Elements Of Data Science - F2020

Week 5: Intro to Machine Learning Models

10/12/2020

TODOs

- Readings:
    - Recommended: https://scikit-learn.org/stable/supervised_learning.html
    - Reference: PML Chapter Chap 3
- Answer and submit Quiz 5
- HW1, Due Thurs Oct 22nd, 11:59pm ET

Today

- Multi-Armed Bandit (previous week's slides)
- Intro to Machine Learning Models
  - Various types of ML
  - Linear models

Git Stash

Git will not allow you to pull new version of files if there is a conflict.

Common source of conflict:

1. Slide notebook is pushed and pulled
2. You make changes to the notebook (encouraged!)
3. I post new updates to the notebook (fixes, etc).

Now your version and the current version on github both have new changes: Conflict!

Solution: Stash your changes

```
$ cd eods-f20
$ git stash
$ git pull
```

Questions?

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

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
69	12.21	1.75	1.28	718.0	1
53	13.77	2.68	1.13	1375.0	0

- 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)

Terms in ML

```
In [3]: df_wine.sample(5,random_state=1)
```

Out[3]:

	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
69	12.21	1.75	1.28	718.0	1
53	13.77	2.68	1.13	1375.0	0

- 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

Variations of ML Tasks

- Supervised vs Unsupervised
    - is there a target/label?
- Regression vs Classification
    - is the target numeric or categorical?
- Interpretation vs Prediction
    - 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

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

Interpretation vs Prediction

- Do we care more about understanding how XX relates to yy?
  - Ex: What happens to tip size as taxi trip length increases?
  - Ex: What is the relationship between debt and loan default?
- Do we care more about generating predictions?
  - Ex: For a given trip, what will the tip size likely be?
  - Ex: For a given loan, will there be a default?

Model Families for Supervised Learning

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

Model Families for Supervised Learning Continued

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

Example: Regression with a Linear Model

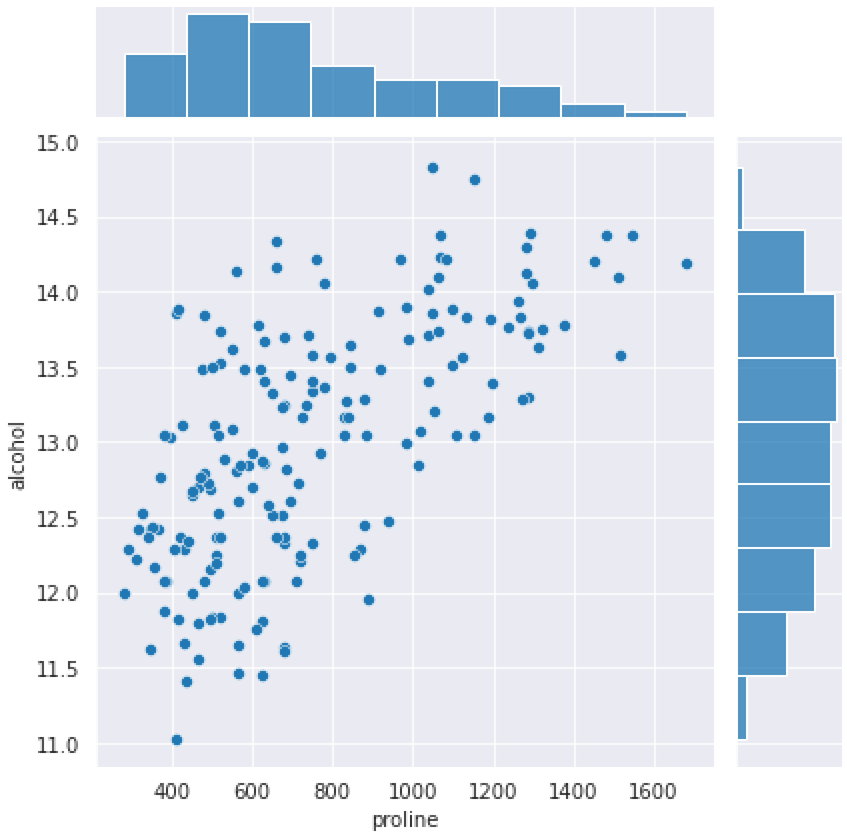
What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

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

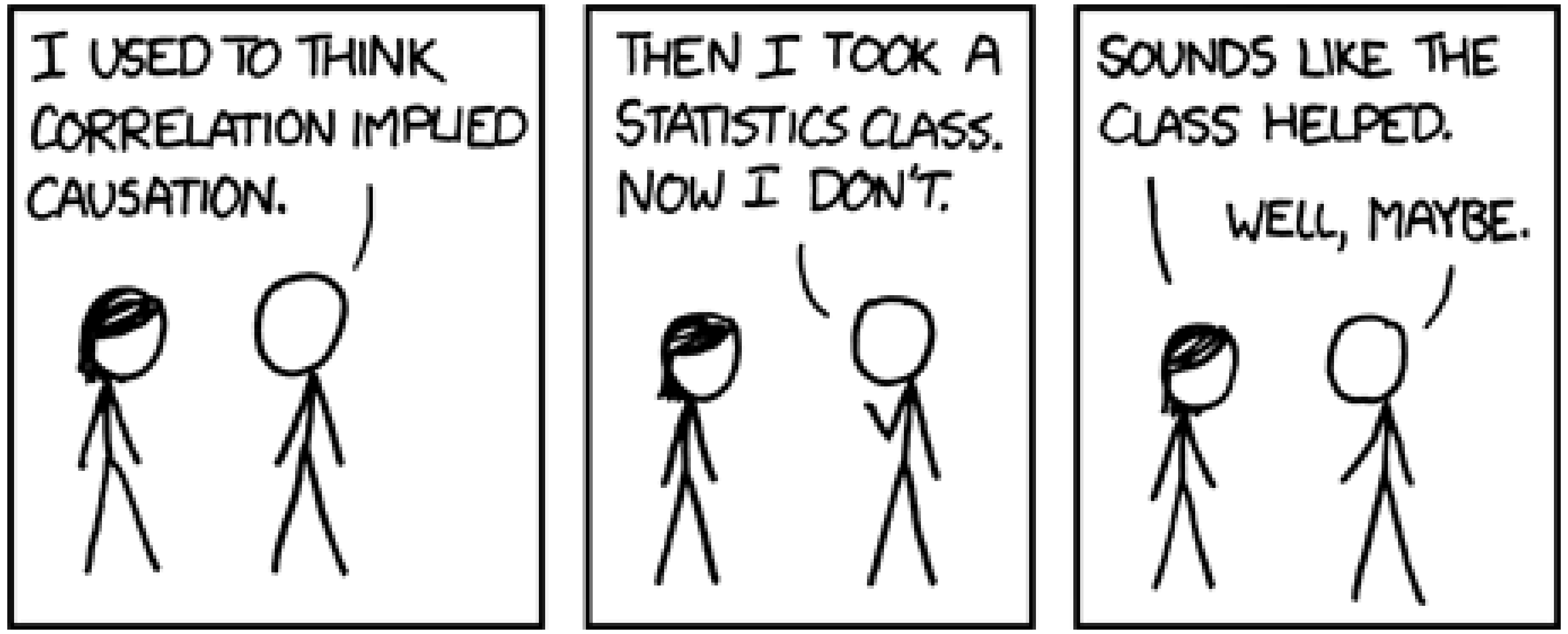
Aside: Correlation

Question: are total_bill and tips correlated?

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



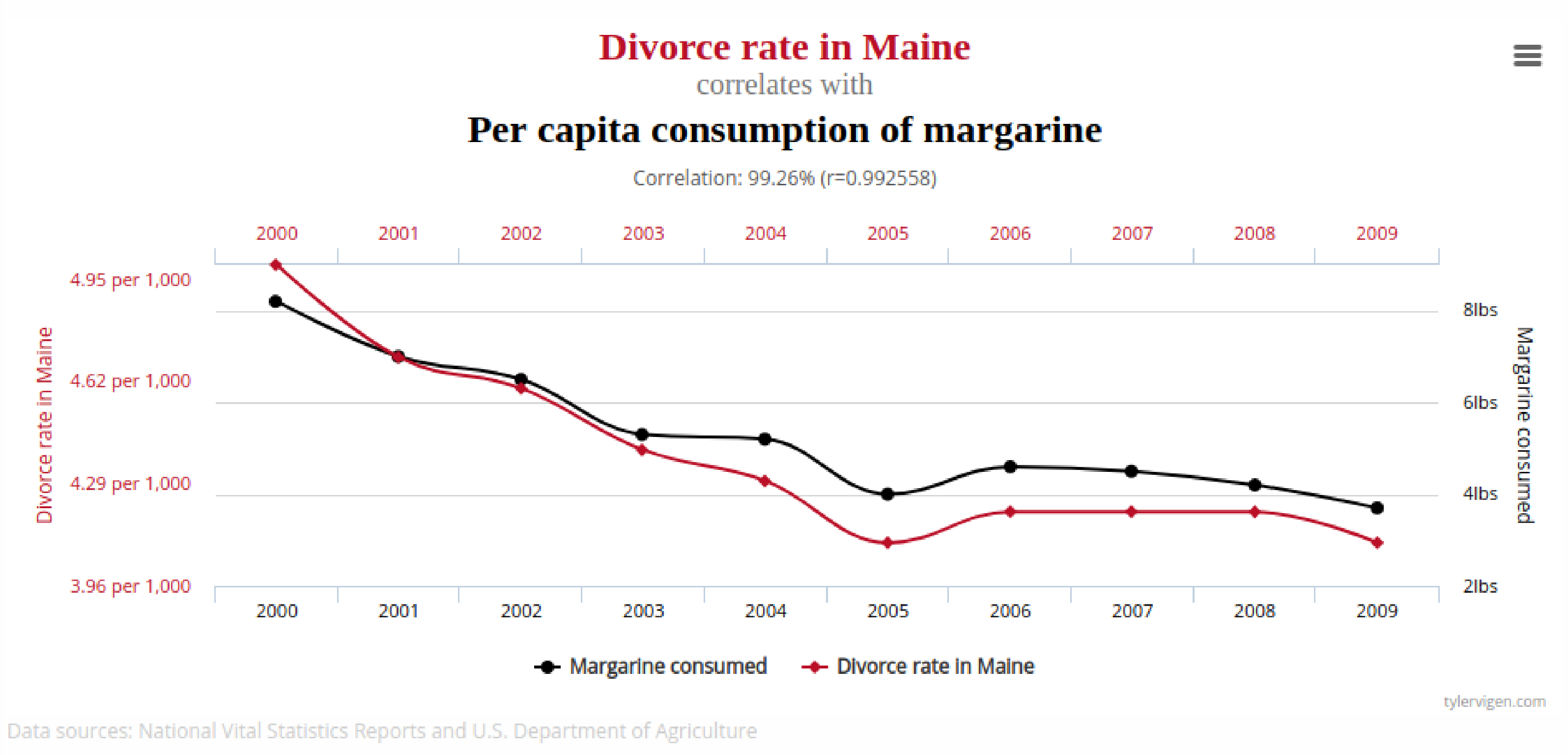
Obligitory Correlation vs. Causation



- 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
- Assumes normally distributed data! (which is not true here)
    - On the Effects of Non-Normality on the Distribution of the Sample Product-Moment Correlation Coefficient

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
```

- 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.

MLXTEND

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

CONDA-FORGE

```
$ conda install --name eods-f20 --channel conda-forge mlxtend
```

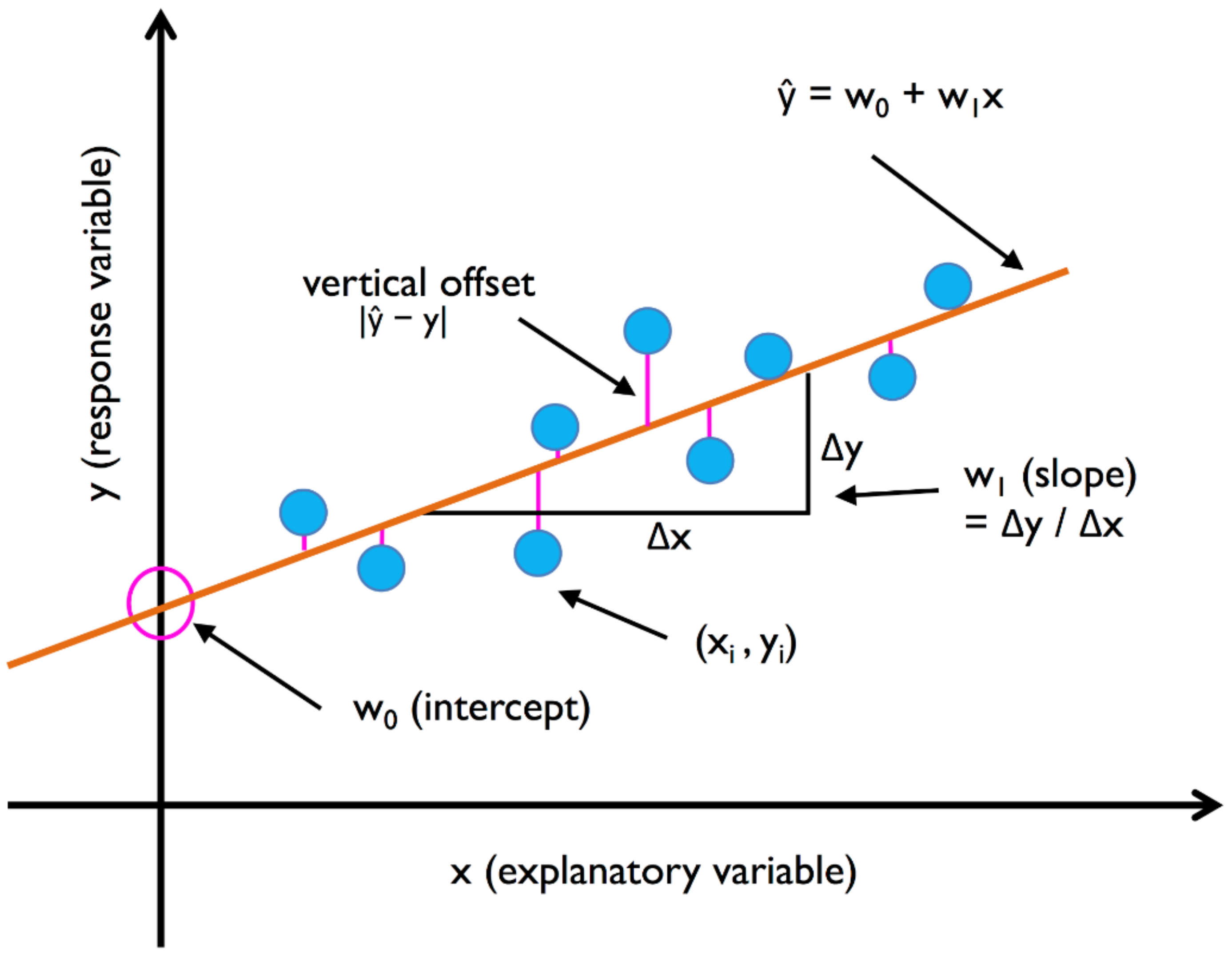
Simple Linear Regression

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

- 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

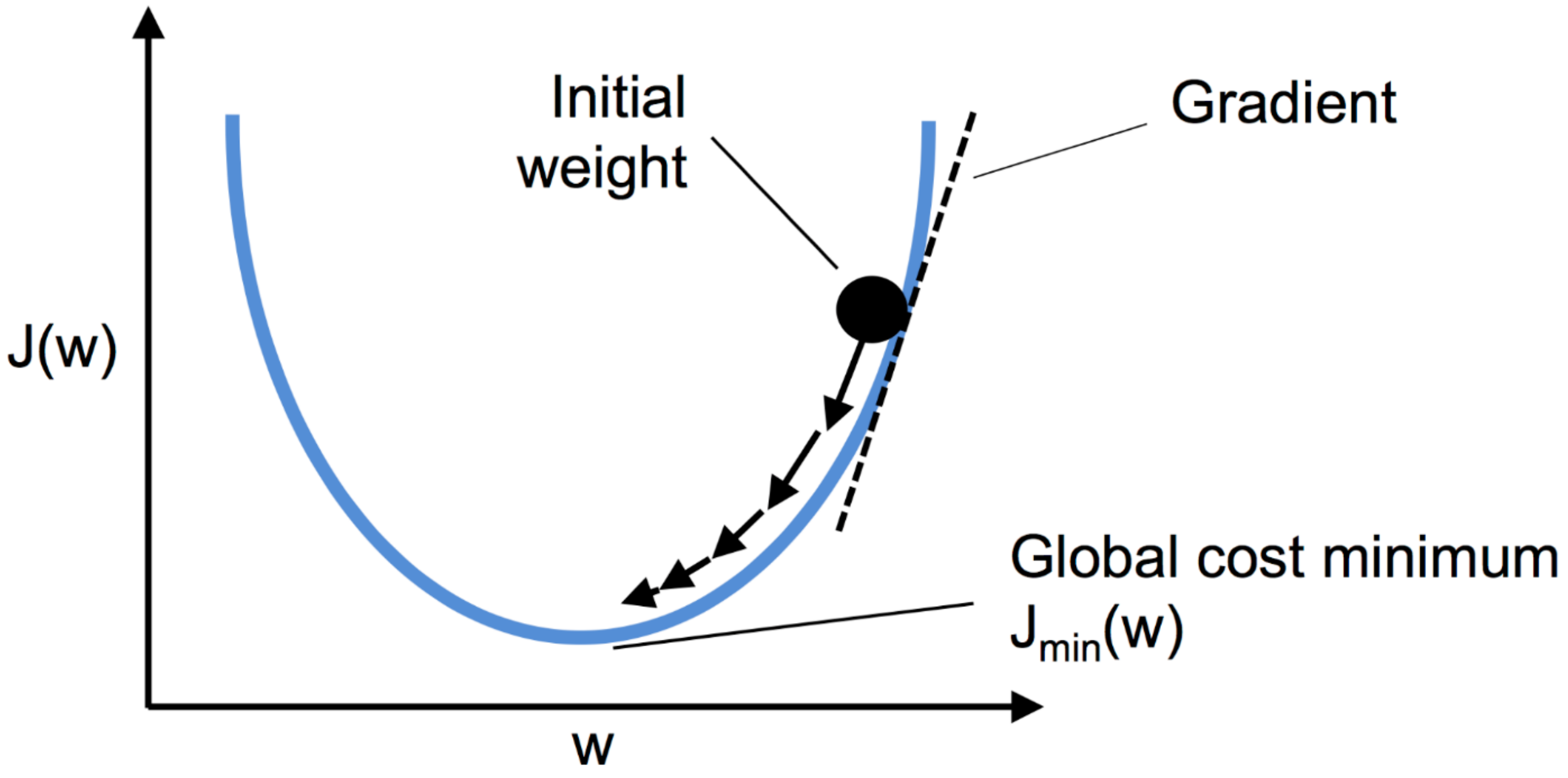
- Want to maximize or minimize something (Ex: squared error)

- **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

Aside: Gradient Descent Cont.



Simple Regression Using scikit-learn

In [7]:
```
# import the model from sklearn
from sklearn.linear_model import LinearRegression
```

In [8]:
```
 # instantiate the model and set hyperparameters
lr = LinearRegression(fit_intercept=True, # by default
                      normalize=False)    # by default
```

In [9]:
```
# fit the model
lr.fit(X=df_wine.proline.values.reshape(-1, 1), y=df_wine.alcohol);
```

In [10]:
```
# display learned coefficients (_ in)
print(lr.coef_)
print(lr.intercept_)
```

```
[0.0016595]
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

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

Out[12]: array([1065., 1050., 1185., 1480.,  735.])

In [13]: df_wine.proline.values.shape

Out[13]: (178,)

In [14]: df_wine.proline.values.reshape(-1,1).shape

Out[14]: (178, 1)
```

-1 means "infer from the data"

Interpreting Coefficients

In [15]:
```
print(f'beta={lr.coef_[0]:0.3f}, alpha={lr.intercept_:0.3f}')
```
```
beta=0.002, alpha=11.761
```

In [16]:
```
print(f'alchohol = {lr.coef_[0]:0.3f}*proline + {lr.intercept_:0.3f}')
```
```
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

In [17]:
```
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

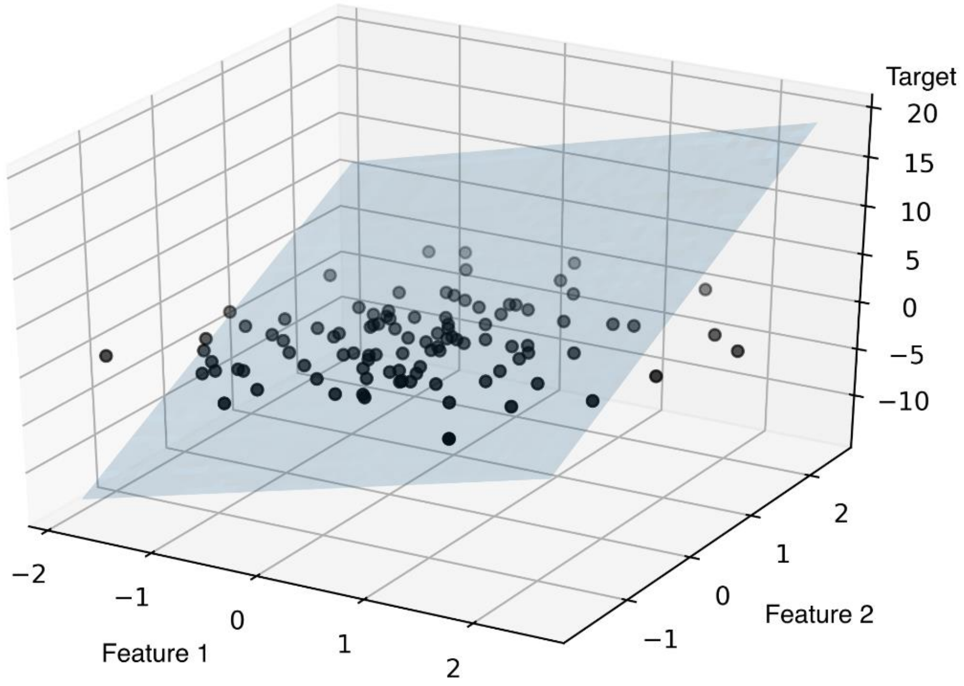
- Including multiple independent variables

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

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

In [18]:
```
mlr = LinearRegression()
mlr.fit(df_wine[['proline','hue']],y=df_wine.alcohol);

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

In [19]:
```
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[19]:

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:	Sun, 11 Oct 2020	**Prob (F-statistic):**	1.15e-24
Time:	17:11:20	**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

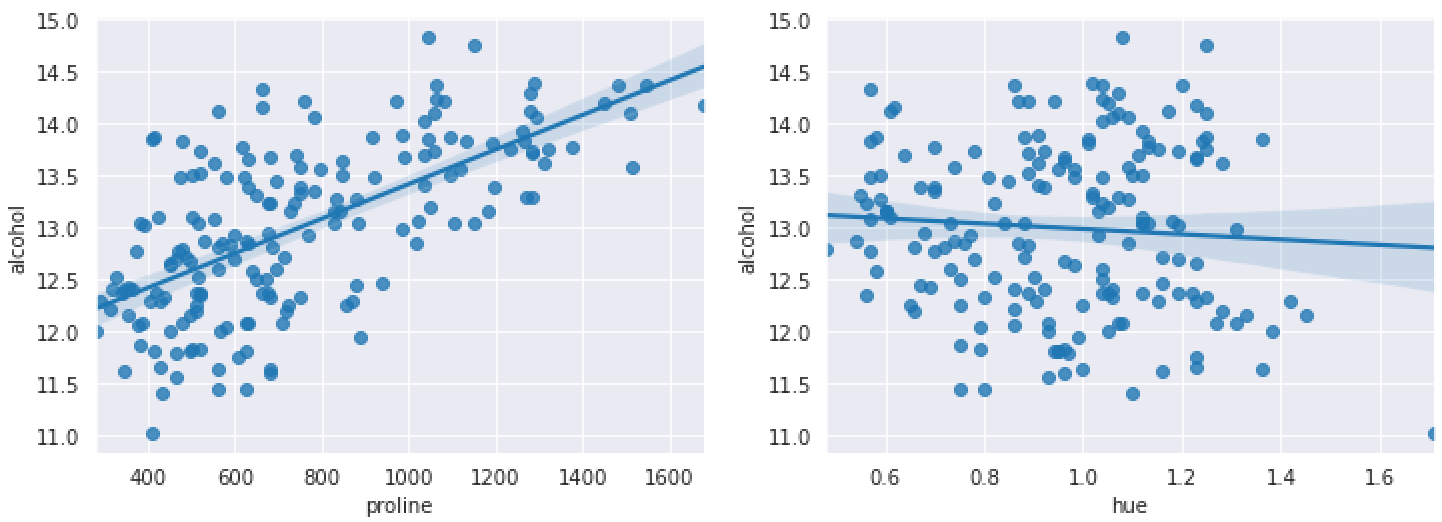
Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Standardizing/Normalizing Features for Interpretation

In [20]:
```
for (name,coef) in zip(['proline','hue'],mlr.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
```

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

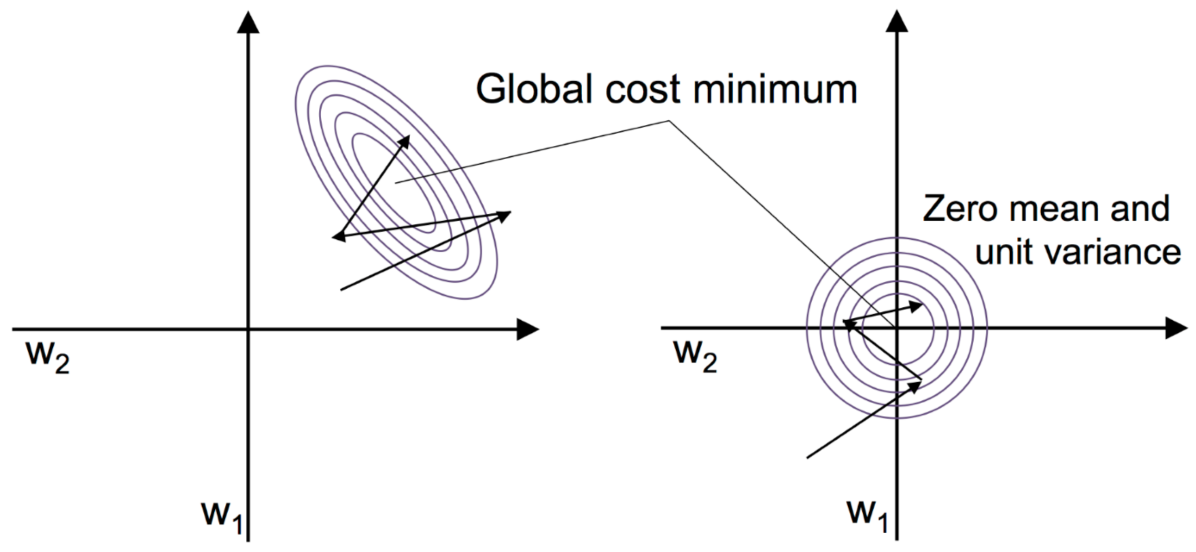
In [21]:
```
fig,ax = plt.subplots(1,2,figsize=(12,4))
sns.regplot(x='proline',y='alcohol',data=df_wine,ax=ax[0])
sns.regplot(x='hue',y='alcohol',data=df_wine,ax=ax[1]);
```



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

Standardizing/Normalizing Features for Gradient Descent

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



From PML

Multiple Linear Regression with Standardization/Normalization

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

In [22]:
```
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}')
```

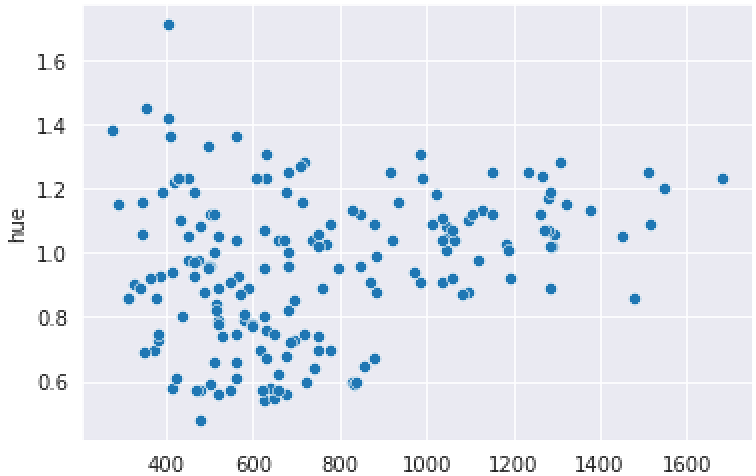
```
proline    :  0.568
hue        : -0.192
```

In [23]:
```
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)

In [24]:
```
sns.scatterplot(x='proline',y='hue',data=df_wine);
```



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

In [25]:
```
df_wine['class'].value_counts()
```

Out[25]:
```
1    71
0    59
2    48
Name: class, dtype: int64
```

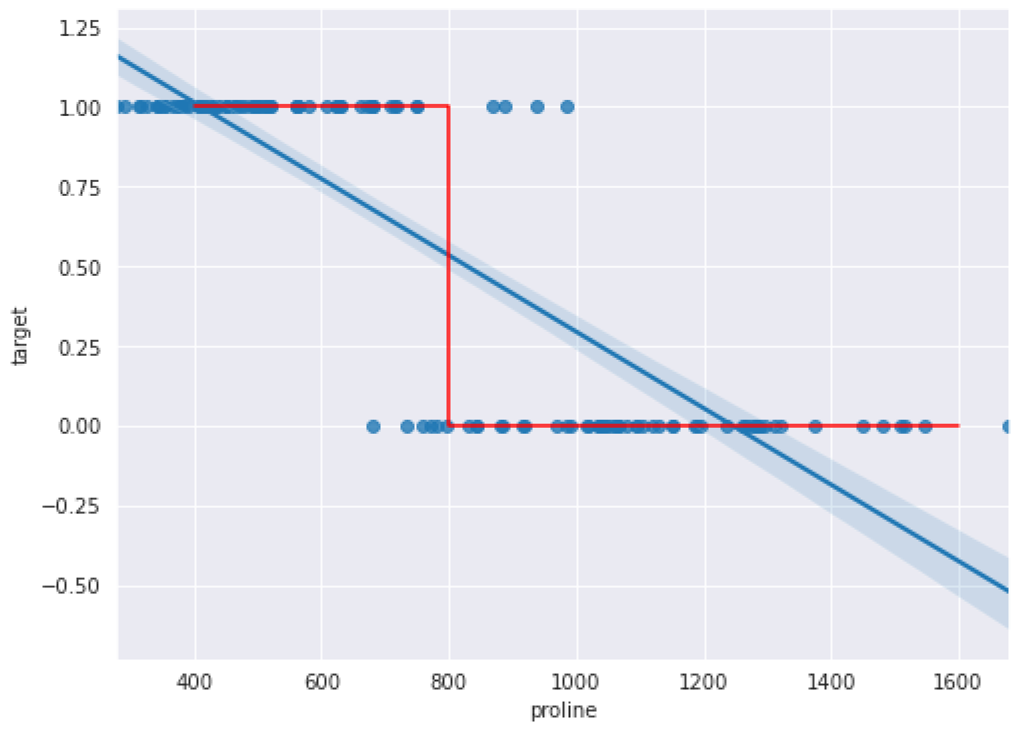
In [26]:
```
# only keep classes 0 and 1
df_wine_2class = df_wine[df_wine['class'] < 2]

# 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[26]:
```
1    71
0    59
Name: target, dtype: int64
```

Classifying Wine with a Linear Model

- Can't use our linear regression model directly

In [27]:
```
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');
```

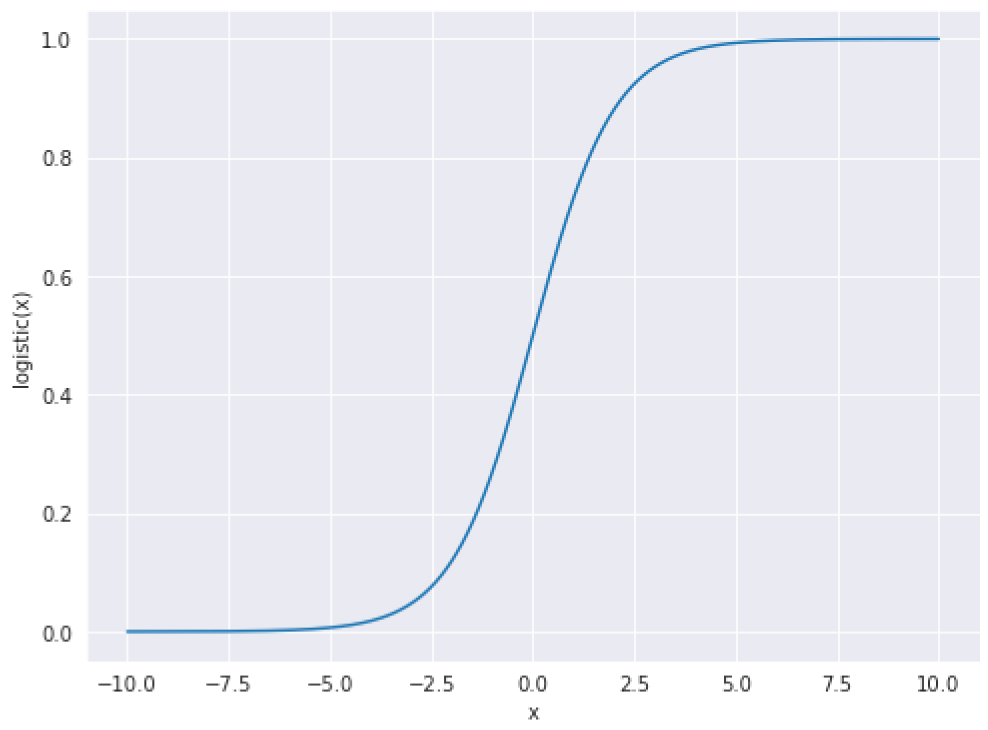


- Want something with that looks like a threshold
- Would like a prediction between 0 and 1

Logistic Regression

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

In [28]:
```python
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)');
```



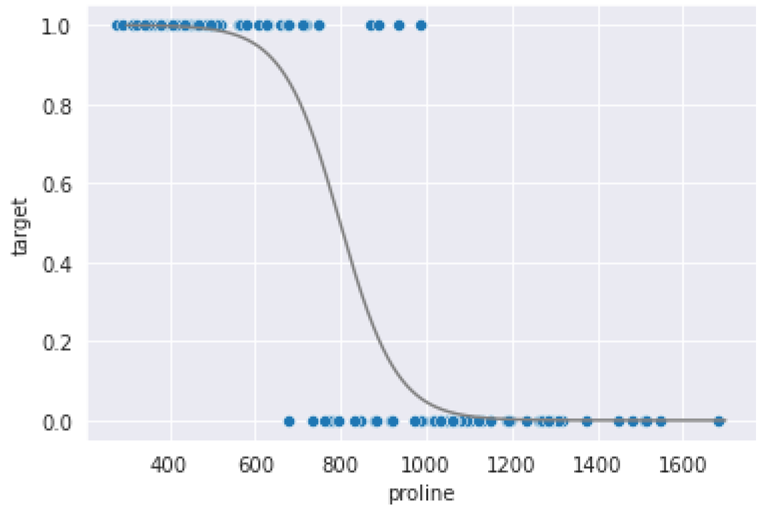
Logistic Regression with sklearn

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

In [29]:
```
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
```

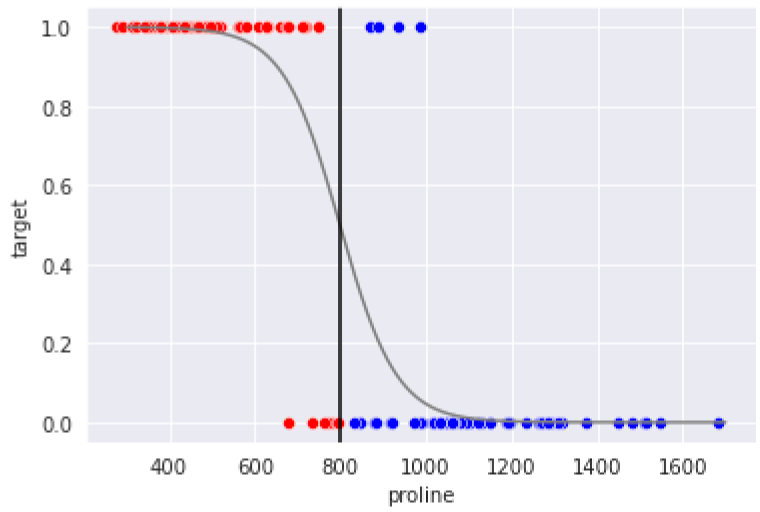
In [30]:
```
fig,ax = plt.subplots(1,1,figsize=(6,4))
x = np.linspace(300,1700,1000)
logistic_x = logistic(x,logr.coef_[0],logr.intercept_)
ax.plot(x,logistic_x,c='gray');
sns.scatterplot(x=df_wine_2class.proline,y=df_wine_2class.target, ax=ax);
```



Adding the Threshold

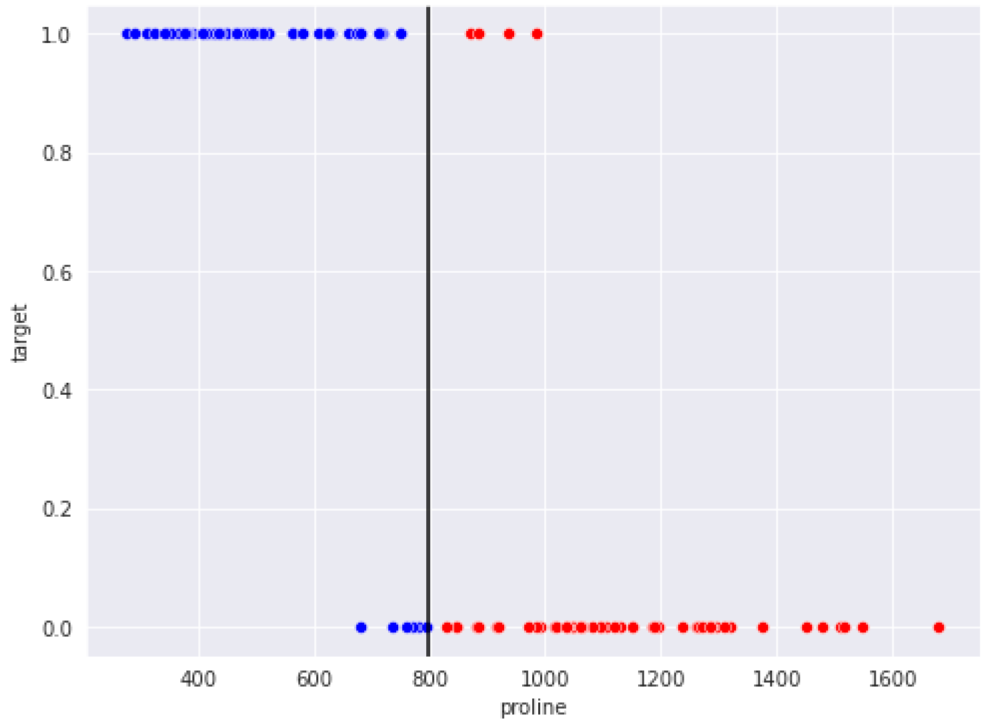
- Can treat the output of the logistic function as $P(y = 1|x)$
- Threshold at .5 (50%) to get class prediction

In [31]:
```
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');
```



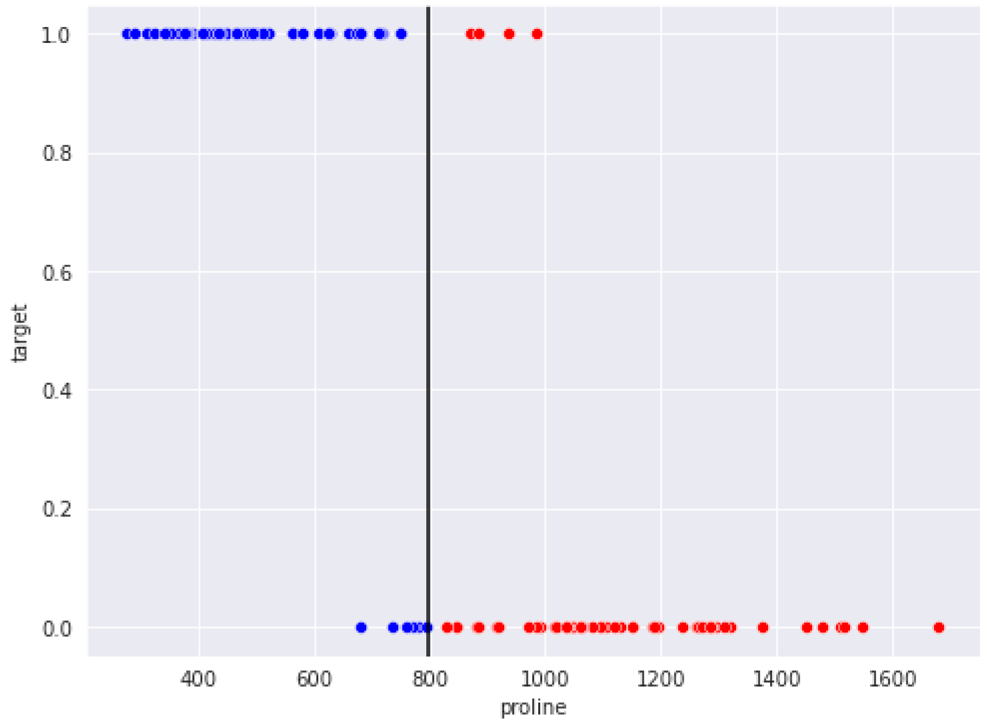
Getting Predictions from sklearn

In [32]:
```
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');
```



Getting Predictions from sklearn

In [32]:
```
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');
```



Note we have some errors!

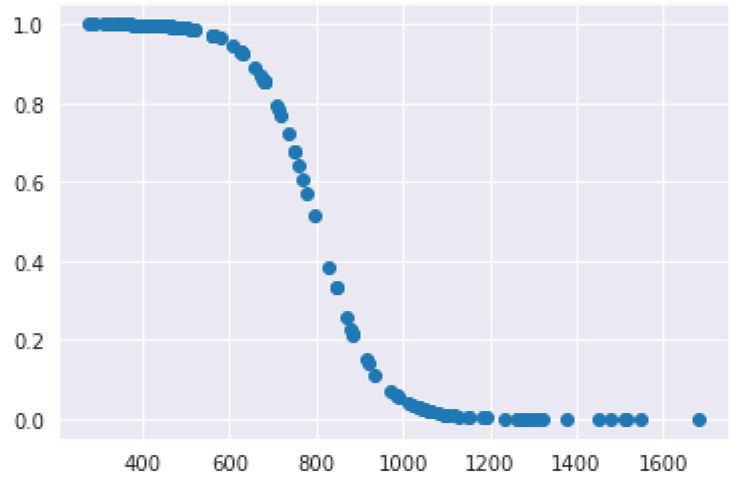
Getting Probabilities from sklearn

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

In [33]:
```
p_y = logr.predict_proba(X)
p_y[:5] # p(y=0|x), p(y=1|x)
```

Out[33]:
```
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]])
```

In [34]:
```
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(5) -> 5/1 -> 5 out of 6 times -> .83
- odds(.2) -> 1/5 -> 1 out of 6 times -> .16

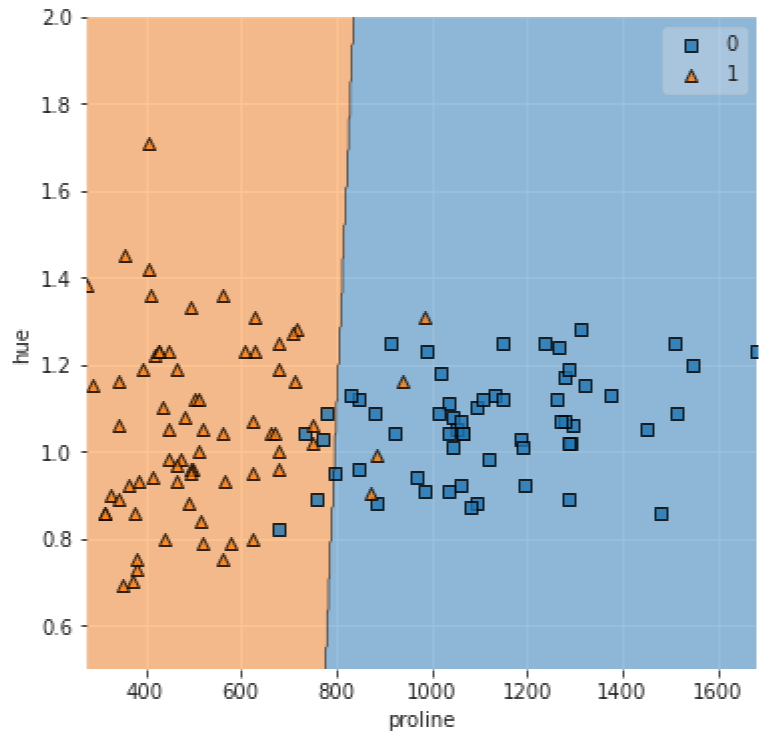
See here for a good explanation

Logistic Regression with Multiple Features

In [35]:
```
X = df_wine_2class[['proline','hue']]
logrm = LogisticRegression().fit(X,y)
for (name,coef) in zip(X.columns,logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')
```

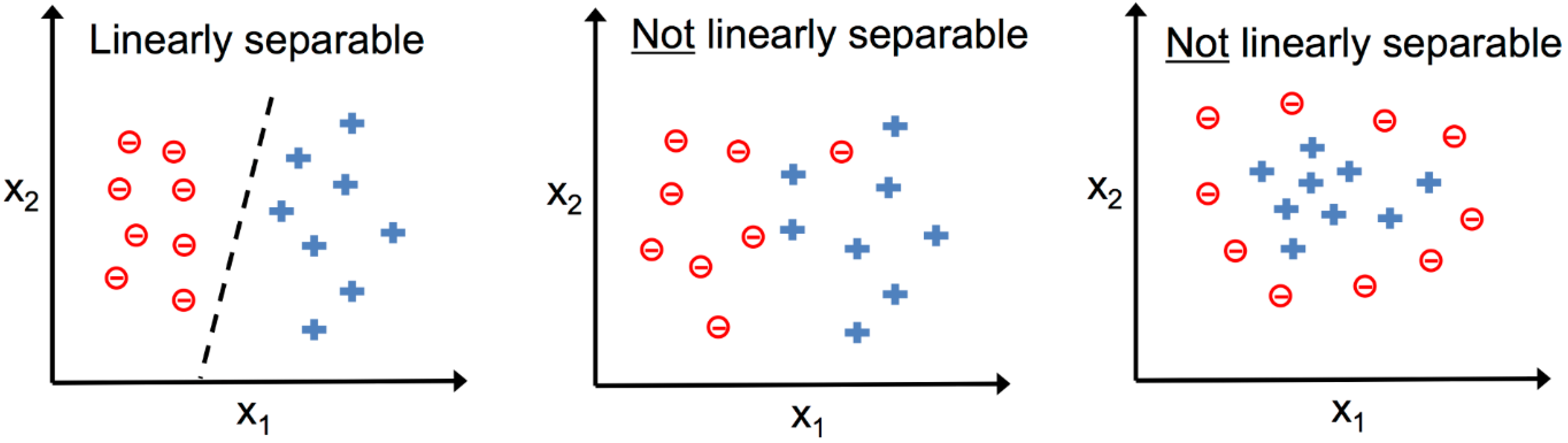
```
proline    : -0.015
hue        :  0.600
```

In [36]:
```
# 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.values, y.values, clf=logrm, ax=ax);
ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
ax.set_ylim(.5,2);
```



Linearly Seperable Data

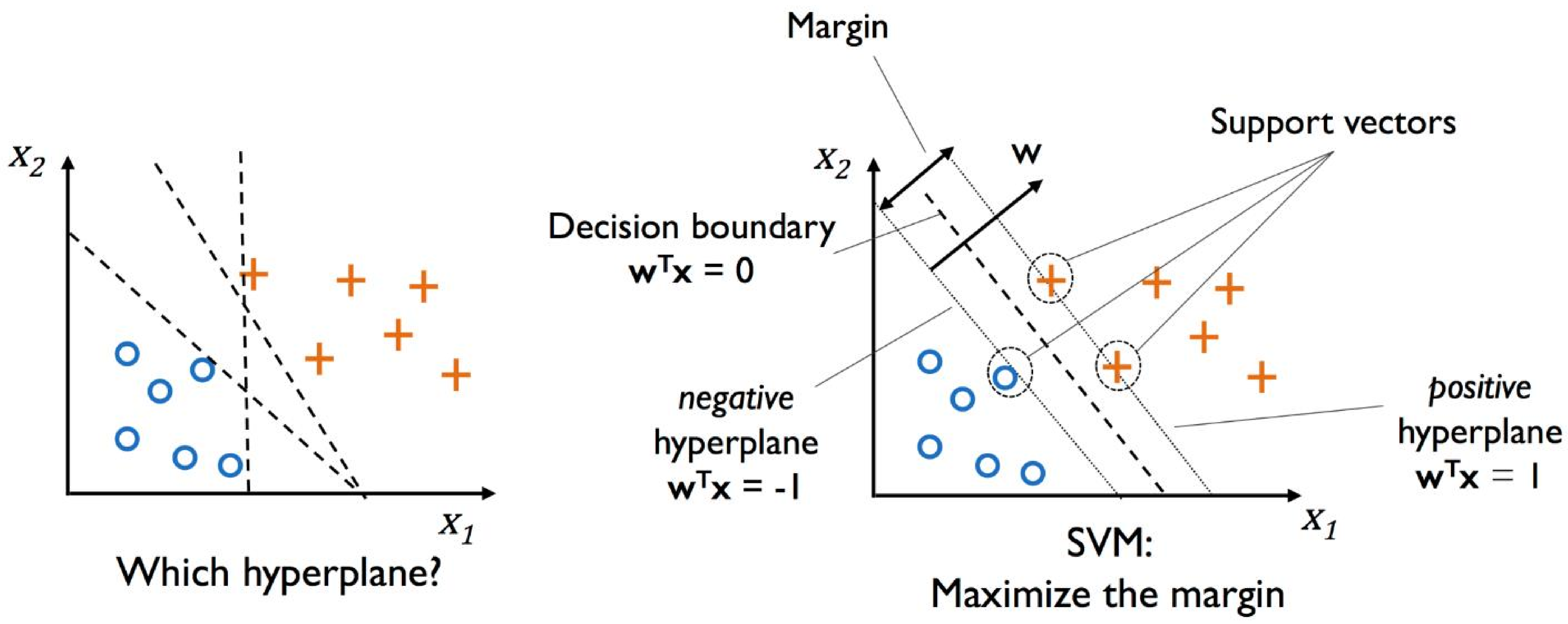
- Logistic Regression depends on data being linearly seperable



From PML

Another Linear Classification Model: SVM

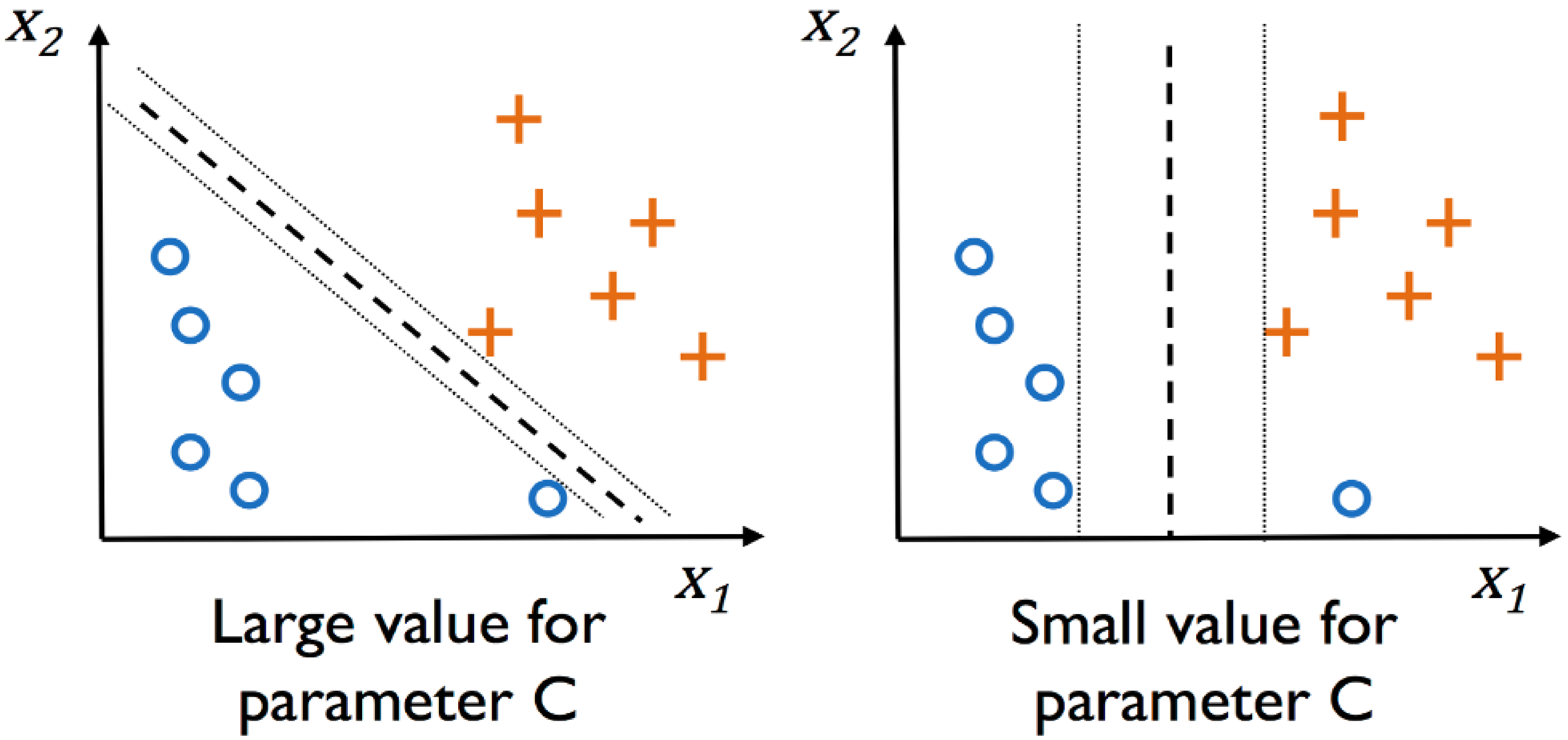
- For a linearly seperable dataset, where should we place the decision boundary?
- Support Vector Machine (SVM) tries to "maximize the margin" between classes



From PML

SVM Hyperparameter C

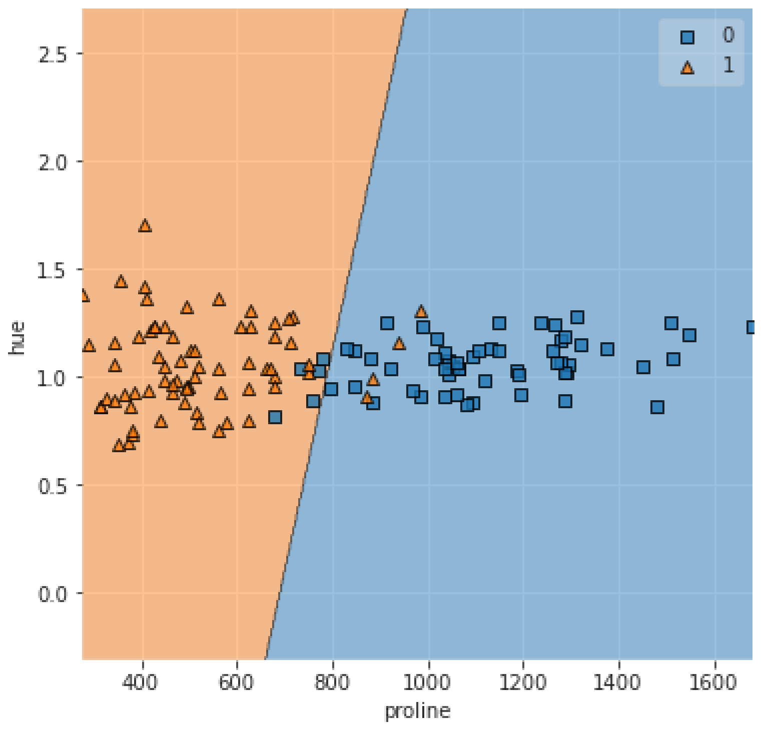
- **Hyperparameter**: Something we set



From PML

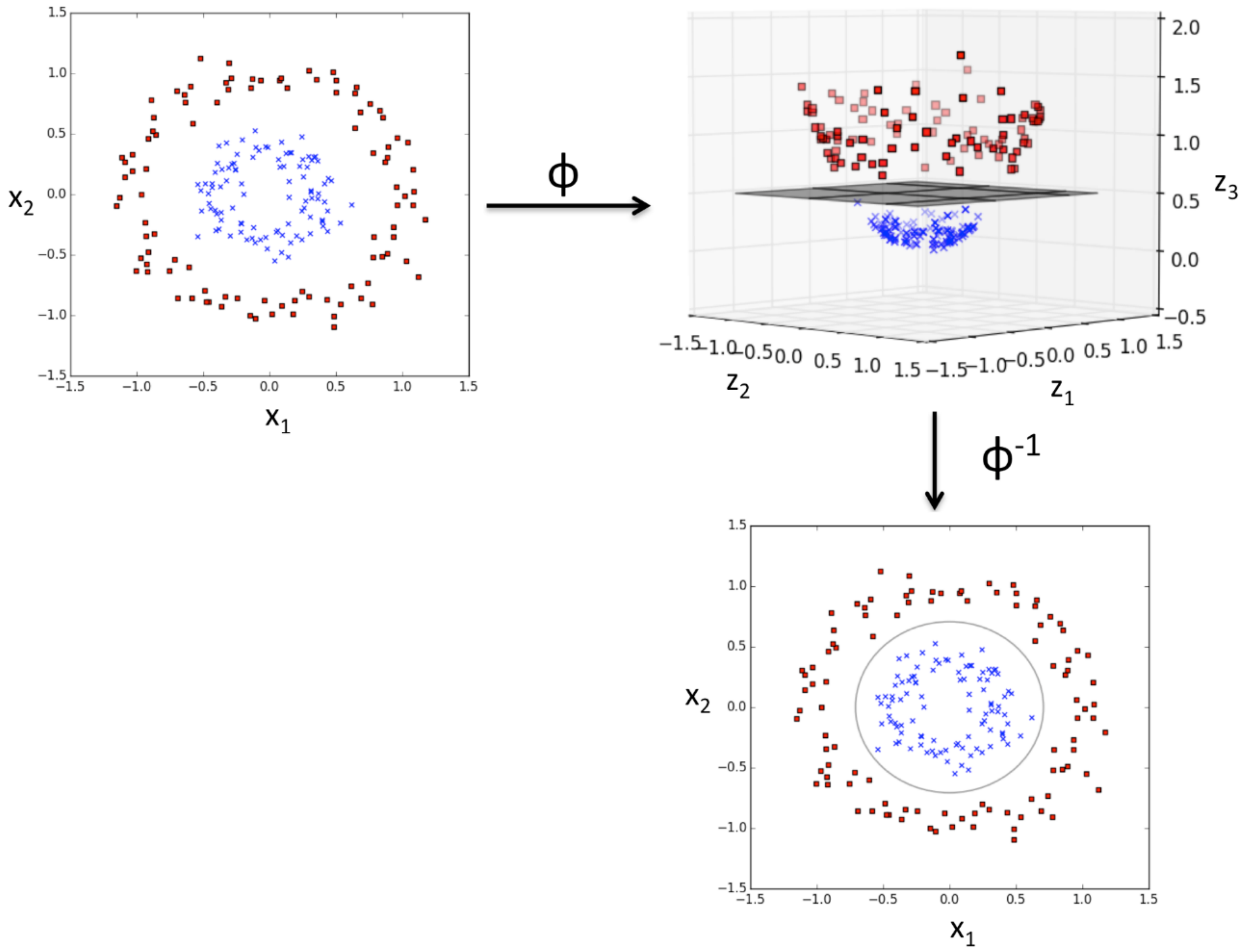
SVM with sklearn

In [37]:
```
from sklearn.svm import SVC
svm_linear = SVC(kernel='linear')
svm_linear.fit(X,y);

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



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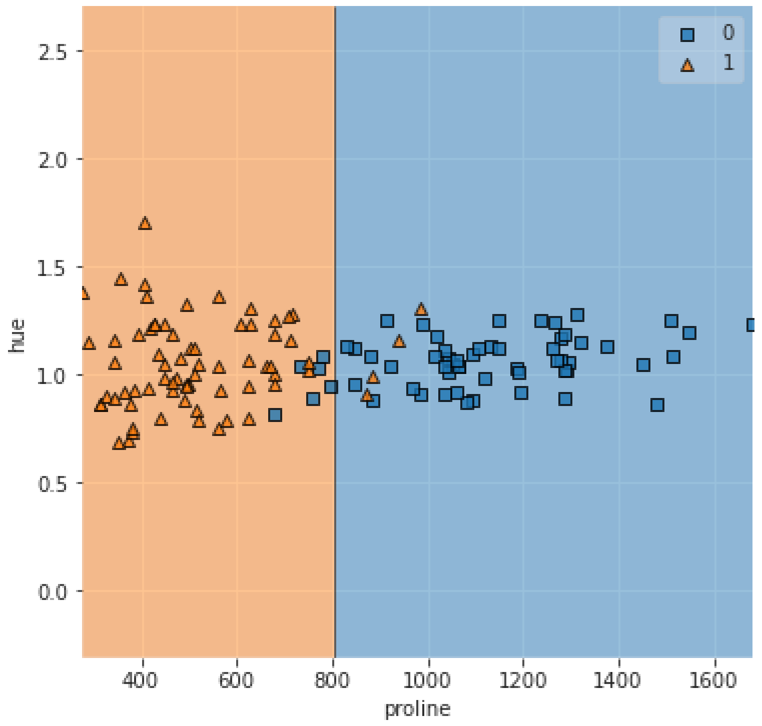
SVM Kernel Trick with RBF Kernel

- RBF (Radial-Basis Function) kernel

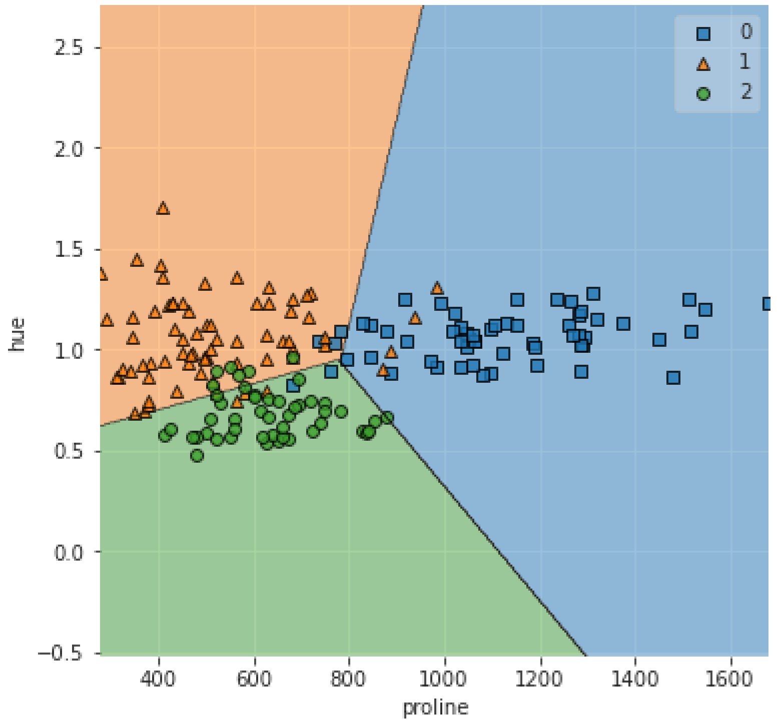
In [38]:
```
svm_rbf = SVC(kernel='rbf')
svm_rbf.fit(X,y);

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



Multiclass/Multilabel Problems with Linear Models

- **One Vs Rest:** train one model per class (ex: 0 vs 1&2, 1 vs 0&2, 2 vs 0&3)

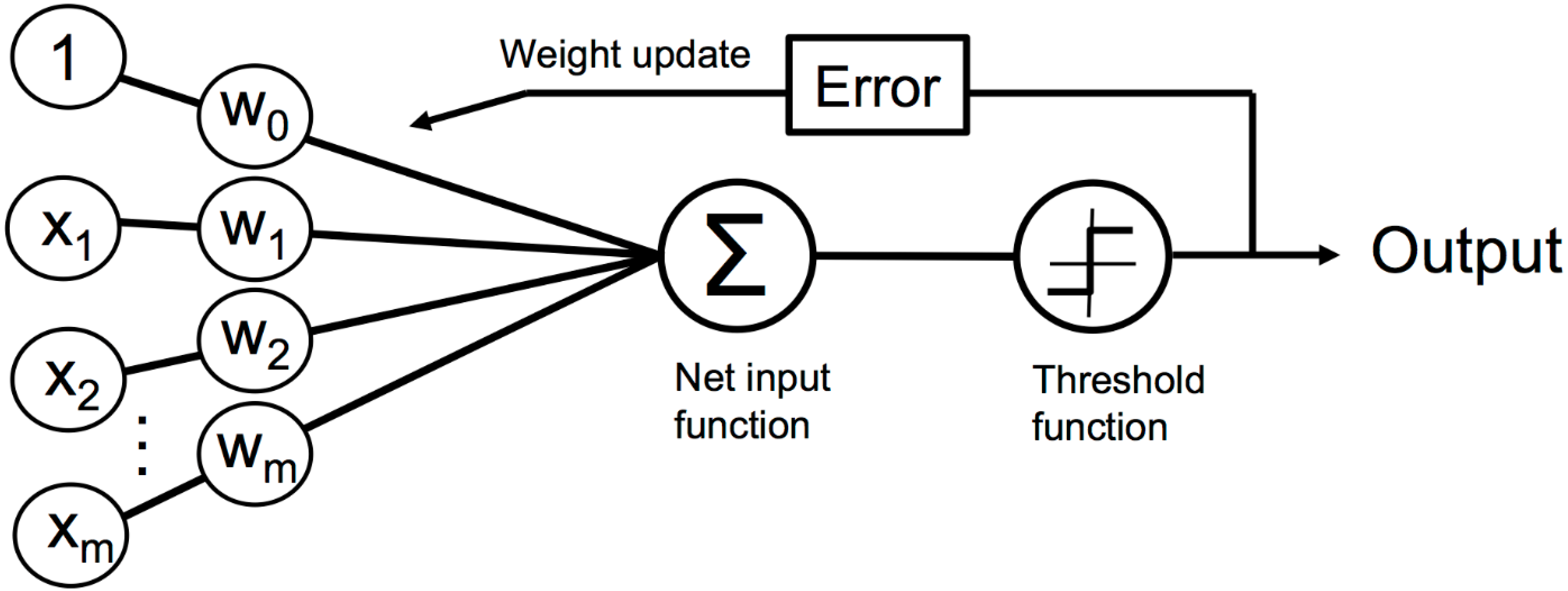
In [39]:
```
X_multiclass = df_wine[['proline','hue']]
y_multiclass = df_wine['class']

svm_rbf_mc = SVC(kernel='linear')
svm_rbf_mc.fit(X_multiclass,y_multiclass);

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



Questions re Classification with Linear Models?

Appendix

Perceptron: Early Neuron Model



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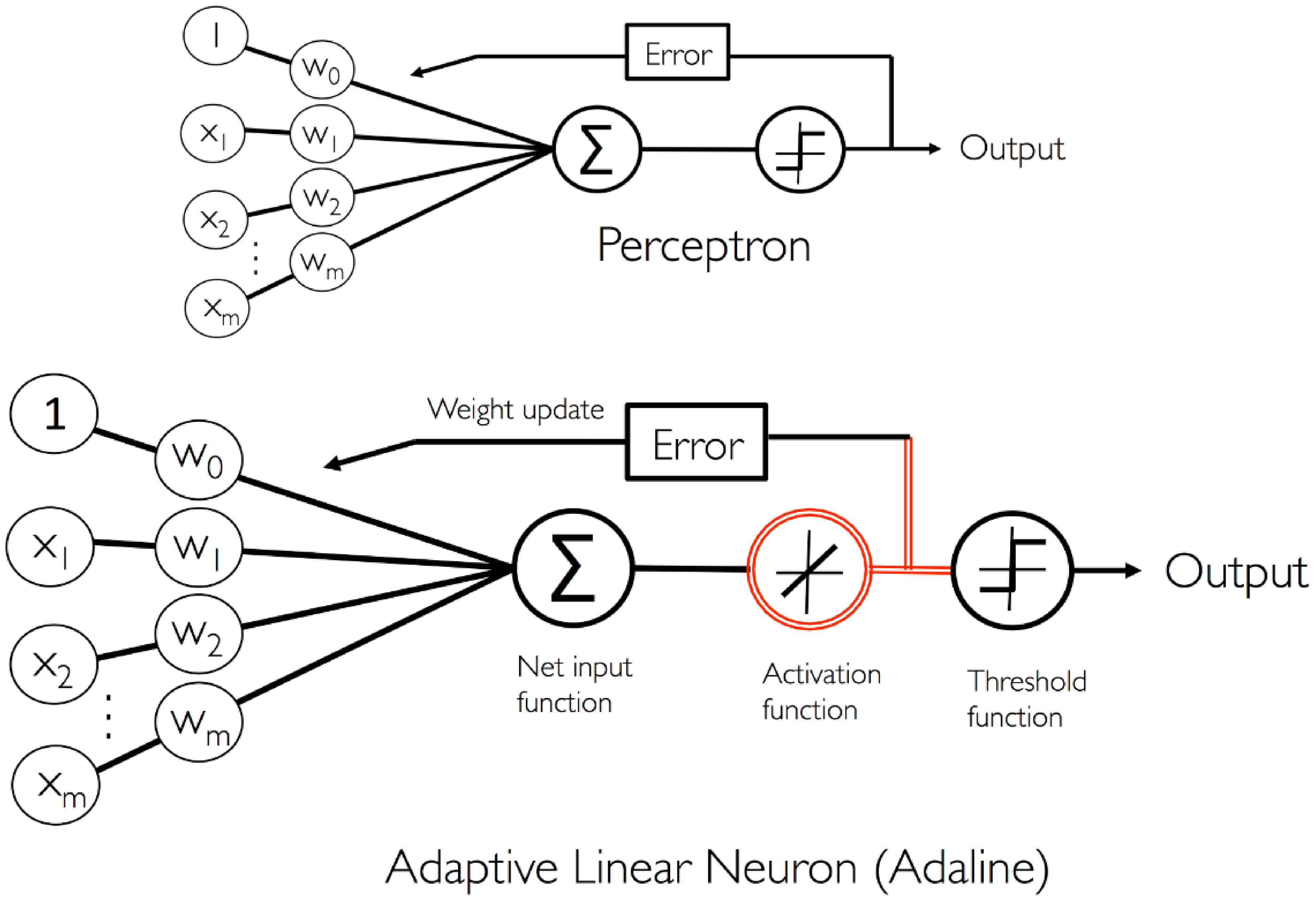
Perceptron to Adaline



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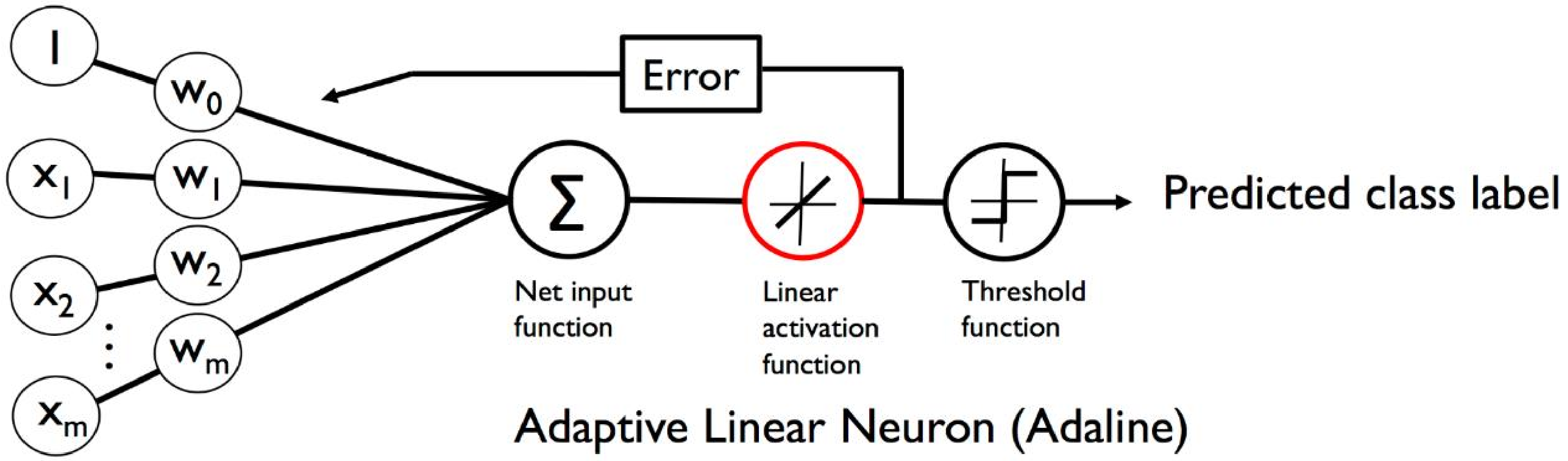
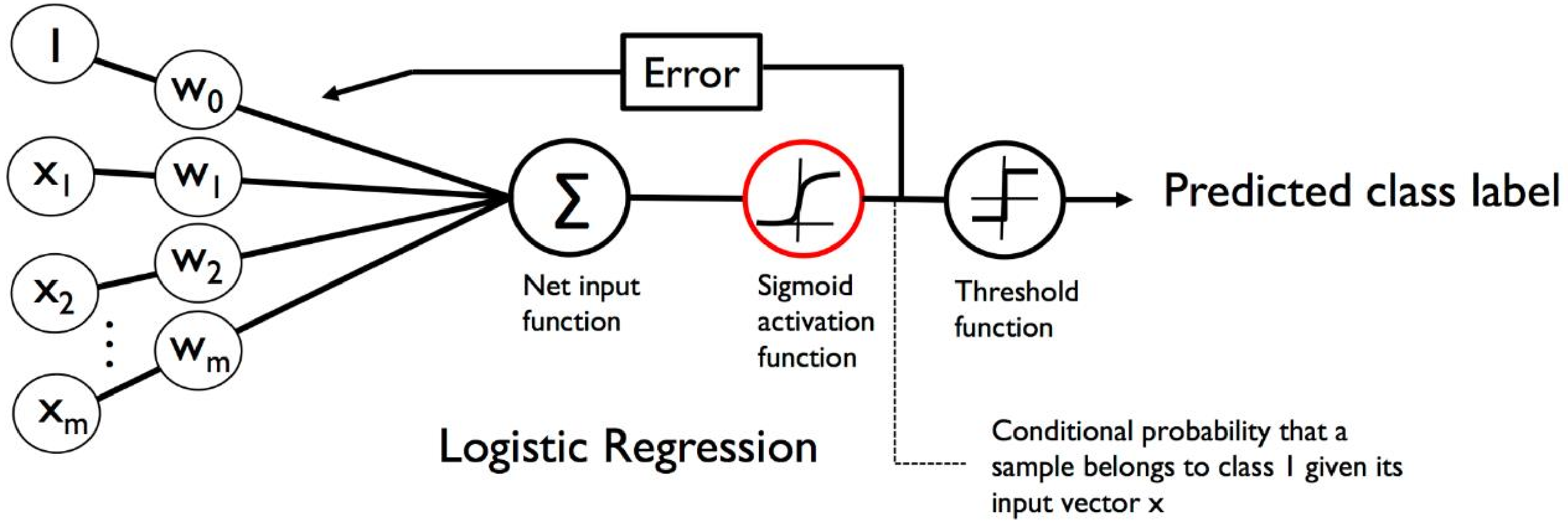
Adaline to Linear Regression





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