Review of linear models

Linear and logistic regression

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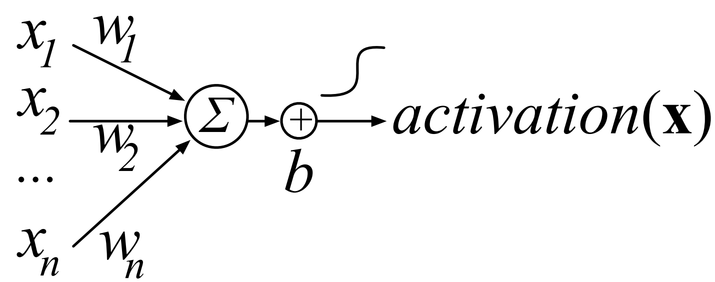
Why do we study linear models?

- 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 with sigmoid activation
- LM can only find separating hyperplane and classes must be contiguous, which is rarely true for more than 1 or 2 vars



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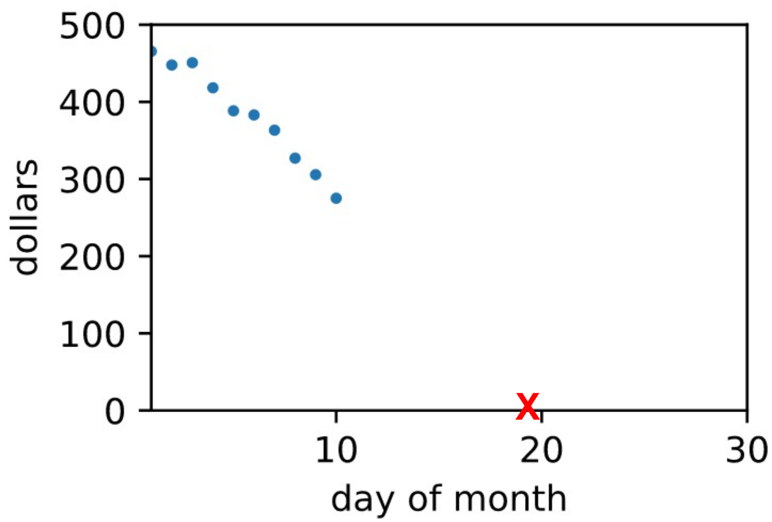
Linear regression

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



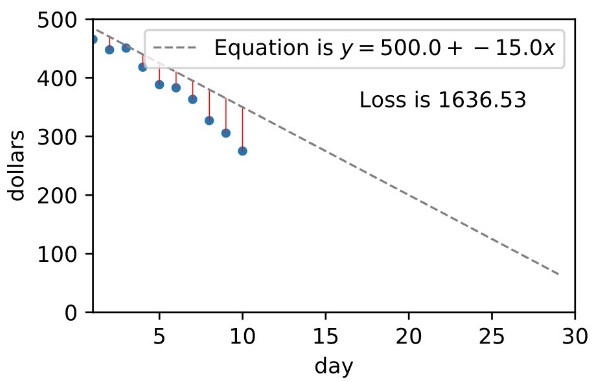
[Car computers that show number of miles remaining are solving the same problem]

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

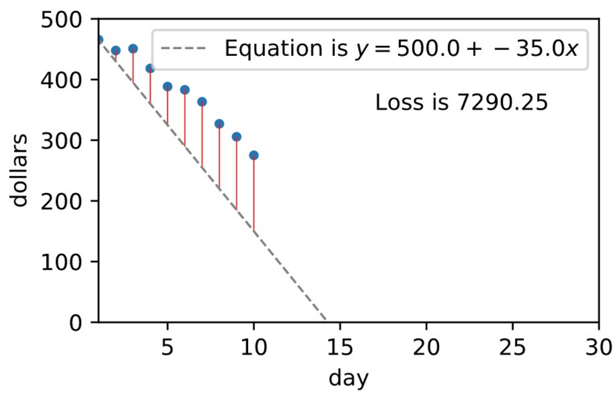
Draw line, manually finding coefficients

- 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 move line around until we find min loss (instead of symbolic solution)

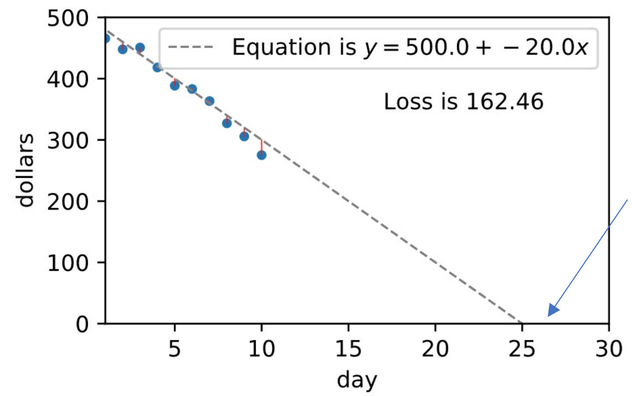
bad fit!



bad fit!



good fit!



must sell blood for 5 days!

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

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 $x^{(i)}$ = $[x_1, x_2, \ldots, x_p]$

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

- In vector notation, $\vec{\beta}$ is column vector $[\beta_1, \beta_2, \ldots, \beta_p]$

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

Augment with “1” trick

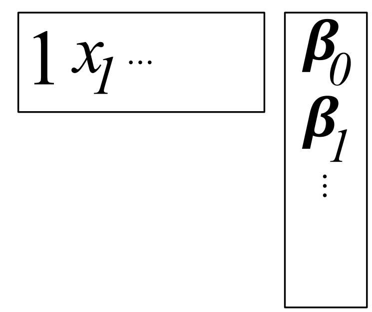
- Adding β_0 is messy so augment $\boldsymbol{x}$ with 1:

$$\boldsymbol{x}' = [1, x_1, x_2, \dots, x_p]$$

then β is column vector

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

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



Training/fitting linear model means finding optimal coefficients

- Finding optimal β amounts to finding vector β that minimizes 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:

rows augmented

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

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 has 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

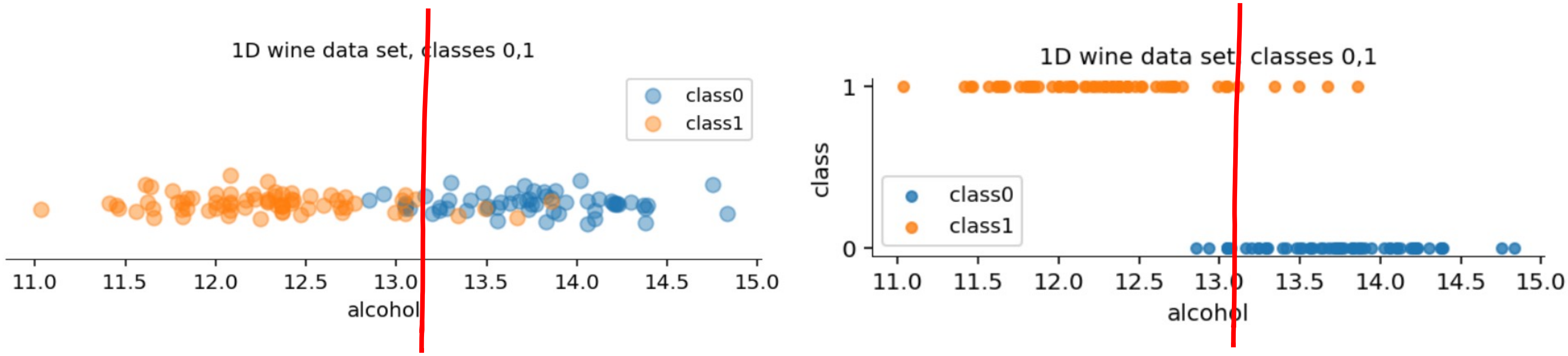
- Boston dataset example into a notebook: https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

```
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

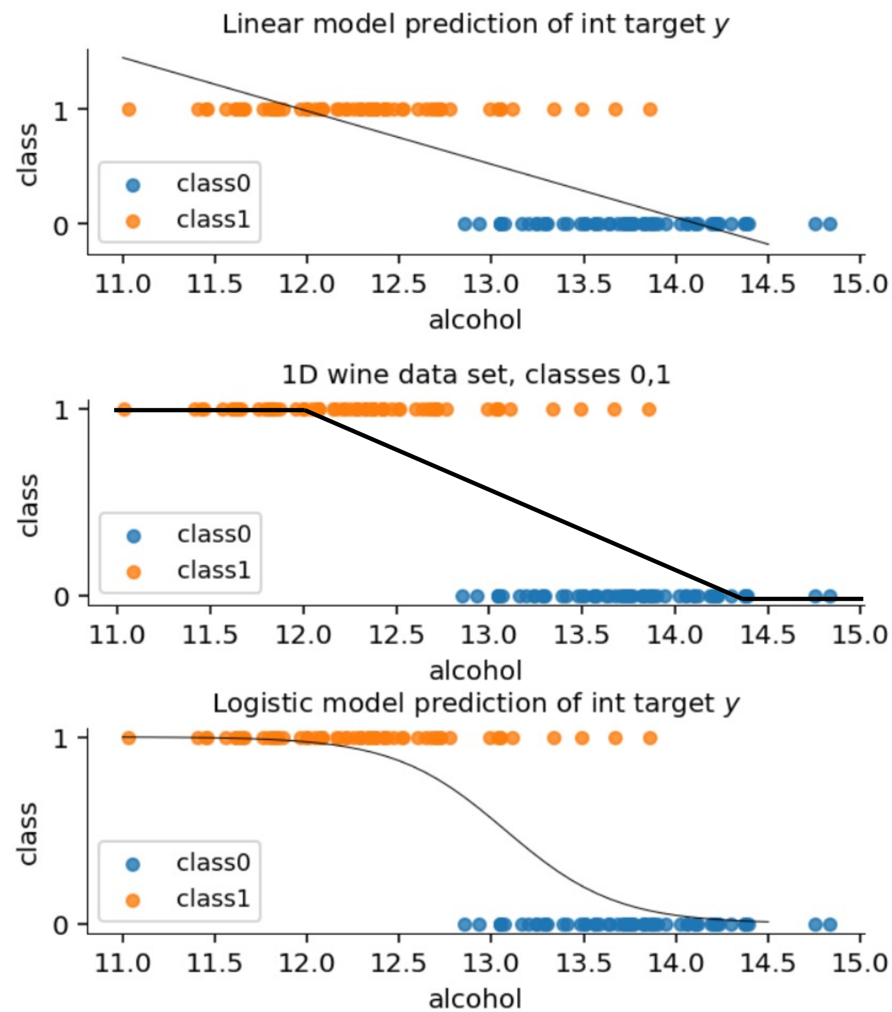
- For classification, response y is discrete int value like {0,1}
- Need separating hyperplane between points in different classes



- Showing hard cutoffs here, but a smooth transition from class 0 to class 1 would be better

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

1D logistic regression

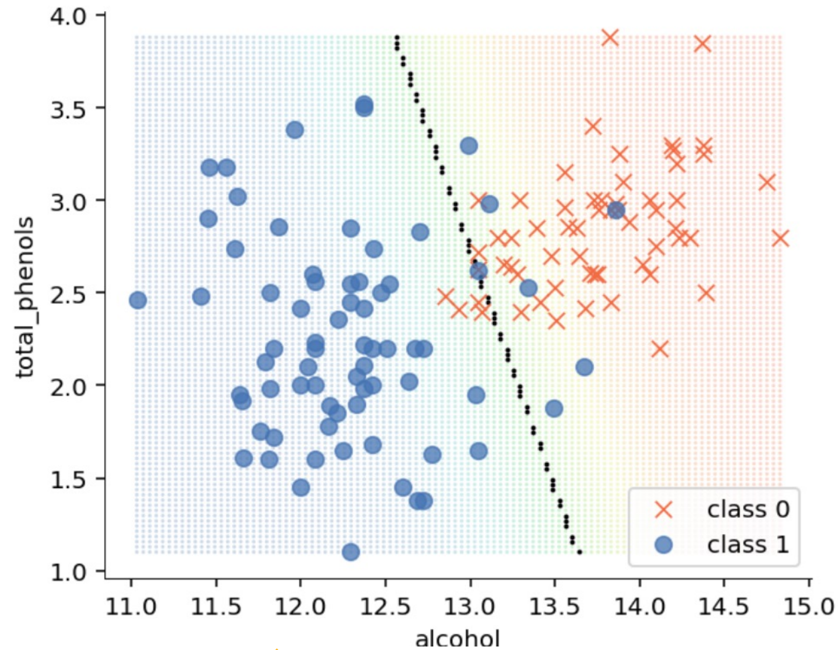


- Could use linear regression, but line would exceed [0,1] range
- Could clip, but discontinuous
- Sigmoid is a much better transition from class 0 to class 1 and gives probability of class 1: $P(y = 1|\boldsymbol{x})$
- Training sends output of linear model into sigmoid then finds coefficients that maximize a max-likelihood loss function

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

2D wine data set example, 2 features

- Logistic regression yields $P(y = 1|\boldsymbol{x})$
- Classifier built on top of logistic prediction; $P(y = 1|\boldsymbol{x}) \geq 0.5$ 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
- Green/yellow shades represent $P(y = 1|\boldsymbol{x})$
- Accuracy 119/130 = 0.92 (threshold, precision, recall) = (0.50, 0.941, 0.901)



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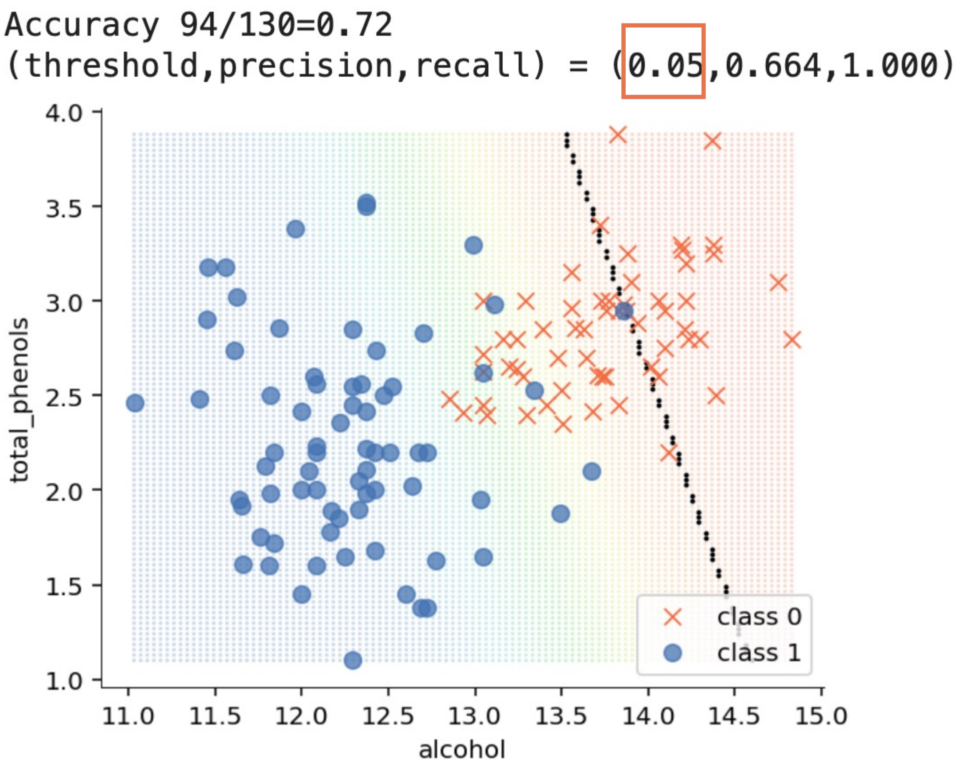
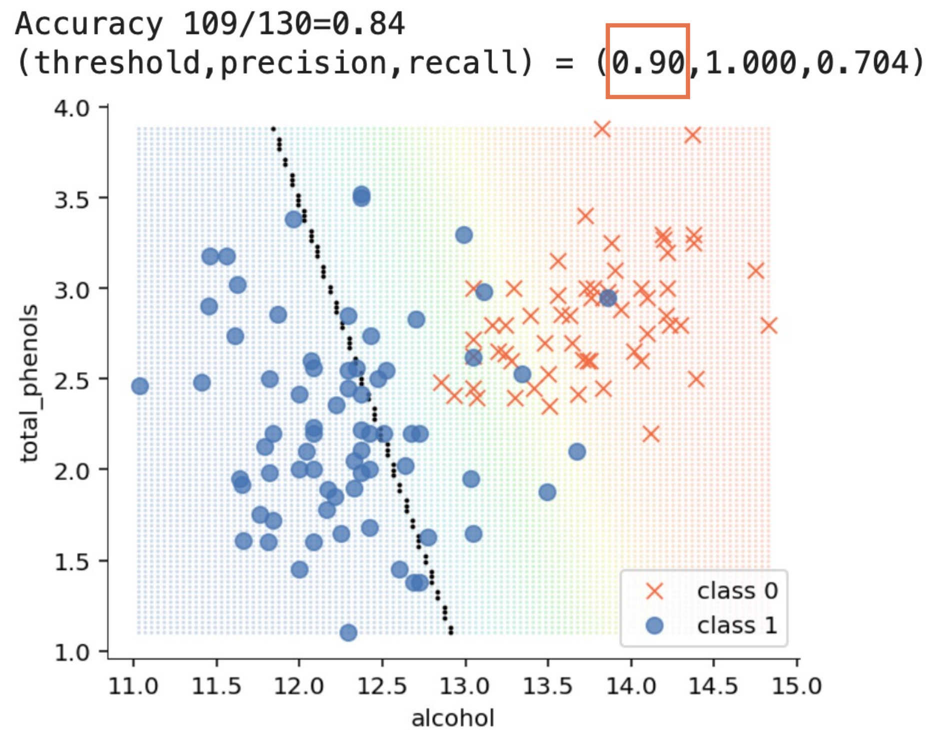
See https://github.com/parrt/msds621/blob/master/notebooks/linear-models/sklearn-linear-models.ipynb

Classifier $P(y = 1|\boldsymbol{x})$ threshold changes

$P(y = 1|\boldsymbol{x}) \geq 0.05$



$P(y = 1|\boldsymbol{x}) \geq 0.9$



Plotting precision and recall for a variety of thresholds yields PR curve (similar to ROC curve)

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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 $p(\mathbf{x}')$, simplify, take log; we get:

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

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

Derivations and intution, see https://github.com/parrt/msds621/raw/master/projects/linreg/linreg.pdf

Solving for logistic model parameters: β

- Same idea as regression: define loss function (negative of max likelihood in this case) and solve for β that gives min loss value
- The likelihood of sigmoid derived from some β fitting the X,y:

$$Likelihood(\beta) = \prod_{i=1}^{n} \begin{cases} P(\mathbf{x}'^{(i)}; \beta) & \text{if } y^{(i)} = 1 \\ 1 - P(\mathbf{x}'^{(i)}; \beta) & \text{if } y^{(i)} = 0 \end{cases}$$

- Flip multiplication to summation via log (log is monotonic):

$$Likelihood(\beta) = \sum_{i=1}^{n} \begin{cases} log(P(\mathbf{x}'^{(i)}; \beta)) & \text{if } y^{(i)} = 1 \\ log(1 - P(\mathbf{x}'^{(i)}; \beta)) & \text{if } y^{(i)} = 0 \end{cases}$$

Derivations and intution, see https://github.com/parrt/msds621/raw/master/projects/linreg/linreg.pdf

Simplifying max likelihood

- Gating the two log terms in and out using $y^{(i)}$ and $(1 - y^{(i)})$ let's us remove the choice operator:

$$Likelihood(\beta) = \sum_{i=1}^{n} \left\{ y^{(i)} log(P(\mathbf{x}'^{(i)}; \beta)) + (1 - y^{(i)}) log(1 - P(\mathbf{x}'^{(i)}; \beta)) \right\}$$

- Simplifies ultimately to:

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

- Logistic regression requires an iterative solution due to sigmoid; solve for min of the negative of that max likelihood $\mathscr{L}(\beta) = -Likelihood(\beta)$

Derivations and intuition, see https://github.com/parrt/msds621/raw/master/projects/linreg/linreg.pdf

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’]

lg = LogisticRegression(solver='lbfgs', max_iter=1000)
lg.fit(X.values, y) # uses regularization by default
lg.score(X.values, y)
```

Lab time

- Plotting decision surfaces for linear models
  https://github.com/parrt/msds621/blob/master/labs/linear-models/decision-surfaces.ipynb