Review of linear models

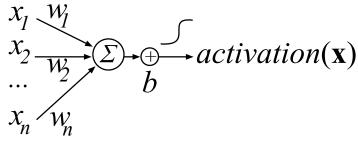
Linear and logistic regression

Terence Parr
MSDS program
University of San Francisco



Why do we study linear models?

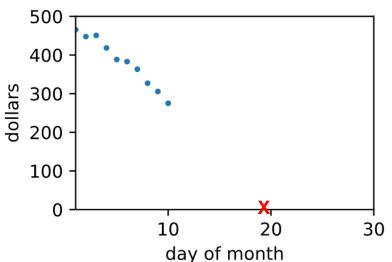
- Simple, interpretable, super fast, can't be beat for linear relationships
- Usually a lower bound on power but they often form the basis of other more powerful techniques, such as LOESS and...
- Combining multiple linear models into a lattice with a nonlinear function as glue yields a neural network; those are insanely useful and powerful
- Logistic regression model is a 1-neuron neural network
- LM can only find separating hyperplane and classes must be contiguous, which is rarely true for more than 1 or 2 vars



Linear regression

What problem are we solving?

- In college, I was given a fixed \$500 for food every month
- I wanted to know, at current rate of pizza consumption, how fast I'd run out of money so I plotted it and "eyeballed" zero x point



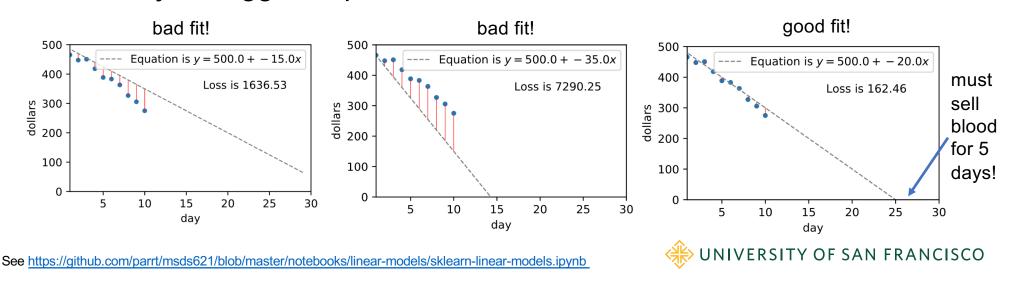
[Car computers that show number of miles remaining are solving the same problem]

♠ UNIVERSITY OF SAN FRANCISCO

See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

Draw line, manually finding coefficients

- I knew to draw line to project into future, but how can we figure out slope of line? (y-intercept is clearly the starting amount)
- Measure cost/loss by computing average squared residual error then just wiggle slope until we find min loss



Review of linear regression notation

- Given (X, y) where X is n x p explanatory matrix and y is target or response vector, we seek coefficients that describe best hyper plane through (X, y) data
- Each row $x^{(i)}$ in X maps to $y^{(i)}$ and $x^{(i)} = [x_1, x_2, ..., x_p]$

$$\hat{y} = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p = \beta_0 + \sum_{i=1}^p \beta_i x_i$$

• In vector notation, β is column vector $[\beta_1, \beta_2, ..., \beta_p]$

$$\hat{y} = \beta_0 + \mathbf{x} \cdot \vec{\beta} = \beta_0 + \mathbf{x} \vec{\beta}$$



Augment with "1" trick

• Adding β_0 is messy so augment x with 1:

$$x' = [1, x_1, x_2, ..., x_p]$$

then β is column vector

$$\beta = [\beta_0, \beta_1, \beta_2, \dots, \beta_p]$$

and we get the much simpler equation: $\hat{y} = \mathbf{x}' \vec{\beta}$

$$\begin{array}{c|c}
\hline
1 x_{l} \cdots \\
\boldsymbol{\beta}_{l} \\
\vdots
\end{array}$$

Training/fitting linear model means finding optimal coefficients

• Finding optimal β amounts to finding vector β that minimize the mean-squared error, which is our *loss* function:

$$MSE(\beta) = \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - \hat{y}^{(i)})^2$$

• Ignoring 1/n and substituting $\hat{y} = \mathbf{x}' \vec{\beta}$, we get:

$$\mathcal{L}(\beta) = \sum_{i=1}^{n} (y^{(i)} - (\mathbf{x}'^{(i)} \cdot \beta))^2 = (\mathbf{y} - \mathbf{X}'\beta) \cdot (\mathbf{y} - \mathbf{X}'\beta)$$

Solutions for finding linear model β

- Loss function is a (convex) quadratic with exact, symbolic solution and you've learned how to solve for coefficients directly
 - Well, if n > p and no weak/nonpredictive columns (X full rank)
- Many regularized and logistic regression loss functions have no direct solutions, though
- You'll use an iterative solution (gradient descent) for all regression problems in your project

Training/testing of linear models in Python

Boston dataset example into a notebook:

https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

```
boston = load_boston()
X, y = boston.data, boston.target

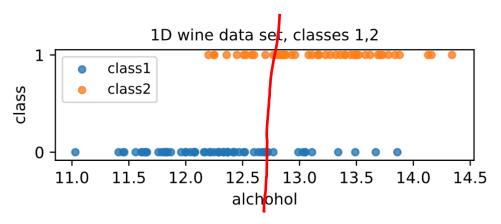
X_train, X_test, y_train, y_test = \
    train_test_split(X, y, test_size=0.2)

lm = LinearRegression()  # OLS
lm.fit(X_train, y_train)
s = lm.score(X_test, y_test) # R^2 = 0.66
```

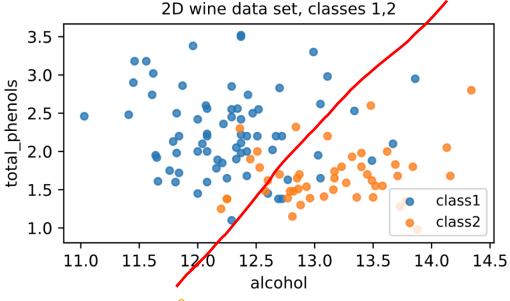
Logistic regression

Review of logistic regression

- For classification, response y is discrete int value like {0,1}
- Need separating hyperplane between points in different classes



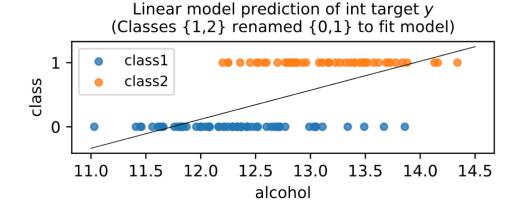
 Showing hard cutoffs but a smooth transition from class 1 to class 2 would be better

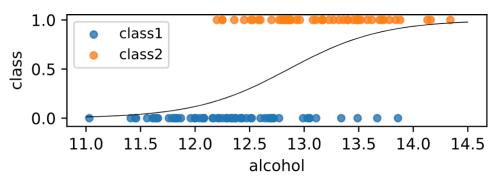


See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

1D logistic regression

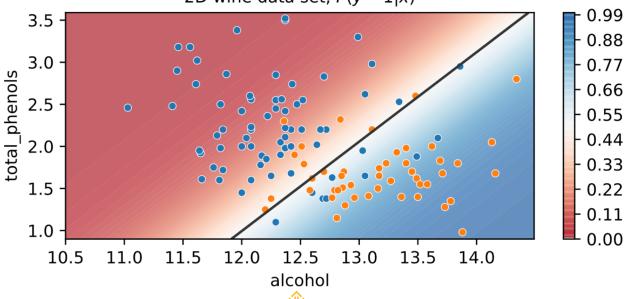
- Could use linear regression, but line would exceed [0,1] range
- Sigmoid is a much better transition from class 0 to class 1 and gives probability of class 1: P(y = 1|x)
- Training sends output of linear model into sigmoid and maximizes max likelihood to find coefficients





2D wine data set example, 2 features

- Logistic regression yields P(y = 1|x)
- Classifier built on top of logistic prediction; $P(y = 1 | x) \ge 0.5$ predict class 1 else predict class 0
- Black line is separating plane, but output of model is smooth transition, not hard threshold, from 0 to 1



See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

Logistic regression notation

Sigmoid function

$$\sigma(z) = \frac{1}{1 + e^{-z}} = \frac{e^z}{1 + e^z}$$

Substituting vectorized linear eqn into sigmoid:

$$p(\mathbf{x}') = \sigma(\mathbf{x}'\beta) = \frac{1}{1 + e^{-\mathbf{x}'\beta}}$$

• Using odds = p/(1-p), subst in p(x'), simplify, take log; we get:

$$log(odds) = \mathbf{x}'\beta$$

BTW, log-odds stuff is interesting but not particularly useful/relevant

Solving for logistic β

- Same idea: define loss function (negative of max likelihood in this case) and solve for β that gives min loss value
- Loss function has nonlinearity in it now though:

$$\mathcal{L}(\beta) = \sum_{i=1}^{n} \left\{ y^{(i)} \mathbf{x}'^{(i)} \beta - \log(1 + e^{\mathbf{x}'\beta}) \right\}$$

 Logistic regression requires an iterative solution because there is no direct, symbolic solution, unlike linear regression

Training/testing of logistic regression models in Python

Wine dataset example from into a notebook:

https://github.com/parrt/msds621/blob/master/notebooks/linear-models/classifier-regularization.ipynb

```
wine = load_wine()
df_wine = pd.DataFrame(data=wine.data,
columns=wine.feature_names)
df_wine['y'] = wine.target
df_wine = df_wine[df_wine['y']<2] # do 2-class problem {0,1}
X, y= df_wine.drop('y', axis=1), df_wine['y']
normalize(X)
lm = LogisticRegression(solver='lbfgs', max_iter=1000)
lm.fit(X.values, y) # uses regularization by default
lm.score(X.values, y)</pre>
```

Lab time

- Plotting decision surfaces for linear models
 https://github.com/parrt/msds621/blob/master/labs/linear-models/decision-surfaces.ipynb
- Note: that link is for viewing since github screws that up; you will need to go to the course repo to get the interactive labs https://github.com/parrt/msds621/tree/master/labs/linear-models