Regularized Linear Regression

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slides of Ryan Henning

- Relate regularization to feature selection in linear regression
- Compare and contrast Lasso and Ridge regression.
- Build test error curve to determine optimal level or regularization

“HELP, my model is overfitting!”

You have a few options.

1. Get more data… (not usually possible/practical)
2. $\boxed{\textbf{Subset Selection:}}$ keep only a subset of your predictors (i.e, dimensions)
3. **Regularization:** restrict your model’s parameter space
4. **Dimensionality Reduction:** project the data into a lower dimensional space

Subset Selection

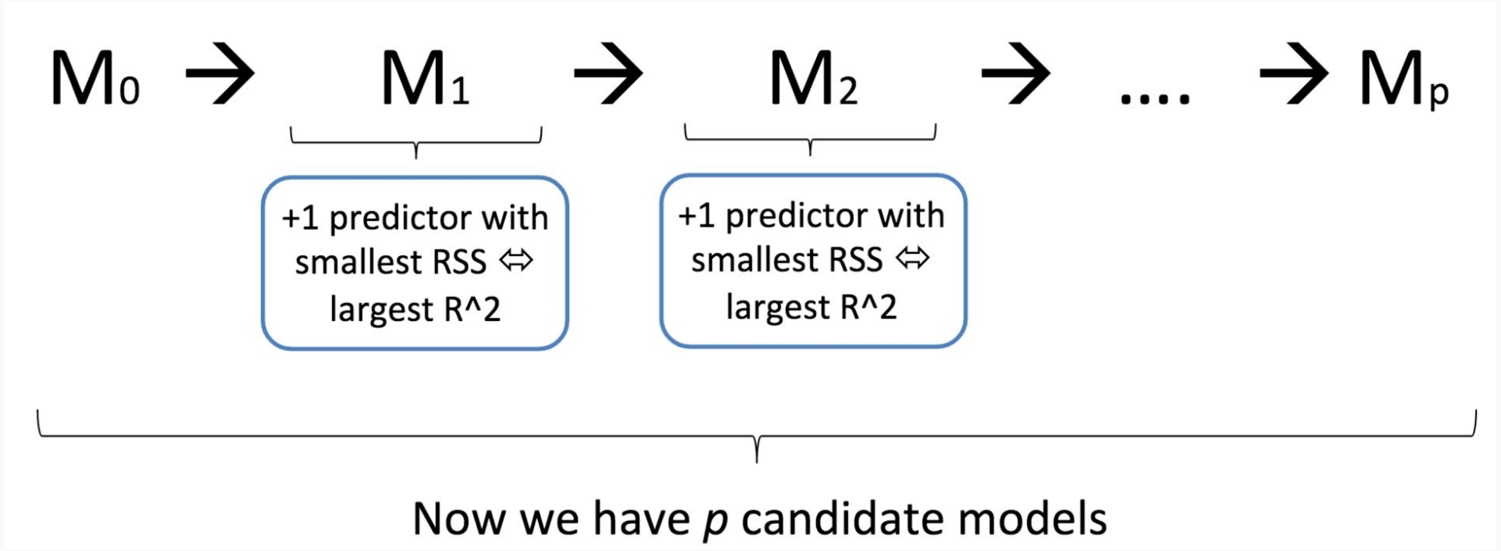
Best subset: Try every model. Every possible combination of *p* predictors

- Computationally intensive. 2^p possible subsets of *p* predictors
- High chance of finding a “good” model by random chance.

Stepwise: Iteratively pick predictors to be in/out of the final model.

- Forward, backward, forward-backward strategies

Forward Stepwise Selection

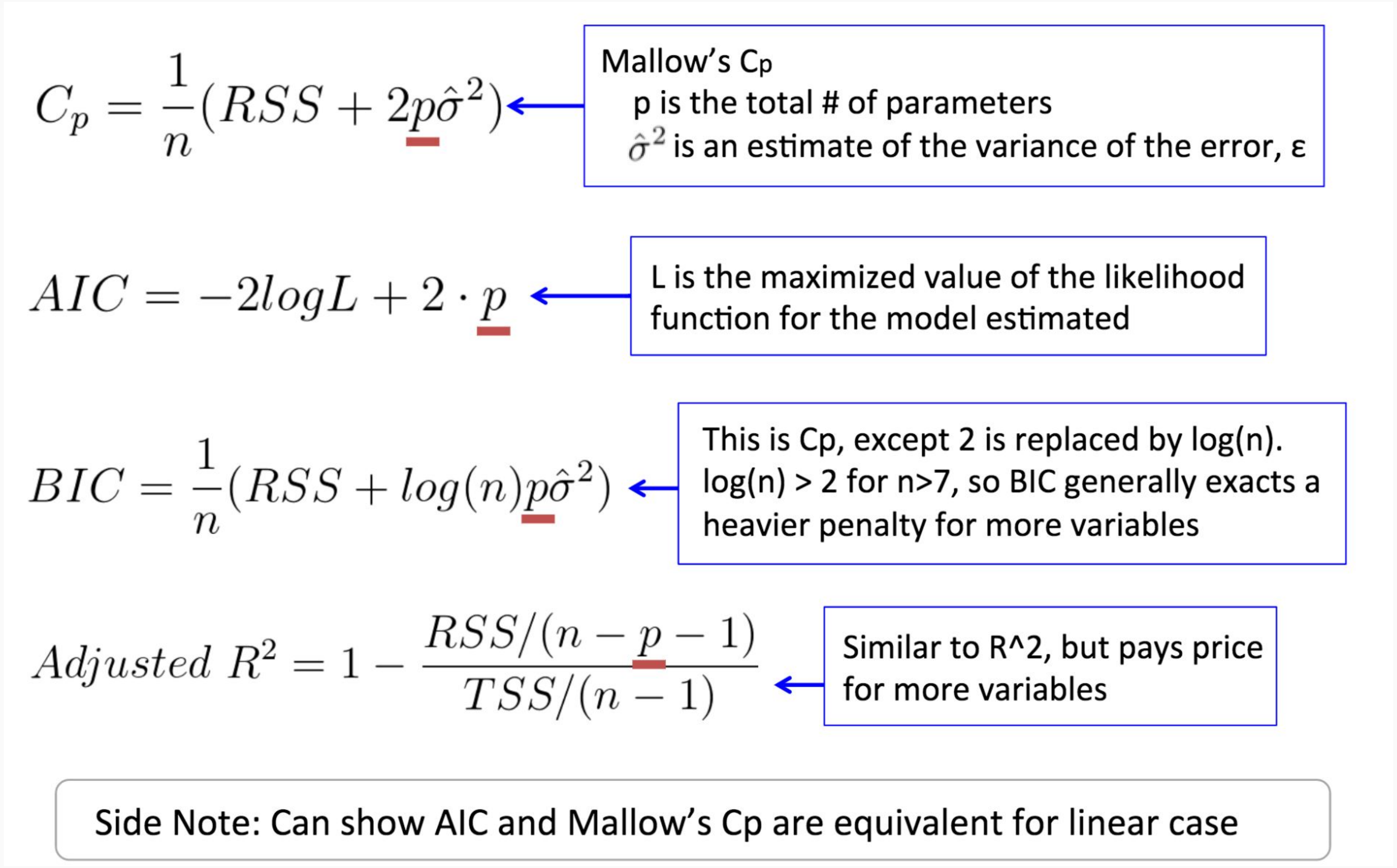

$M_0 \rightarrow M_1 \rightarrow M_2 \rightarrow .... \rightarrow M_p$
+1 predictor with smallest RSS ⇔ largest R^2
+1 predictor with smallest RSS ⇔ largest R^2
Now we have *p* candidate models

Are RSS and R^2 good ways to decide amongst the resulting *(p+1)* candidates?

Answer: Don't use RSS or R^2 for this part.
Use Mallow's C_p, or AIC, or BIC, or Adjusted R^2.

… or just use cross-validation with any error measurement.

Subset Selection: Comparing models of varying number of predictors...



$$C_p = \frac{1}{n}(RSS + 2\underline{p}\hat{\sigma}^2)$$

Mallow's Cp
p is the total # of parameters
$\hat{\sigma}^2$ is an estimate of the variance of the error, ε

$$AIC = -2logL + 2 \cdot \underline{p}$$

L is the maximized value of the likelihood function for the model estimated

$$BIC = \frac{1}{n}(RSS + log(n)\underline{p}\hat{\sigma}^2)$$

This is Cp, except 2 is replaced by log(n). log(n) > 2 for n>7, so BIC generally exacts a heavier penalty for more variables

$$Adjusted\ R^2 = 1 - \frac{RSS/(n - \underline{p} - 1)}{TSS/(n-1)}$$

Similar to R^2, but pays price for more variables

Side Note: Can show AIC and Mallow's Cp are equivalent for linear case

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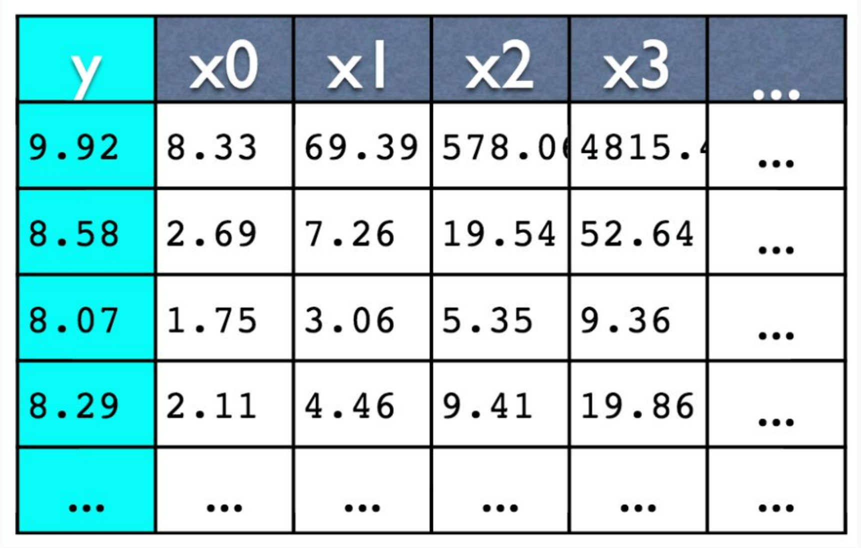
Linear Regression Example

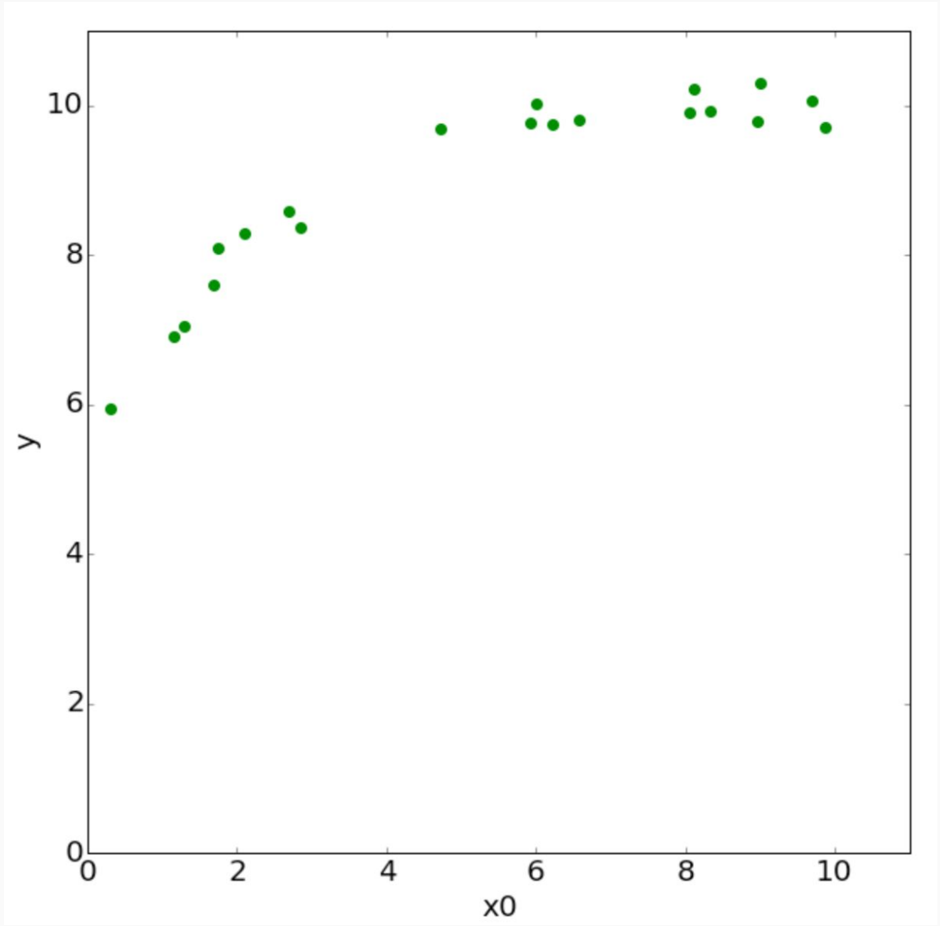
Data: 20 examples x 10 features

Predict: *y*

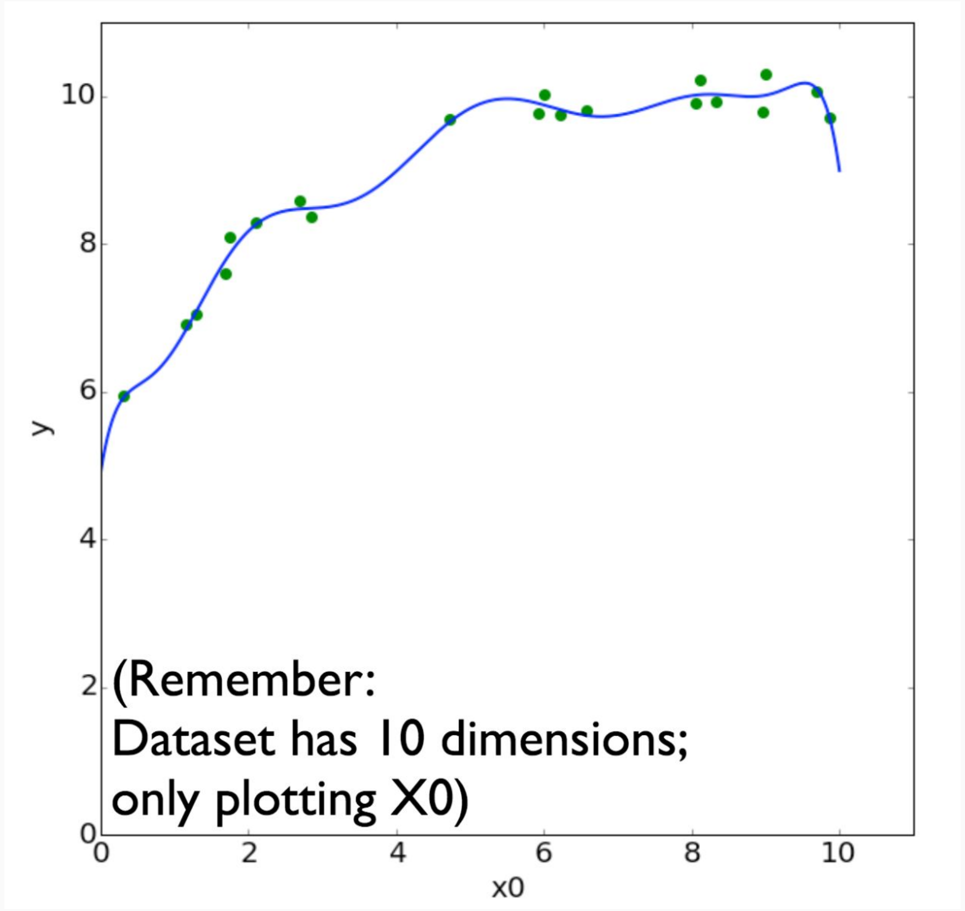


y	x0	x1	x2	x3	...
9.92	8.33	69.39	578.0	4815.	...
8.58	2.69	7.26	19.54	52.64	...
8.07	1.75	3.06	5.35	9.36	...
8.29	2.11	4.46	9.41	19.86	...
...	...	...	...	...	...

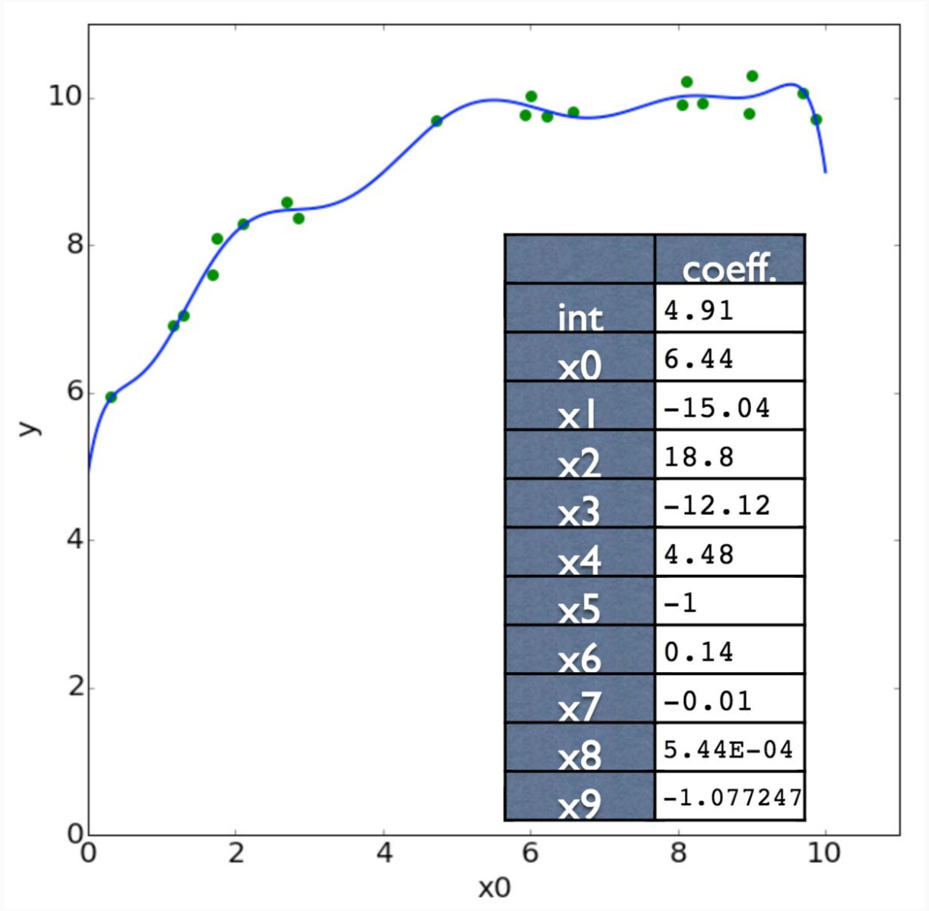
Linear Regression Example (x0 vs y)



Linear Regression Example (x0 vs y, model over all features)

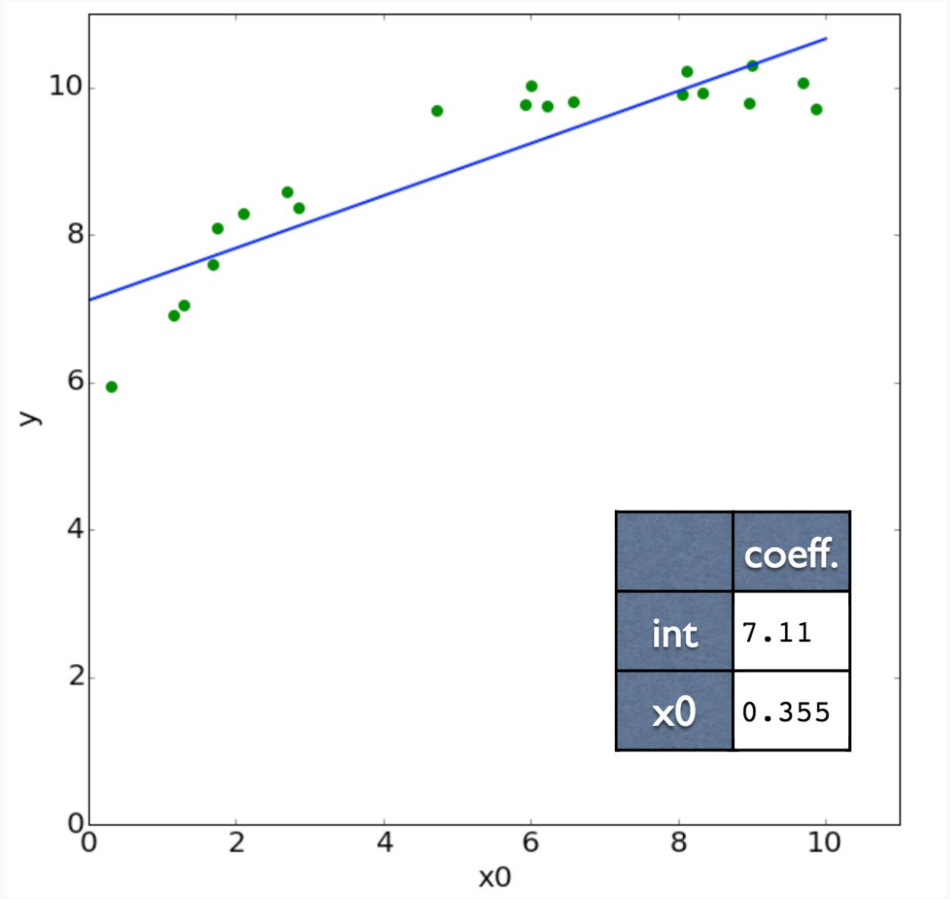


Linear Regression Example (x0 vs y, model over all features)



	coeff.
int	4.91
x0	6.44
x1	-15.04
x2	18.8
x3	-12.12
x4	4.48
x5	-1
x6	0.14
x7	-0.01
x8	5.44E-04
x9	-1.077247

Linear Regression Example (x0 vs y, model over only x0 features)



	coeff.
int	7.11
x0	0.355

In high dimensions, data is (usually) sparse

Again… the **Curse of Dimensionality** bites us.
(we'll talk more about this is a later lecture)

Linear regression can have high variance (i.e. tends to overfit) on high dimensional data…
We'd like to restrict ("normalize", or "regularize") the model so that it has less variance.

Take the 20 example x 10 feature dataset as an example… when we fit over all features, the complexity of the model grew dramatically.
(and keep in mind, some datasets have thousands of features)

Linear Regression (another review)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

We estimate the model parameters by minimizing:

$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2$$

Ridge Regression
(Linear Regression w/ Tikhonov (L2) Regularization)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

(same as before)

We estimate the model parameters by minimizing:

(the "regularization" parameter)

$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \underbrace{\boxed{\lambda}\sum_{i=1}^{p}\hat{\beta}_i^2}$$

(new term!)

Ridge Regression

$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$$

What if we set the lambda equal to zero?

What does the new term accomplish?

What happens to a features whose corresponding coefficient value (beta) is zero?

Ridge Regression

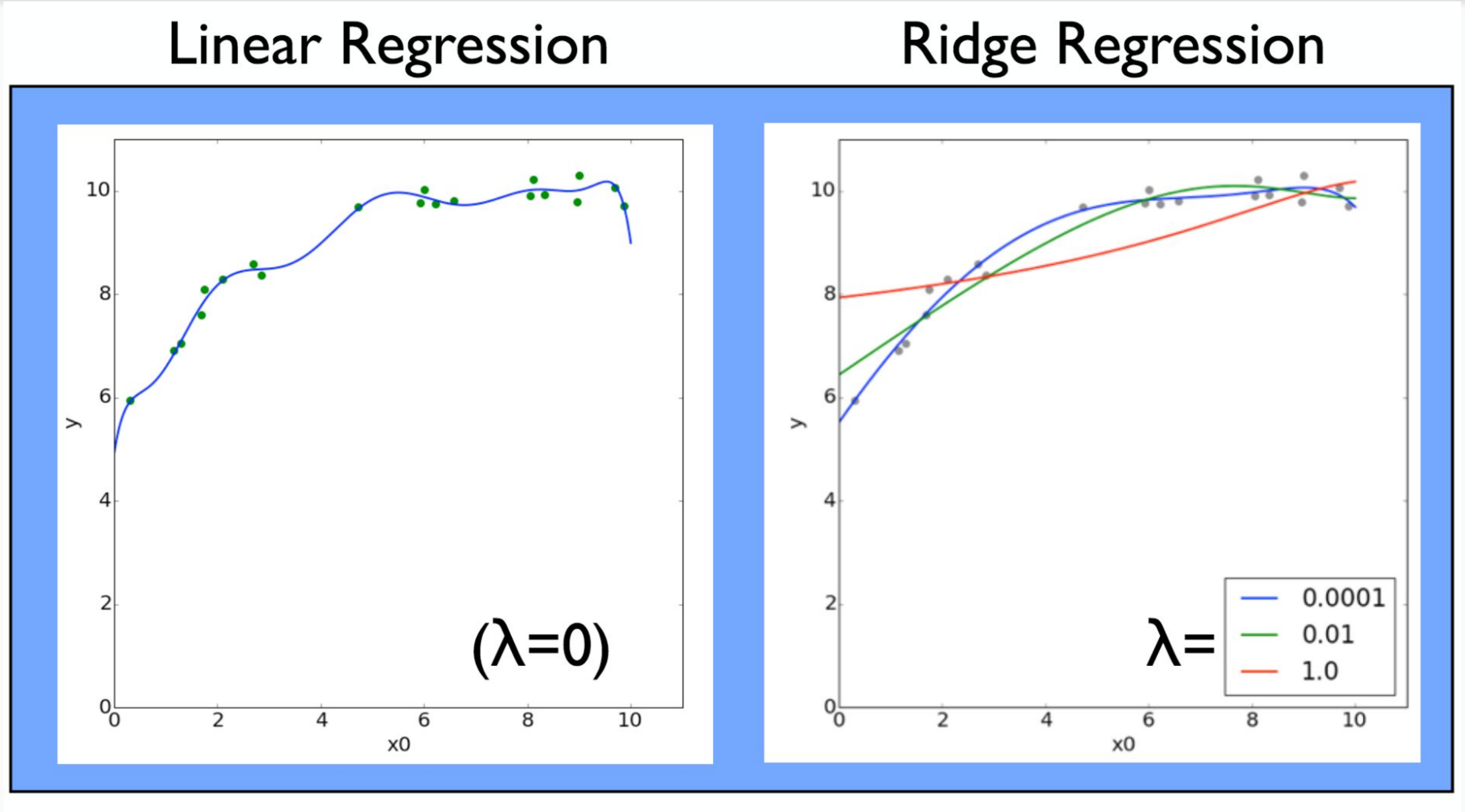
$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$$

Notice, we do not penalize B_0.

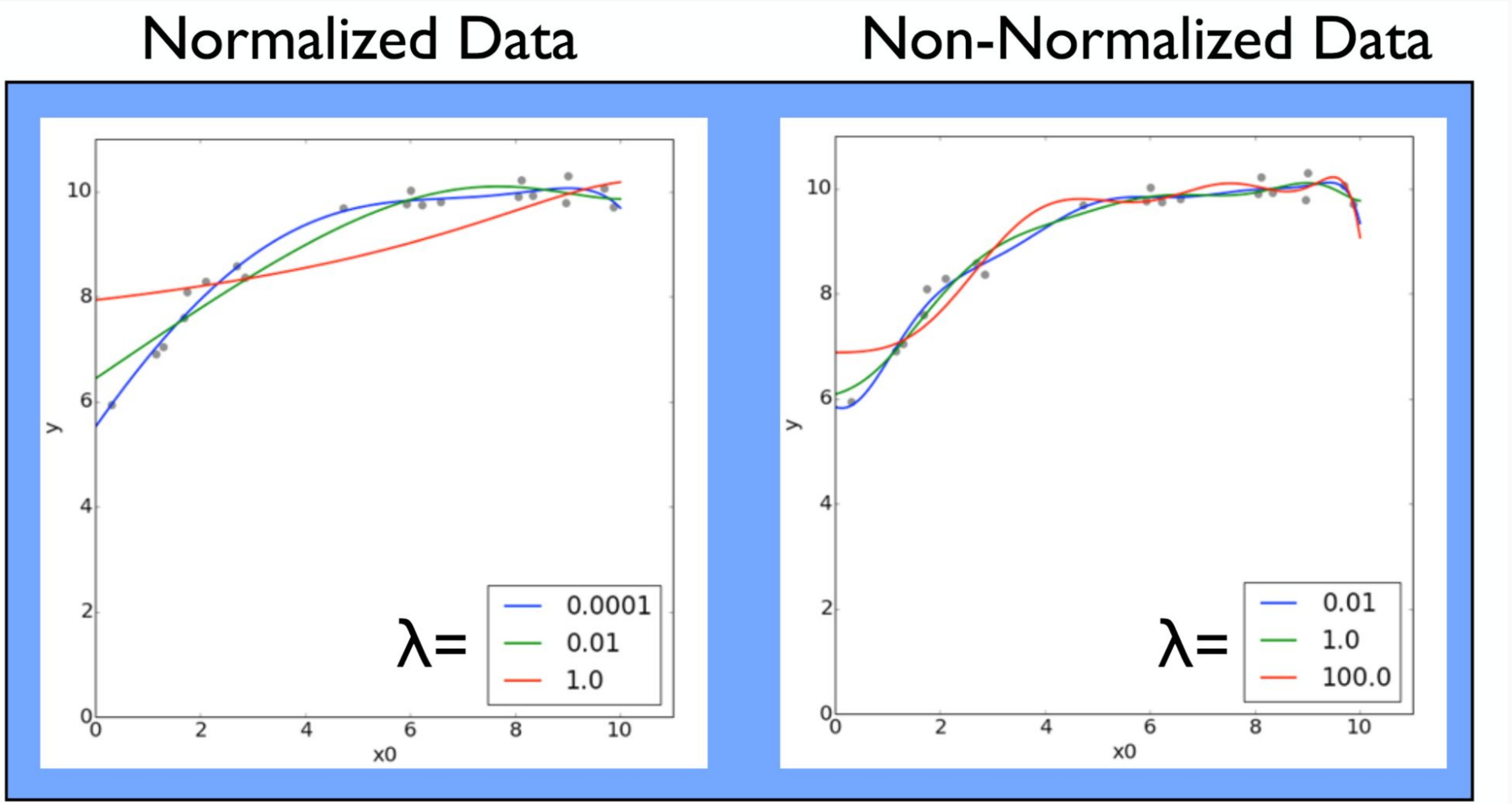
Changing lambda changes the amount that large coefficients are penalized.

Increasing lambda increases the model's bias and decreases its variance. ← this is cool!

Ridge Regression



Ridge Regression



Single value for λ assumes features are on the same scale!!

LASSO Regression
(Linear Regression w/ LASSO (L1) Regularization)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

(same as before)

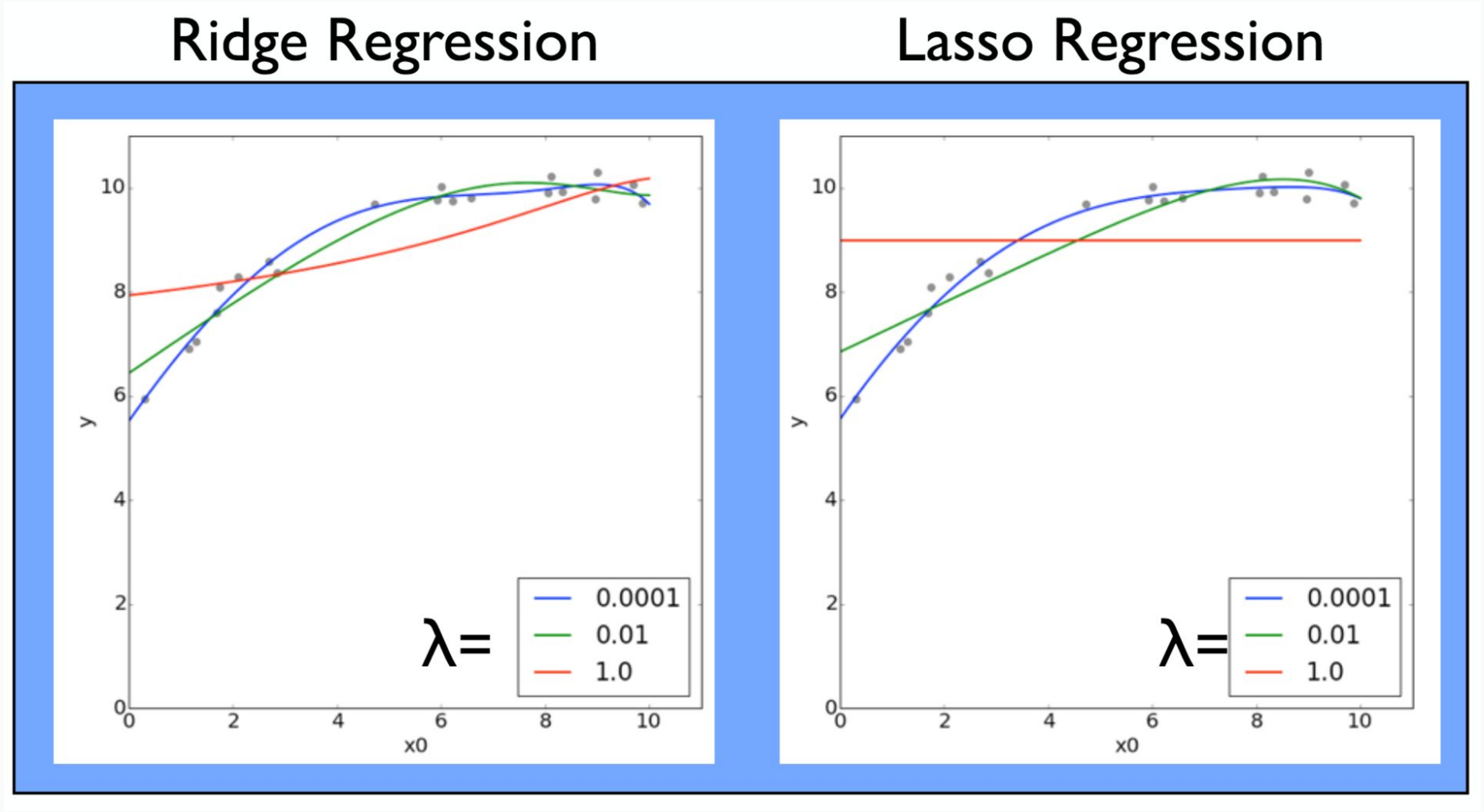
We estimate the model parameters to minimizing:

(the “regularization” parameter)

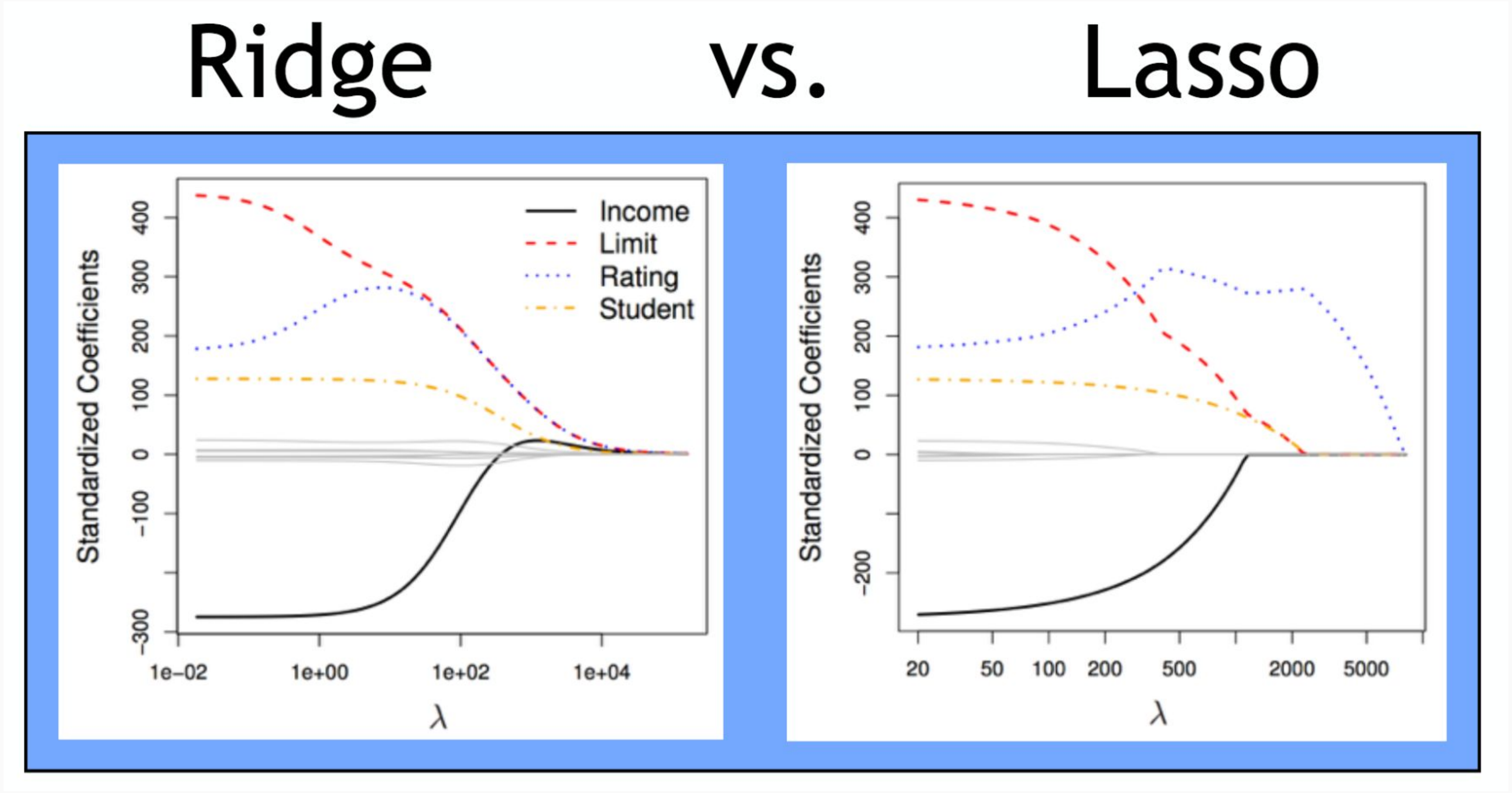
$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \boxed{\lambda}\sum_{i=1}^{p}\boxed{|\hat{\beta}_i|}$$

(absolute value instead of squared)

Lasso Regression



Ridge vs LASSO

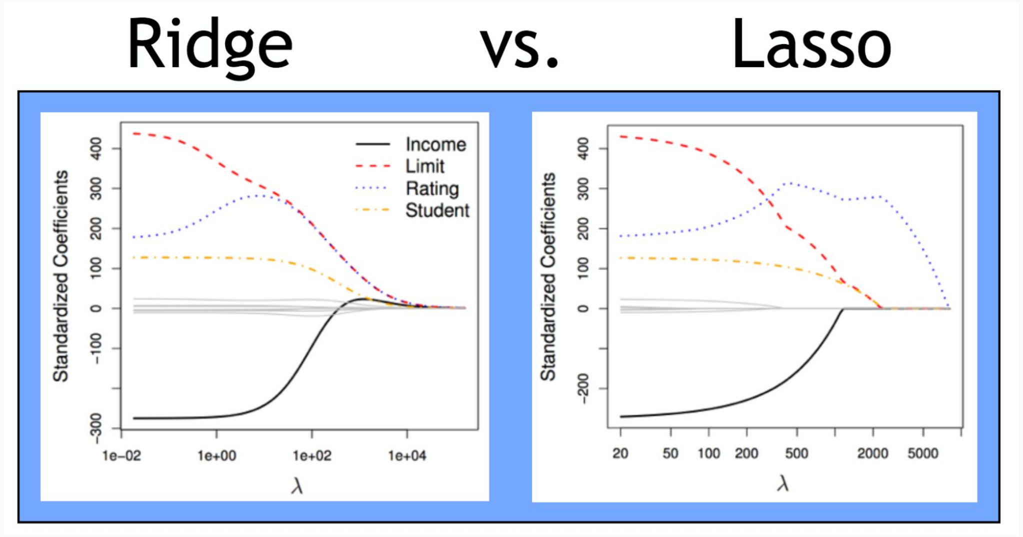


Ridge vs LASSO

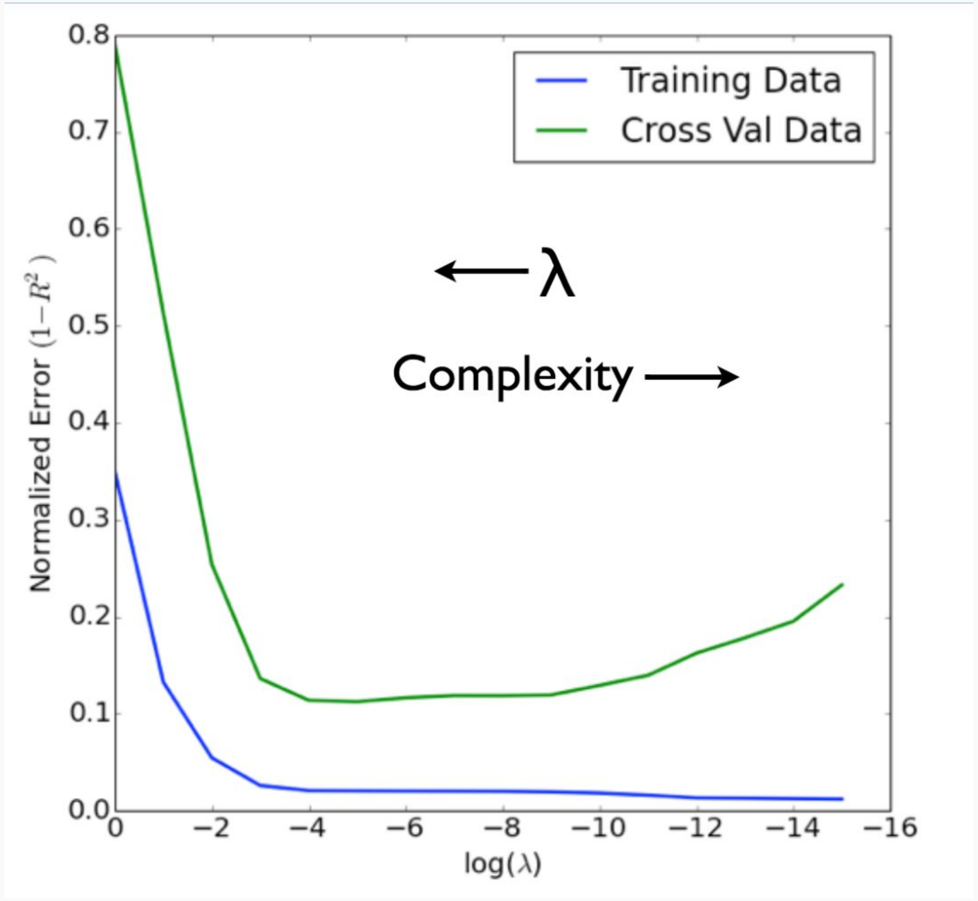
- Ridge forces parameters to be small + Ridge is computationally easier because it is differentiable
- Lasso tends to set coefficients exactly equal to zero
    - This is useful as a sort-of “automatic feature selection” mechanism,
    - leads to “sparse” models, and
    - serves a similar purpose to stepwise features selection

Which is better depends on your dataset!

True sparse models will benefit from lasso; true dense models will benefit from ridge.



Chose lambda via Cross-Validation



scikit-learn

Classes:

- sklearn.linear_model.**LinearRegression**(...)
- sklearn.linear_model.**Ridge**(alpha=my_alpha, …)
- sklearn.linear_model.**Lasso**(alpha=my_alpha, …)

All have these methods:

- fit(X, y)
- predict(X)
- score(X, y)