Regularization

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Objectives

- Define and describe regularization for regression models
- Write the regularized loss function
- Describe how regularization affects regression coefficients
- Describe the differences between the Lasso, Ridge, and ElasticNet models
- Implement and visualize the penalties using `sklearn`

Warmup

With a partner, describe what overfitting is and how it occurs. What is the impact of overfitting?

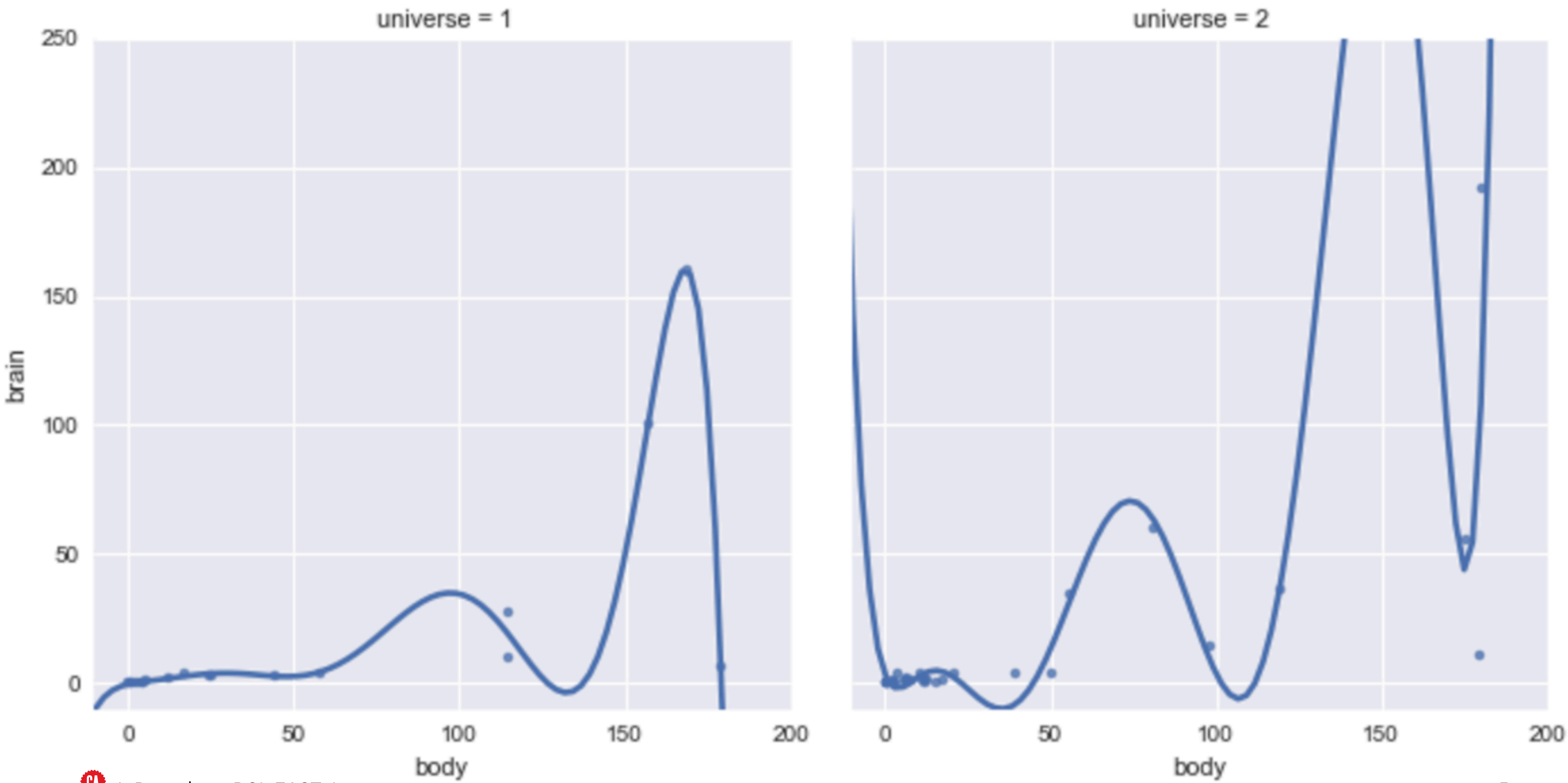
Overfitting

Overfitting means building a model that matches the training data "too closely." The model ends up training on noise rather than signal.

— Usually cause by model that is too complex

— Overfit model does not generalize

— Low bias/high variance models


universe = 1
universe = 2
brain
body
body
250
200
150
100
50
0
0
50
100
150
200

Do I need to worry about overfitting with Linear Regression**?**

"Good" properties

— Low complexity

— High bias/low variance

— Does not tend to overfit

Do I need to worry about overfitting with Linear Regression**?**

Danger zone

— Including irrelevant features (signal v noise)

— p (number of features) is close to n (number of observations)

— Correlated inputs

— Numerically large coefficients

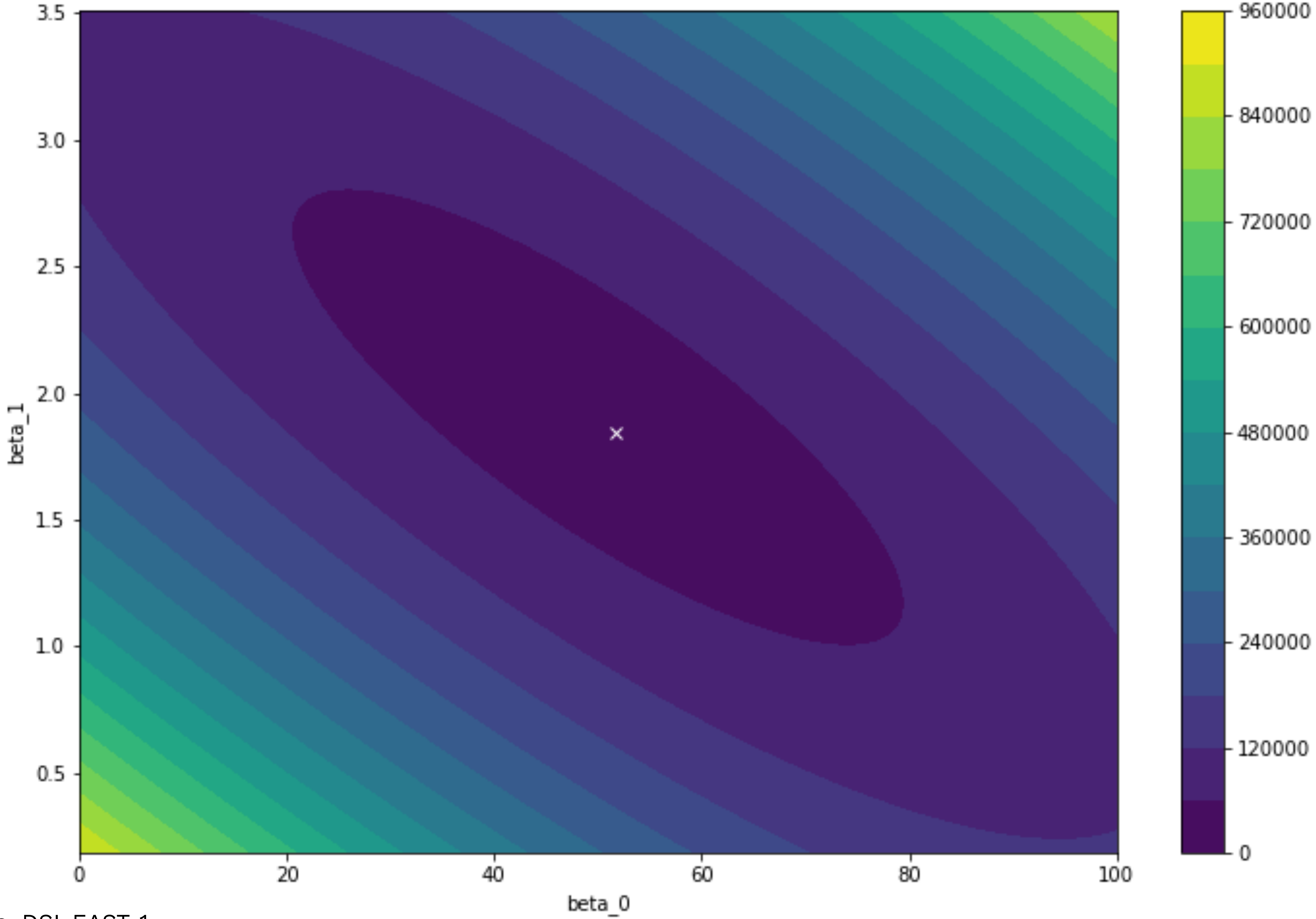
What Do I Do Now

Error and the Loss Function

$$
\begin{aligned}
RSS(\beta_0, \beta_1) &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^{n} (\hat{y}_i - \beta_0 - \beta_1 x_i)^2
\end{aligned}
$$

The goal of training is to minimize $RSS(\beta_0, \beta_1)$, i.e.

$$\beta_0, \beta_1 = \arg\min RSS(\beta_0, \beta_1)$$


3.5
3.0
2.5
2.0
1.5
1.0
0.5
beta_1
0
20
40
60
80
100
beta_0
960000
840000
720000
600000
480000
360000
240000
120000
0

Ridge Regression

(a.k.a. Tikhonov regularization, weight decay, L_2 regularization)

$$J(\beta_0, \beta_1) = RSS(\beta_0, \beta_1) + \alpha\beta_1^2$$

Ridge regression penalizes the model for having large coefficients. As α increases, β_1 will decay.

α acts as a "tuning" parameter.

Ridge Regression (general case)

$$J(\beta_0, \beta_1, \ldots, \beta_p) = RSS(\beta_0, \beta_1, \ldots, \beta_p) + \alpha \sum_{i=1}^{p} \beta_i^2$$

Ridge shrinks the regression coefficients.

Ridge Regression

Get ready to roll (down the loss function!)

Check: Find the `sklearn` documentation on Ridge Regression. Locate the model description (inputs, outputs, parameters, methods), and the discussion of the theory with examples.

1. How do you set the regularization strength?
2. How can you get the values of the regularized regression coefficients?

Lasso Regression

a.k.a. L_1 regularization

$$J(\beta_0, \beta_1) = RSS(\beta_0, \beta_1) + \alpha\,|\beta_1|$$

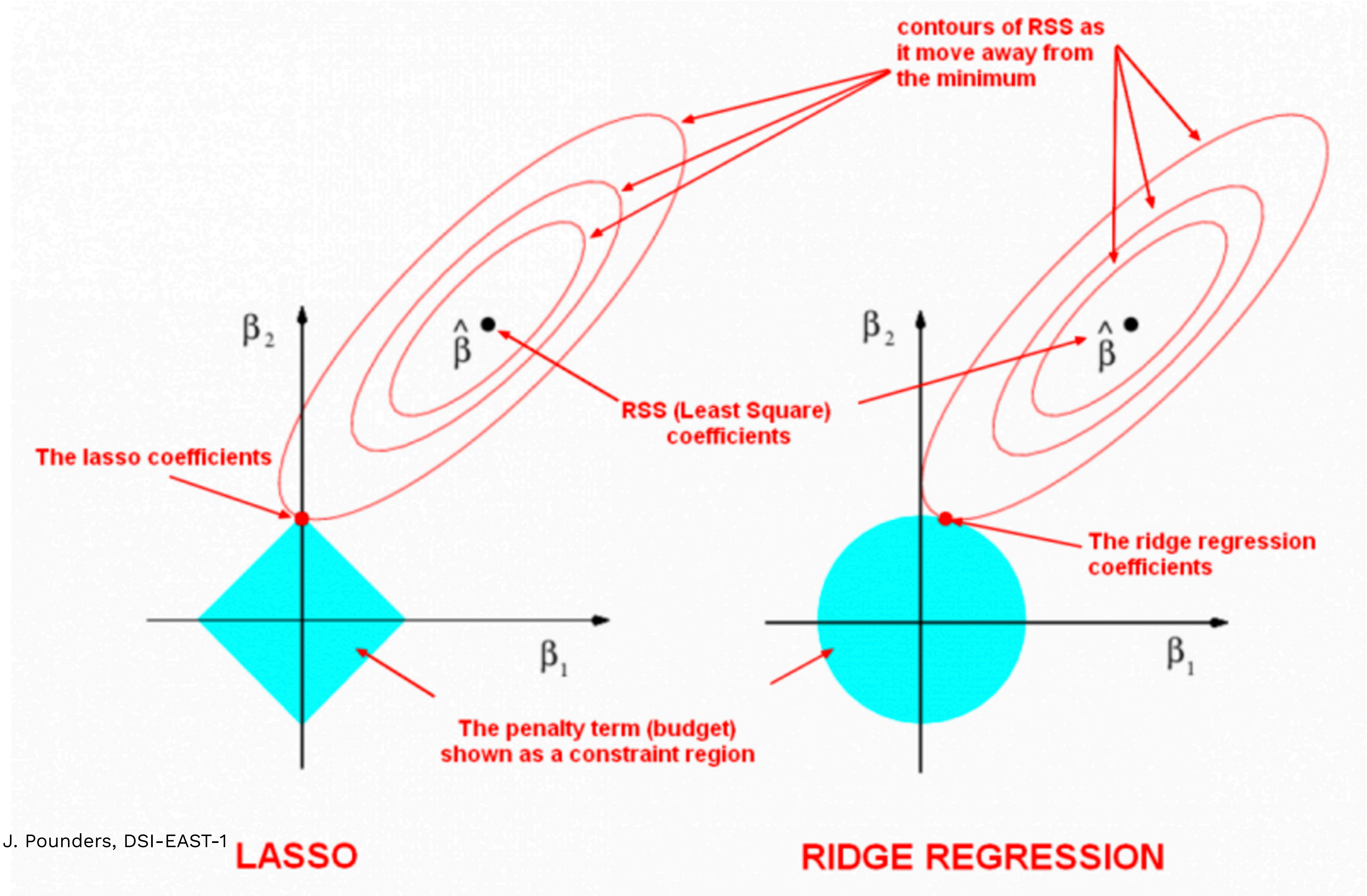
Lasso regression penalizes the model for having large coefficients. As α increases, β_1 will decrease, even to the point of zero.

α acts as a "tuning" parameter.

Lasso Regression (general case)

$$J(\beta_0, \beta_1, \ldots, \beta_p) = RSS(\beta_0, \beta_1, \ldots, \beta_p) + \alpha \sum_{i=1}^{p} |\beta_i|$$

Ridge shrinks the regression coefficients, and may "zero-out" unimportant features.


contours of RSS as
it move away from
the minimum
β_2
$\hat{\beta}$
RSS (Least Square)
coefficients
The lasso coefficients
β_1
β_2
$\hat{\beta}$
The ridge regression
coefficients
β_1
The penalty term (budget)
shown as a constraint region
LASSO
RIDGE REGRESSION

Tuning Bias vs Variance with Regularization

Alert!! Key takeaway!

- Increase α (turn **up** regularization)
  - Increase bias
  - Decrease variance
- Decrease α (turn **down** regularization)
  - Decrease bias
  - Increase variance

Additional Considerations

- Features (inputs) should be standardized in regularized models
  - Why?
- Ridge vs Lasso?
  - Maybe have irrelevant features? **Lasso**
  - Just want the best prediction? **Try both**
  - Want to use both? **ElasticNet**

Elastic Net Regression

$$J(\beta_0, \beta_1) = RSS(\beta_0, \beta_1) + \alpha_1 \left|\beta_1\right| + \alpha_2 \beta_1^2$$

Elastic net combines Ridge and Lasso penalties

α_1 and α_2 both act as "tuning" parameters

Elastic Net Regression

A second (equivalent formulation) used by `sklearn`

$$J(\beta_0, \beta_1) = RSS(\beta_0, \beta_1) + \alpha\rho\,|\beta_1| + \frac{\alpha(1-\rho)}{2}\beta_1^2$$

Elastic net combines Ridge and Lasso penalties

— $\alpha =$ penalty strength

— $\rho =$ Lasso (L_1) ratio

Elastic Net Regression

A second (equivalent formulation) used by `sklearn`

$$J(\beta_0, \beta_1) = RSS(\beta_0, \beta_1) + \alpha\rho\,|\beta_1| + \frac{\alpha(1-\rho)}{2}\beta_1^2$$

Elastic net combines Ridge and Lasso penalties

Check: what values of ρ lead to (a) Ridge and (b) Lasso regression?

Elastic Net Regression (general case)

$$J(\beta_0, \beta_1, \ldots, \beta_p) = RSS(\beta_0, \beta_1, \ldots, \beta_p) + \alpha\rho \sum_{i=1}^{p} |\beta_i| + \frac{\alpha(1-\rho)}{2} \sum_{i=1}^{p} \beta_i^2$$

[Elastic Net] allows for learning a sparse model where few of the weights are non-zero like Lasso, while still maintaining the regularization properties of Ridge.

— `sklearn` docs

Turn and Talk

With a partner, discuss and summarize...

1. What is Ridge regularization?
2. What is Lasso regularization?
3. What is Elastic Net regularization?

After 4 minutes, I will call on volunteers to summarize one of these responses.

Python Time