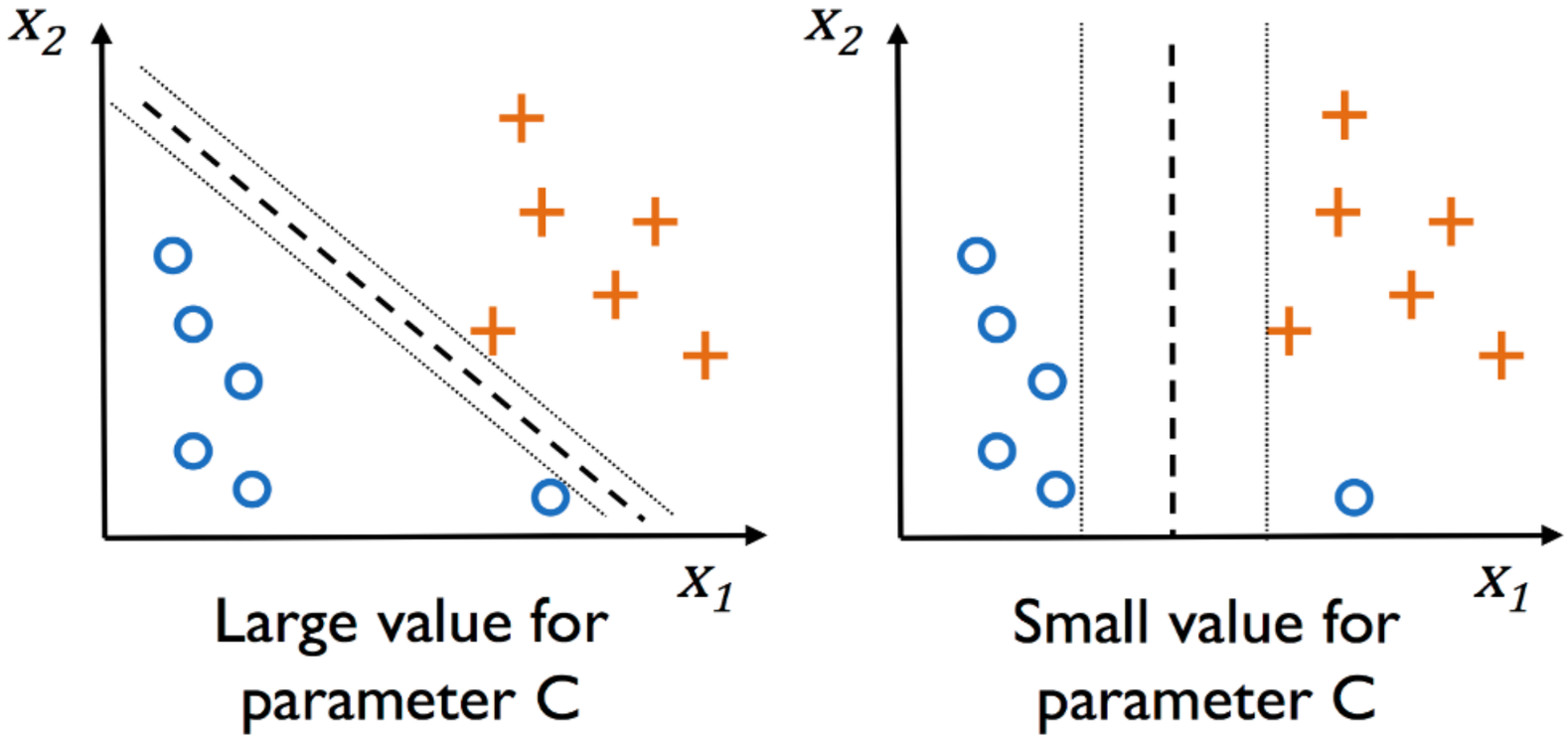
Which hyperplane?



SVM:
Maximize the margin

SVM Hyperparameter C

- **Hyperparameter**: Something we set

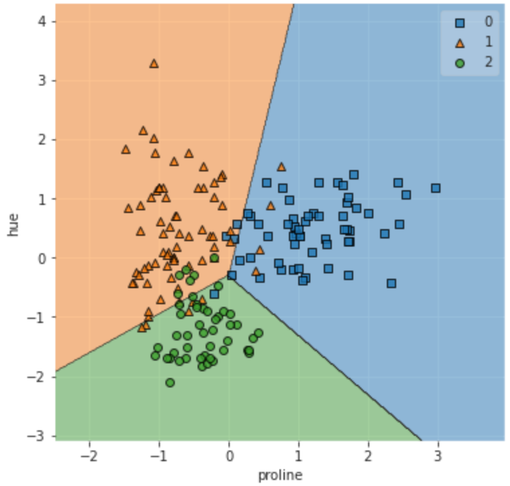


From PML

SVM with sklearn

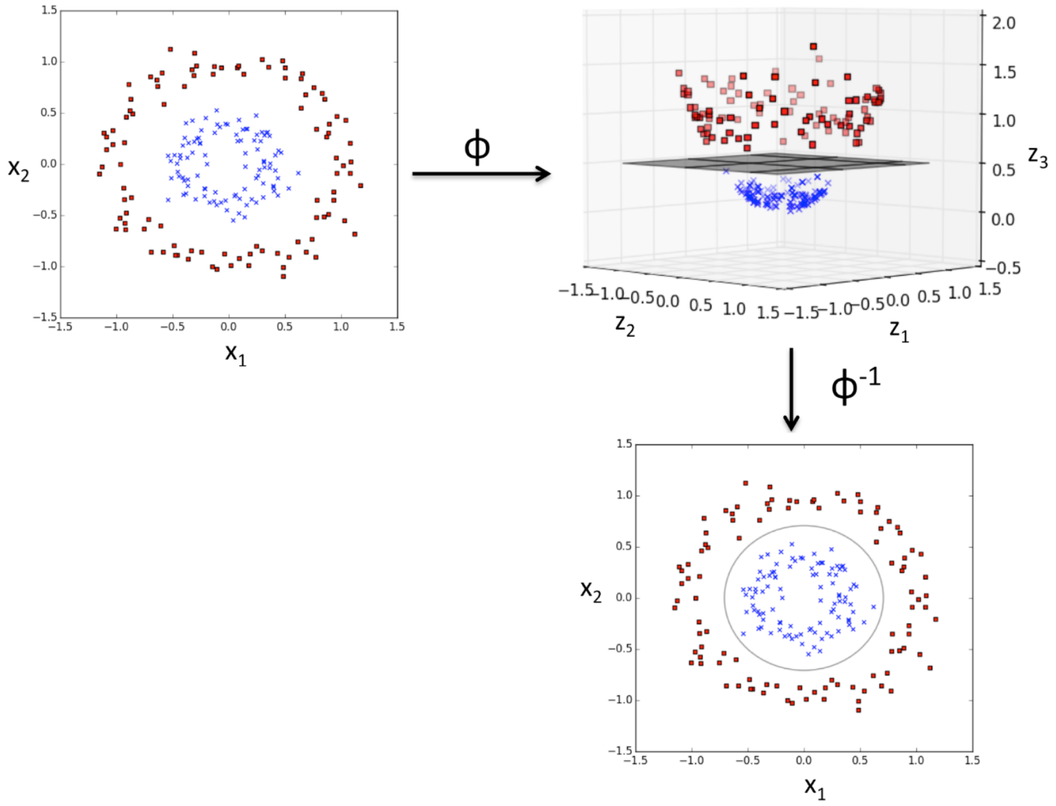
SVM with sklearn

In [57]:
```
from sklearn.svm import SVC
svm_linear = SVC(kernel='linear')
svm_linear.fit(X_zscore,y);

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



Non-Linear Boundaries with SVMs Kernel Trick

- **Kernel Trick**: Map data to a higher dimensional space and find linear boundary there



From PML

SVM Kernel Trick with RBF Kernel

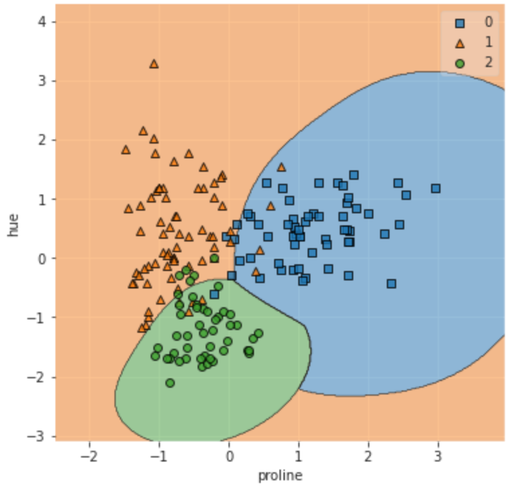
SVM Kernel Trick with RBF Kernel

- RBF (Radial-Basis Function) kernel

SVM Kernel Trick with RBF Kernel

- RBF (Radial-Basis Function) kernel

In [58]:
```
svm_rbf = SVC(kernel='rbf')
svm_rbf.fit(X_zscore,y);

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



Questions?