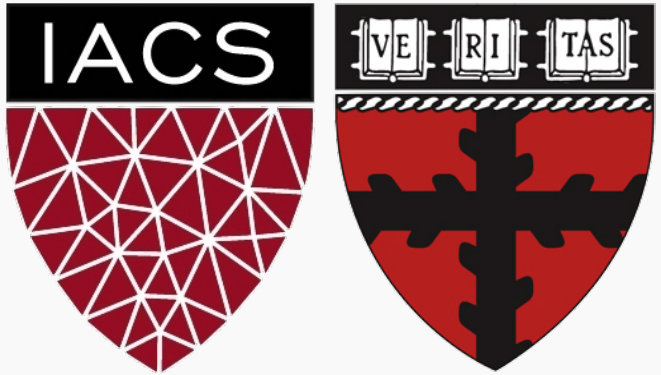
Lecture 8a: Regularization

CS109A Introduction to Data Science

Pavlos Protopapas, Kevin Rader and Chris Tanner

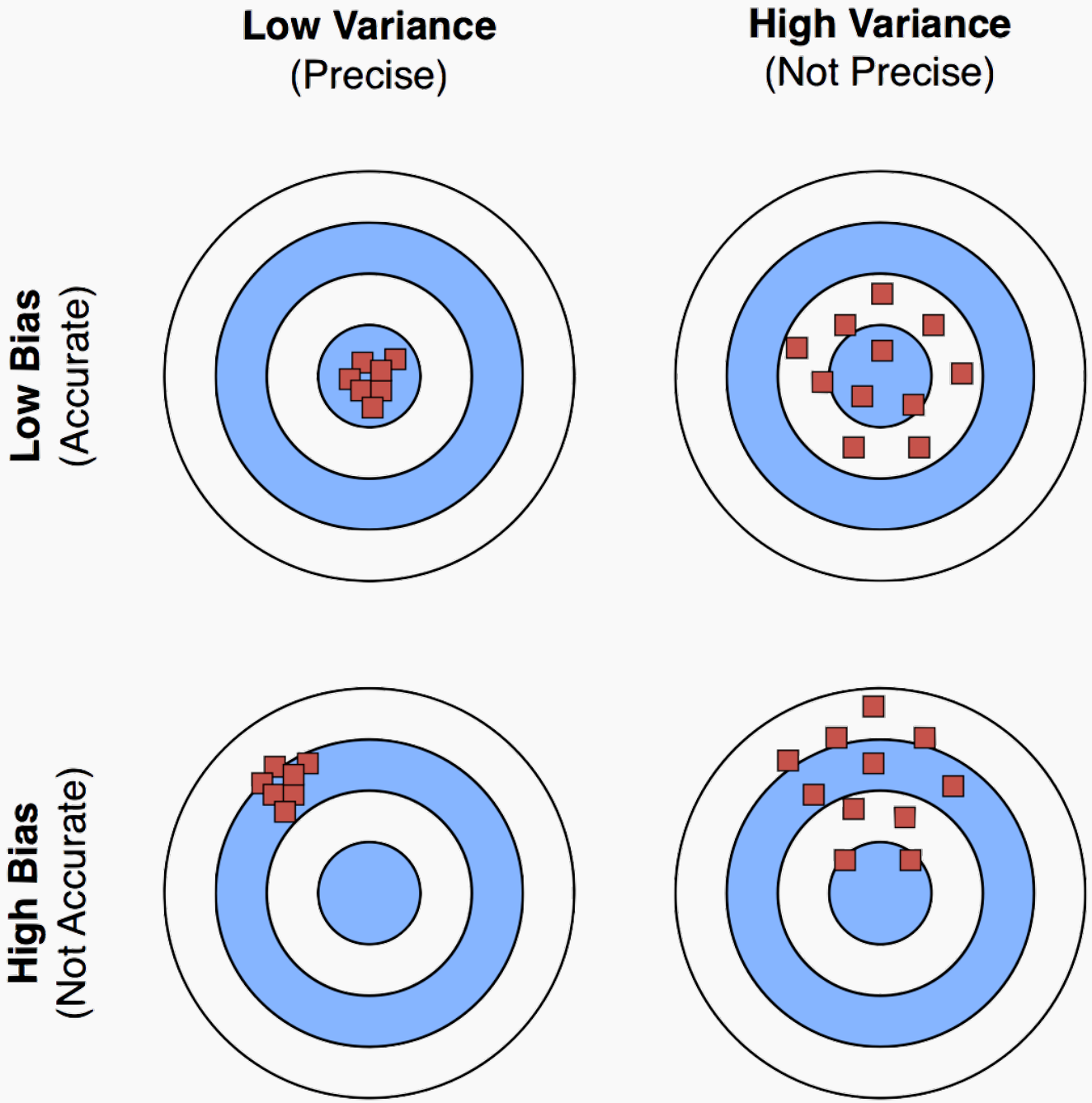


ANNOUNCEMENTS

- Religious Holidays: please contact if this affects your HW due dates.
- For 209 students:
  - please submit 209 HW separately from 109 HW in different assignments on Canvas.
  - A-sec this week: optional to cover 2nd part from last week (Bayesian perspective).

ANNOUNCEMENTS

- Milestone 1: Due this Friday, Oct 4 (see Canvas instructions).
- Study break: Wednesday 6-8pm in TBD?
- Recall Course Requirements: “You are expected to have programming experience at the level of CS 50 or above, and statistics knowledge at the level of Stat 100 or above (Stat 110 recommended).”

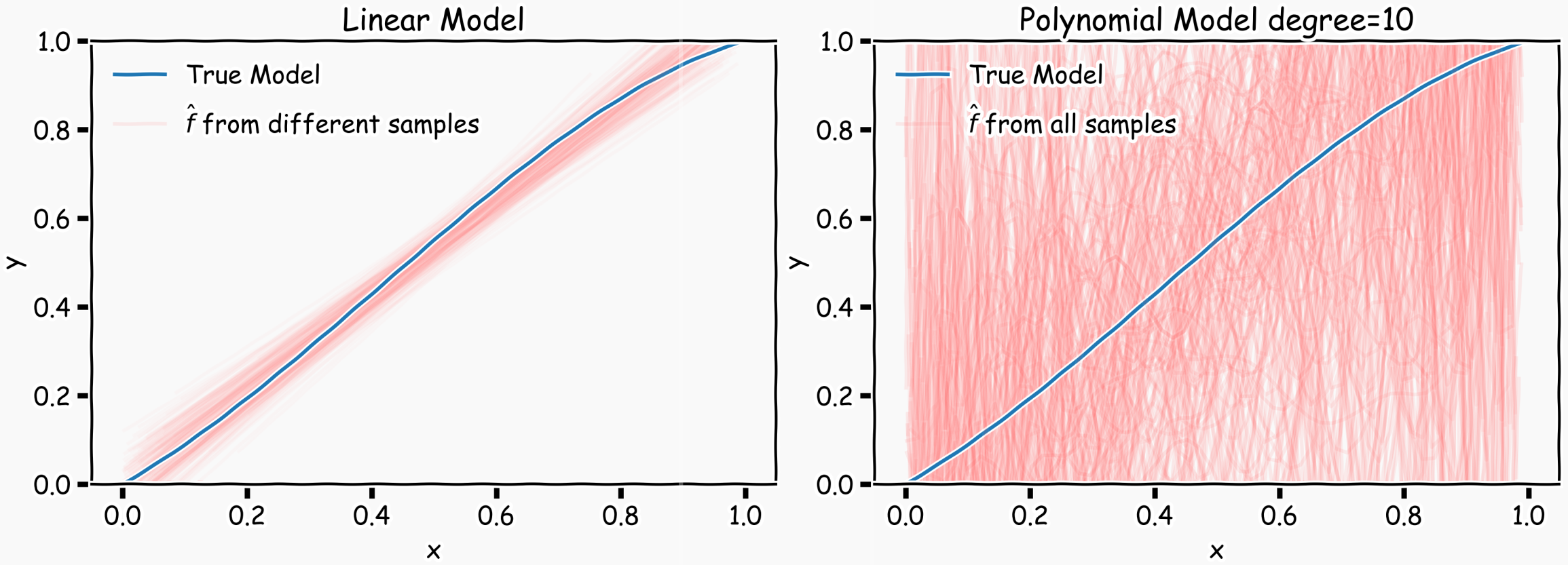

Low Variance
(Precise)
High Variance
(Not Precise)
Low Bias
(Accurate)
High Bias
(Not Accurate)

Bias vs Variance

Left: 2000 best fit straight lines, each fitted on a different 20 point training set.

Right: Best-fit models using degree 10 polynomial

You have lots of variation in f depending on realization of the data

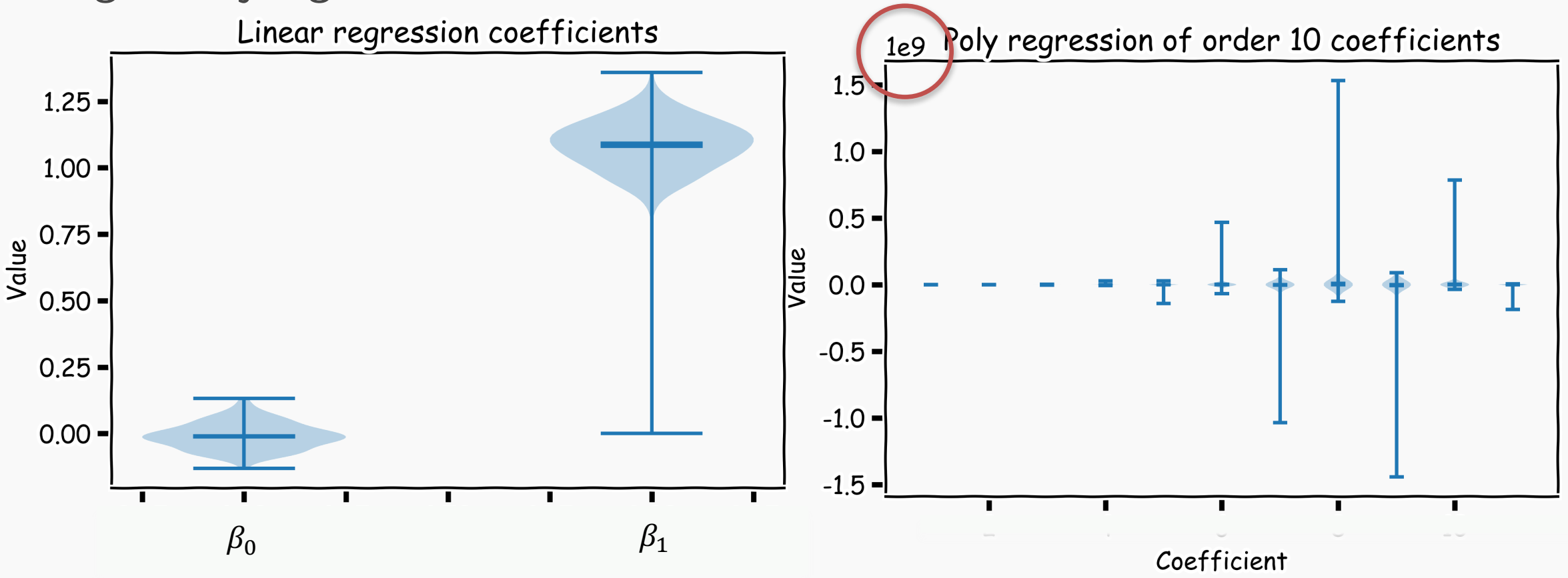


Bias vs Variance

Left: Linear regression coefficients

Right: Poly regression of order 10 coefficients

Huge range in the coefficient values



Lecture Outline

Regularization: LASSO and Ridge

Geometric Interpretation

Regularization: An Overview

The idea of regularization revolves around modifying the loss function L; in particular, we add a regularization term that penalizes some specified properties of the model parameters

Balance variance with bias - we want best MSE without getting coefficients too large

Complex models fit data well (low MSE) but have large coefficients - we will try to find a compromise by penalizing large coefficients in complex models

$$L_{reg}(\beta) = L(\beta) + \lambda R(\beta),$$

where λ is a scalar that gives the weight (or importance) of the regularization term.

Fitting the model using the modified loss function L_{reg} would result in model parameters with desirable properties (specified by R).

LASSO Regression

Since we wish to discourage extreme values in model parameter, we need to choose a regularization term that penalizes parameter magnitudes. For our loss function, we will again use MSE.

Together our regularized loss function is:

$$L_{LASSO}(\beta) = \frac{1}{n}\sum_{i=1}^{n}|y_i - \boldsymbol{\beta}^\top \boldsymbol{x}_i|^2 + \lambda \sum_{j=1}^{J}|\beta_j|.$$

Note that $\sum_{j=1}^{J}|\beta_j|$ is the $\boldsymbol{l_1}$ norm of the vector $\boldsymbol{\beta}$

$$\sum_{j=1}^{J}|\beta_j| = \|\boldsymbol{\beta}\|_1$$

Ridge Regression

Alternatively, we can choose a regularization term that penalizes the squares of the parameter magnitudes. Then, our regularized loss function is:

$$L_{Ridge}(\beta) = \frac{1}{n}\sum_{i=1}^{n}|y_i - \boldsymbol{\beta}^\top \boldsymbol{x}_i|^2 + \lambda \sum_{j=1}^{J} \beta_j^2.$$

Note that $\sum_{j=1}^{J}|\beta_j|^2$ is the square of the $\boldsymbol{l_2}$ norm of the vector $\boldsymbol{\beta}$

$$\sum_{j=1}^{J} \beta_j^2 = \|\boldsymbol{\beta}\|_2^2$$

Choosing λ

In both ridge and LASSO regression, we see that the larger our choice of the **regularization parameter** λ, the more heavily we penalize large values in $\boldsymbol{\beta}$,

- If λ is close to zero, we recover the MSE, i.e. ridge and LASSO regression is just ordinary regression.
- If λ is sufficiently large, the MSE term in the regularized loss function will be insignificant and the regularization term will force $\boldsymbol{\beta}_{\text{ridge}}$ and $\boldsymbol{\beta}_{\text{LASSO}}$ to be close to zero.

To avoid ad-hoc choices, we should select λ using cross-validation.

Ridge, LASSO - Computational complexity

Solution to ridge regression:

Has analytical solution - can calculate B that minimize regularization and MSE terms

$$\beta = (X^T X + \lambda I)^{-1} X^T Y$$

The solution to the LASSO regression:

practical solution: sklearn! not as computationally efficient as ridge regression

LASSO has no conventional analytical solution, as the L1 norm has no derivative at 0. We can, however, use the concept of subdifferential or subgradient to find a manageable expression. See a-sec2 for details.

Regularization Parameter with a Validation Seet

The solution of the Ridge/Lasso regression involves three steps:

- Select λ
- Find the minimum of the ridge/Lasso regression loss function (using the formula for ridge) and record the *MSE* **on the test set**.

Validation set

- Find the λ that gives the smallest *MSE* on the validation set

L (loss function) = Lmse + Lreg
record Lmse only for validation set - you just want to minimize the MSE

The Geometry of Regularization (LASSO)

full loss function

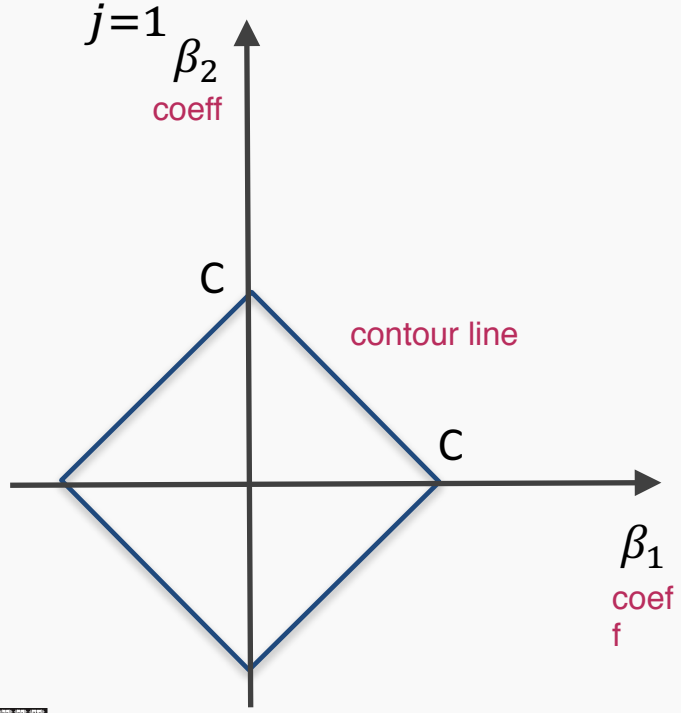
$$L_{LASSO}(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=1}^{n} |y_i - \boldsymbol{\beta}^T \boldsymbol{x}|^2 + \lambda \sum_{j=1}^{J} |\beta_j|$$

Lmse

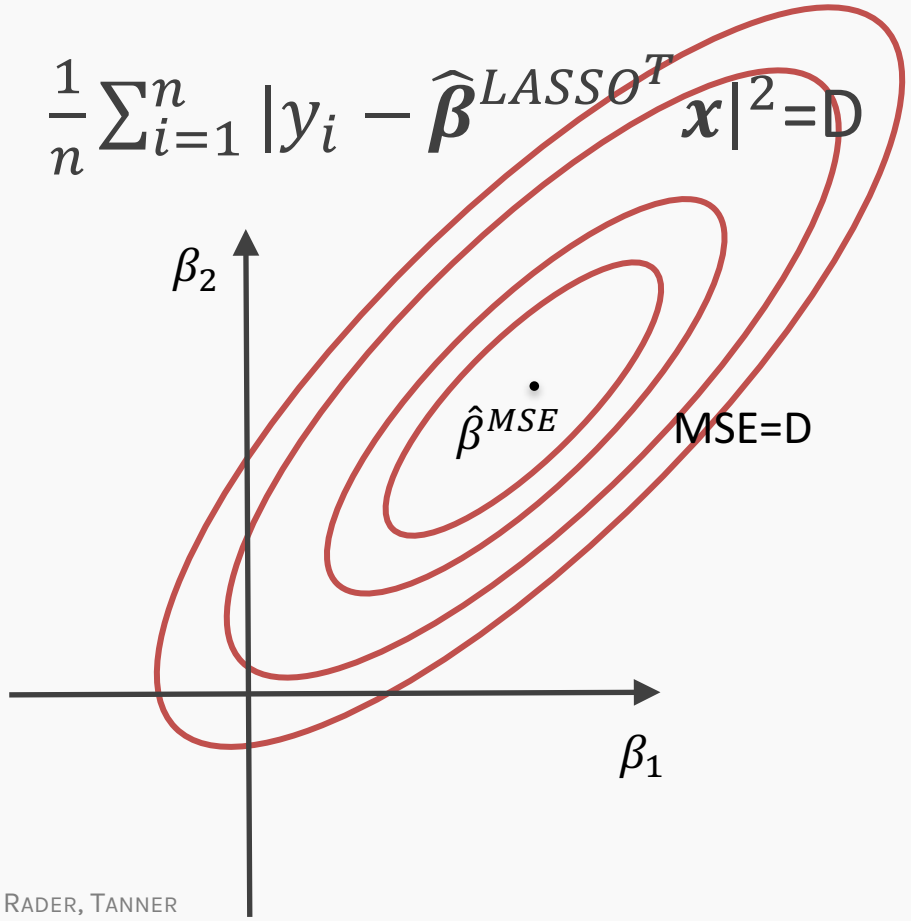
Lreg

$$\hat{\boldsymbol{\beta}}^{LASSO} = \text{argmin}\, L_{LASSO}(\boldsymbol{\beta})$$

$$\lambda \sum_{j=1}^{J} |\hat{\beta}_j^{LASSO}| = C$$



$$\frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{\boldsymbol{\beta}}^{LASSO^T} \boldsymbol{x}|^2 = D$$

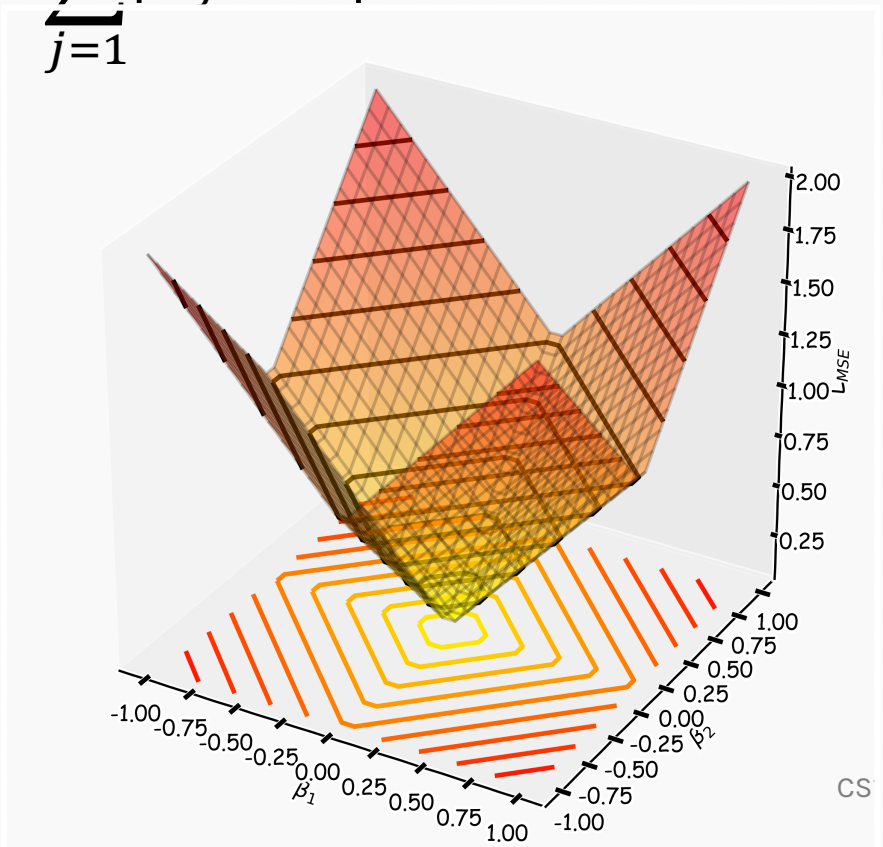


The Geometry of Regularization (LASSO)

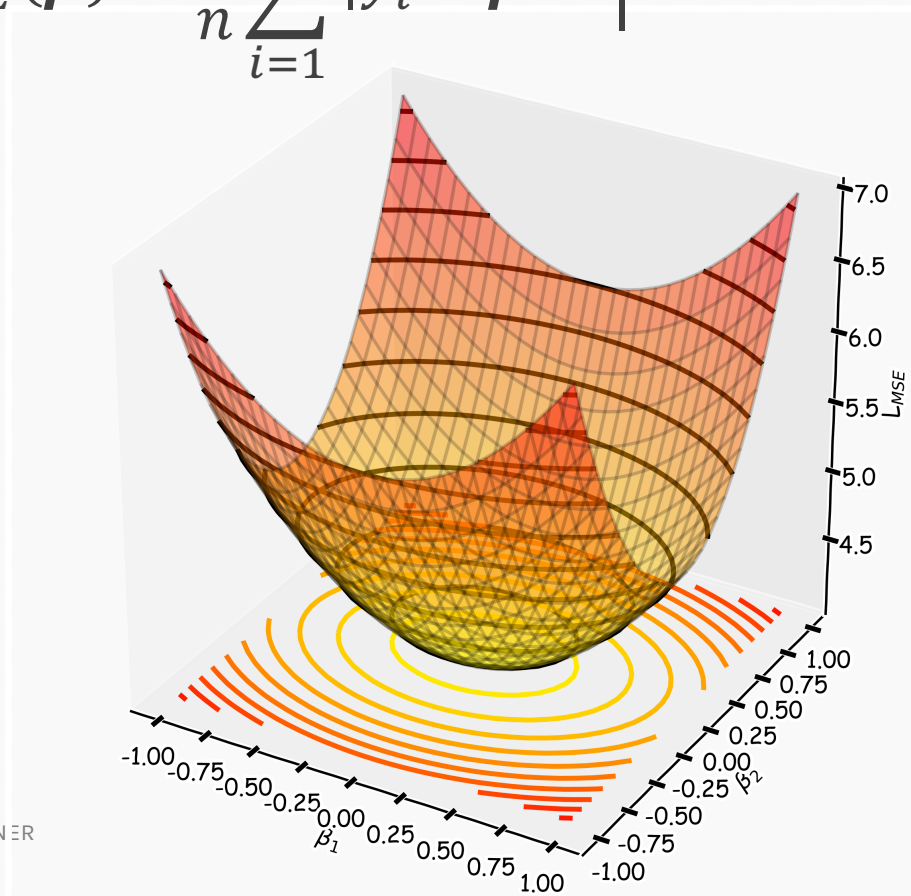
$$L_{LASSO}(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=1}^{n} |y_i - \boldsymbol{\beta}^T \boldsymbol{x}\Big|^2 + \lambda \sum_{j=1}^{J} |\beta_j|$$

$$\widehat{\boldsymbol{\beta}}^{LASSO} = \operatorname{argmin} L_{LASSO}(\boldsymbol{\beta})$$

$$L_1 = \lambda \sum_{j=1}^{J} |\hat{\beta}_j^{LASSO}|$$



$$L_{MSE}(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=1}^{n} |y_i - \boldsymbol{\beta}^T \boldsymbol{x}\Big|^2$$

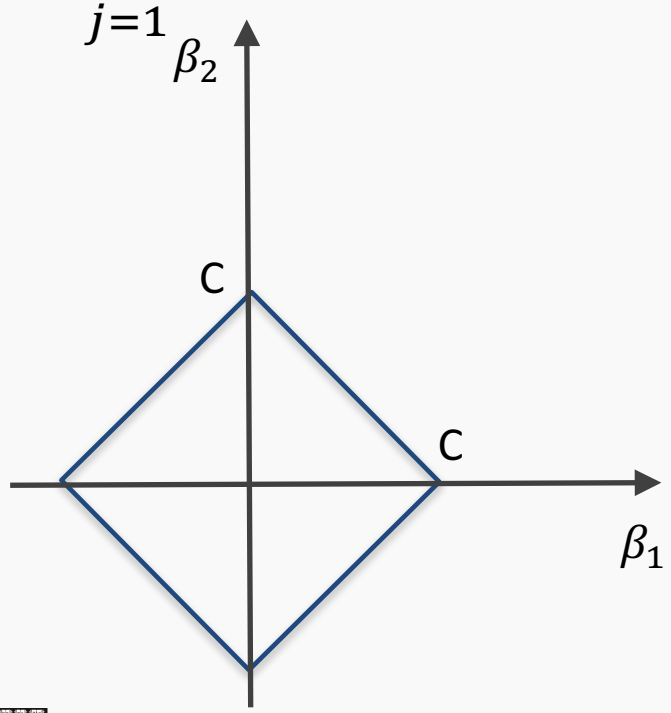


The Geometry of Regularization (LASSO)

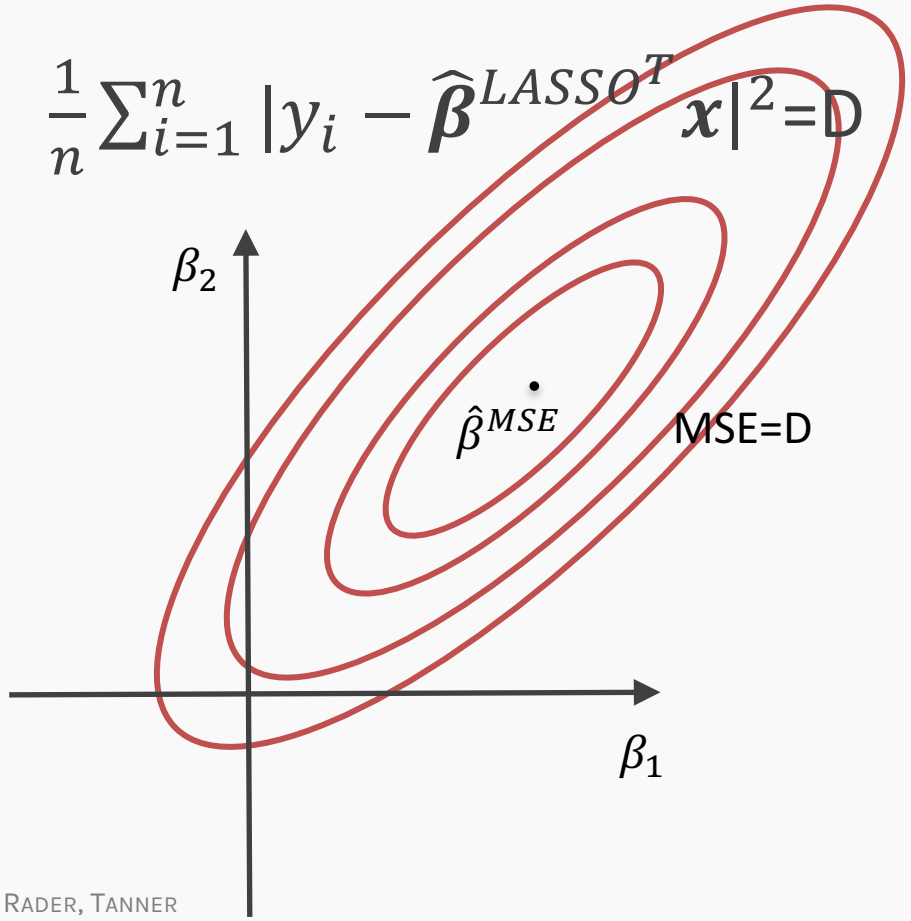
$$L_{LASSO}(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=1}^{n} |y_i - \boldsymbol{\beta}^T \boldsymbol{x}|^2 + \lambda \sum_{j=1}^{J} |\beta_j|$$

$$\widehat{\boldsymbol{\beta}}^{LASSO} = \text{argmin}\, L_{LASSO}(\boldsymbol{\beta})$$

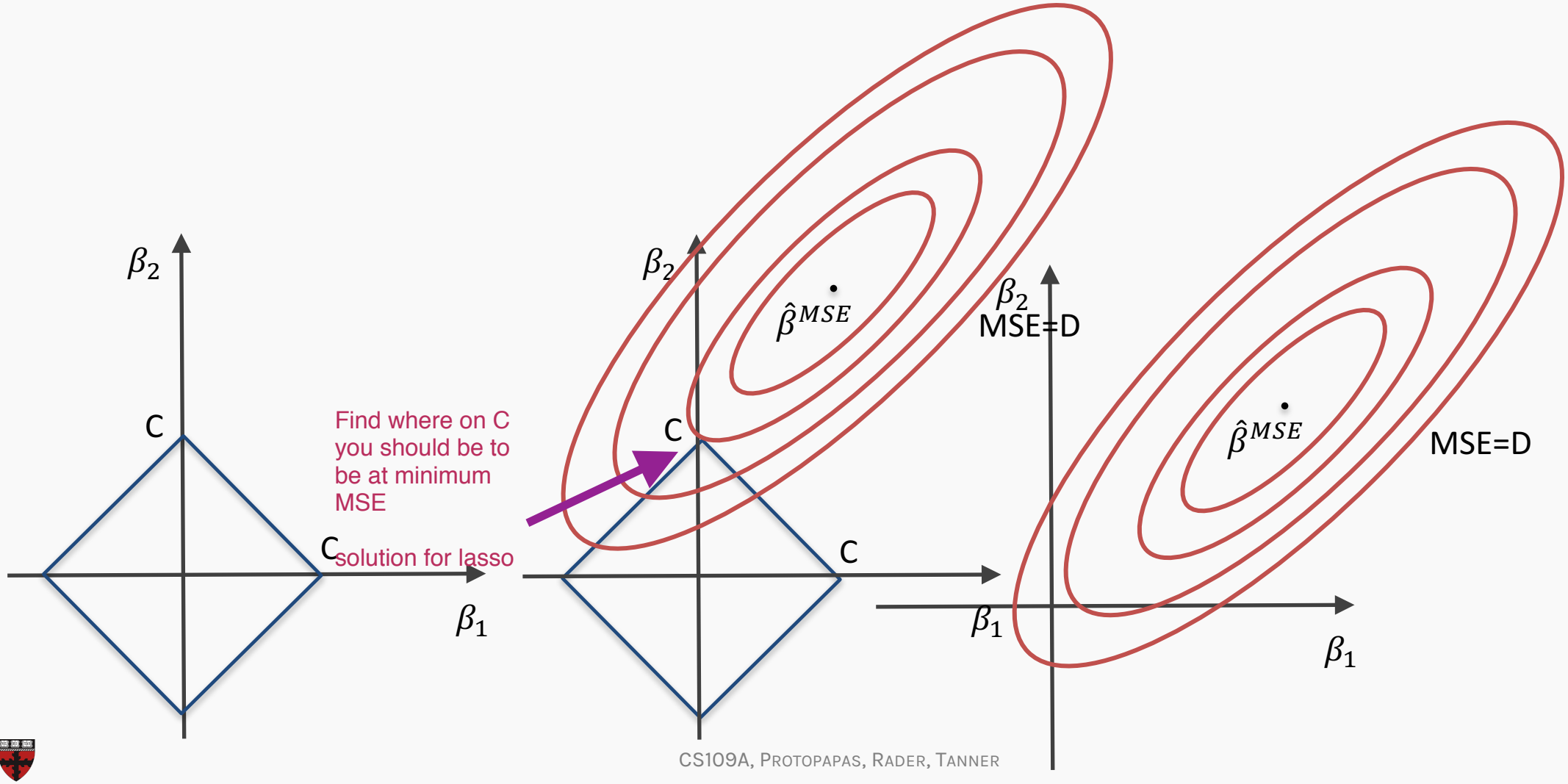
$$\lambda \sum_{j=1}^{J} |\hat{\beta}_j^{LASSO}| = C$$



$$\frac{1}{n}\sum_{i=1}^{n} |y_i - \widehat{\boldsymbol{\beta}}^{LASSO^T} \boldsymbol{x}|^2 = D$$



The Geometry of Regularization (LASSO)

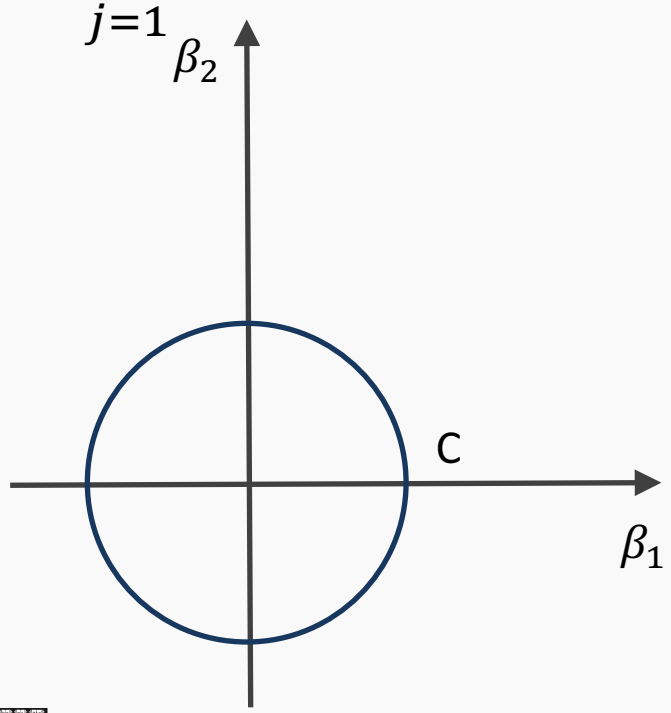


The Geometry of Regularization (Ridge)

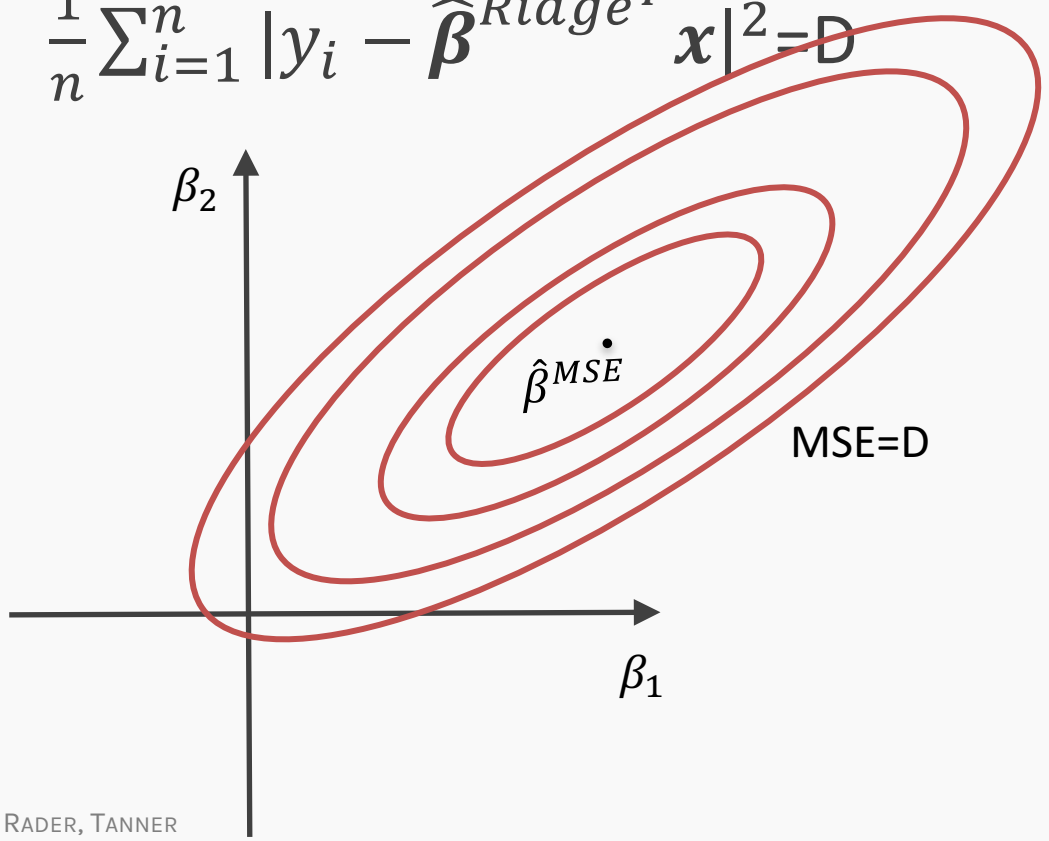
$$L_{Ridge}(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=1}^{n} |y_i - \boldsymbol{\beta}^T \boldsymbol{x}\Big|^2 + \lambda \sum_{j=1}^{J} (\beta_j)^2$$

$$\widehat{\boldsymbol{\beta}}^{Ridge} = \text{argmin}\, L_{Ridge}(\boldsymbol{\beta})$$

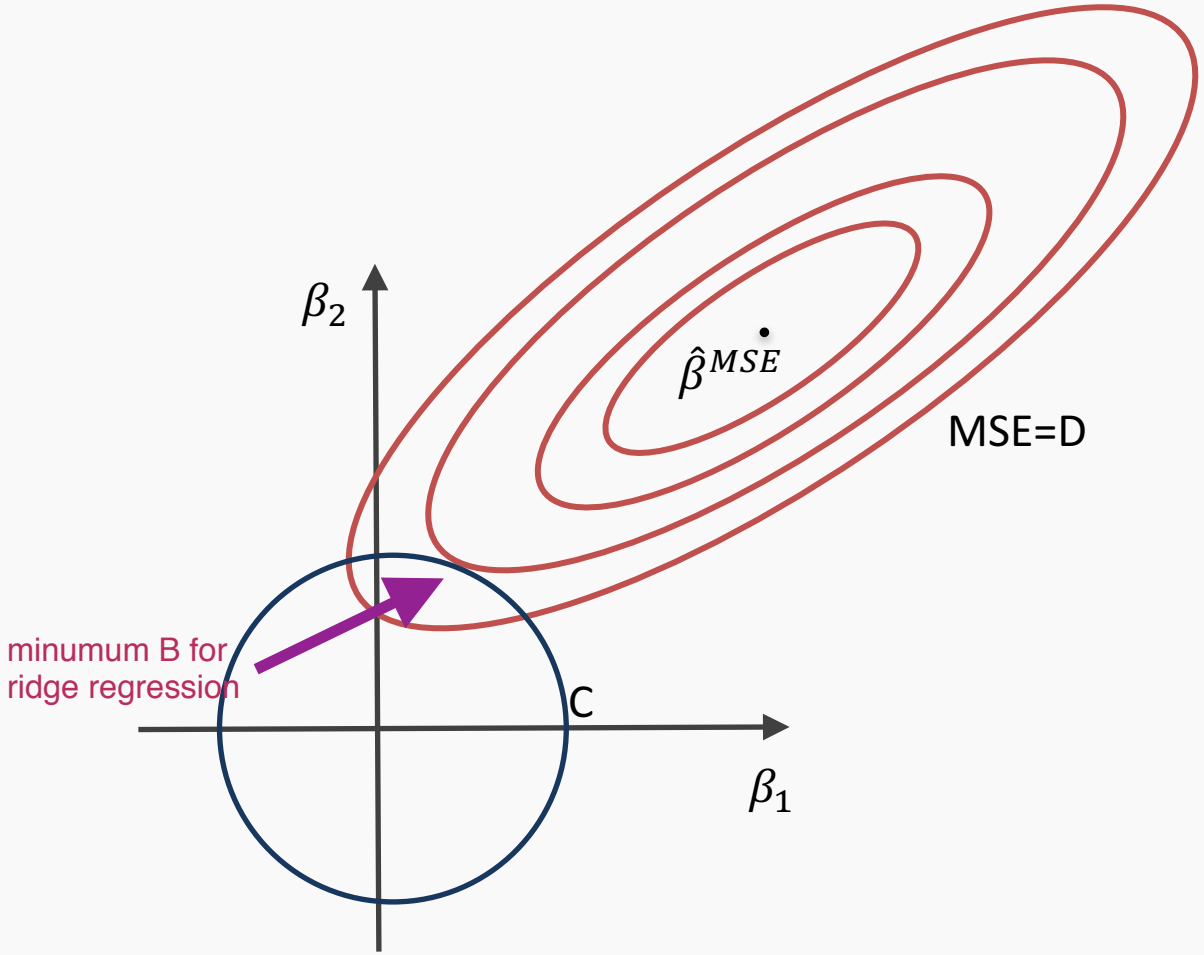
$$\lambda \sum_{j=1}^{J} \Big|\hat{\beta}_j^{Ridge}\Big|^2 = C$$



$$\frac{1}{n}\sum_{i=1}^{n} |y_i - \widehat{\boldsymbol{\beta}}^{Ridge^T} \boldsymbol{x}|^2 = D$$

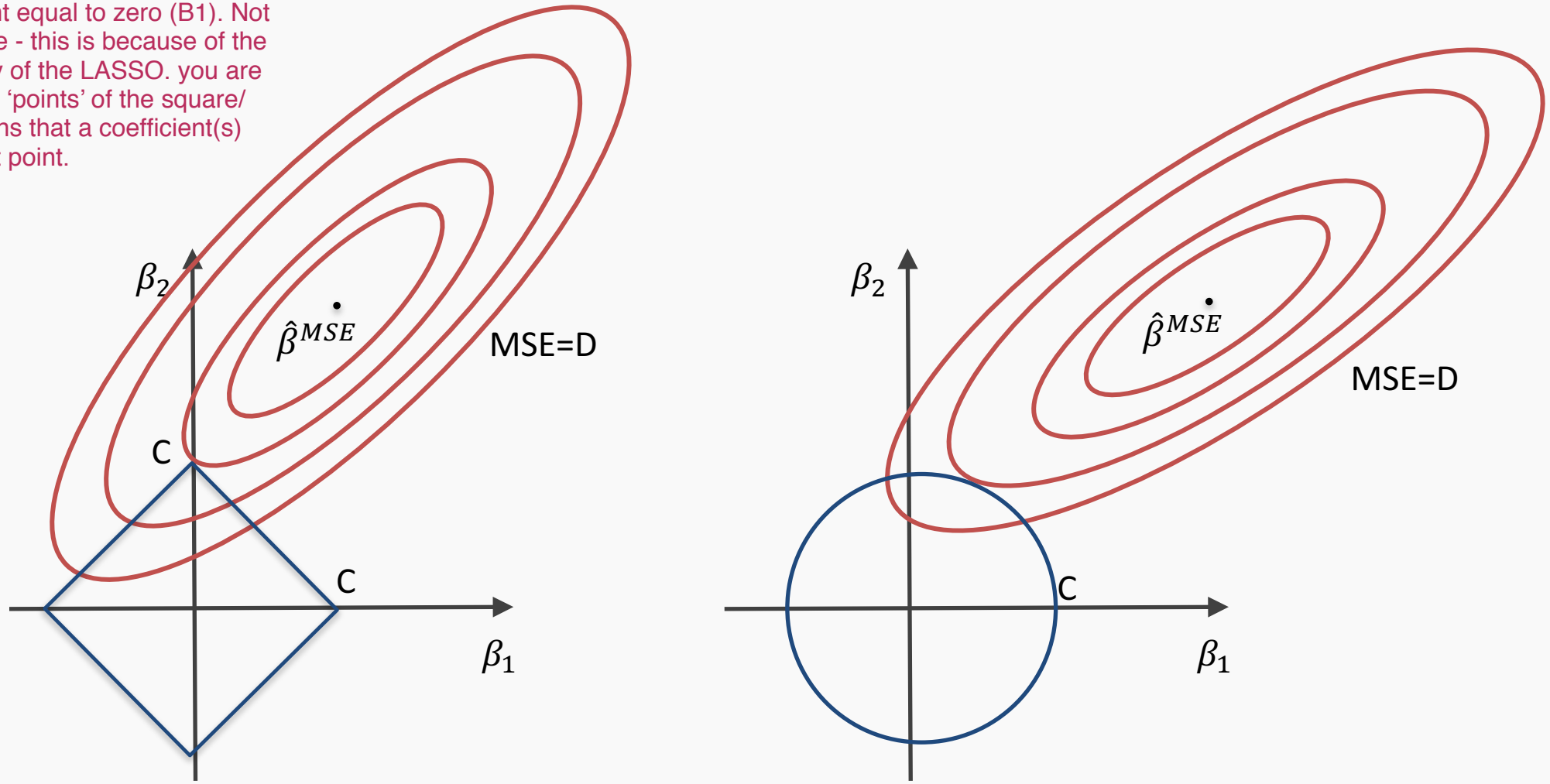


The Geometry of Regularization (Ridge)



The Geometry of Regularization

For LASSO there is a solution that will have a coefficient equal to zero (B1). Not the case for ridge - this is because of the 'pointy' geometry of the LASSO. you are touching that the 'points' of the square/ cube which means that a coefficient(s) must be 0 at that point.



Examples

In [ ]:
```
from sklearn.linear_model import Lasso
```

Lasso can be used for variable selection - you turn variables to zero and you can throw them away

In [22]:
```
lasso_regression = Lasso(alpha=1.0, fit_intercept=True)
lasso_regression.fit(np.vstack((X_train, X_val)), np.hstack((y_train, y_val)))

print('Lasso regression model:\n {} + {}^T . x'.format(lasso_regression.intercept_, lasso_regression.coe
```

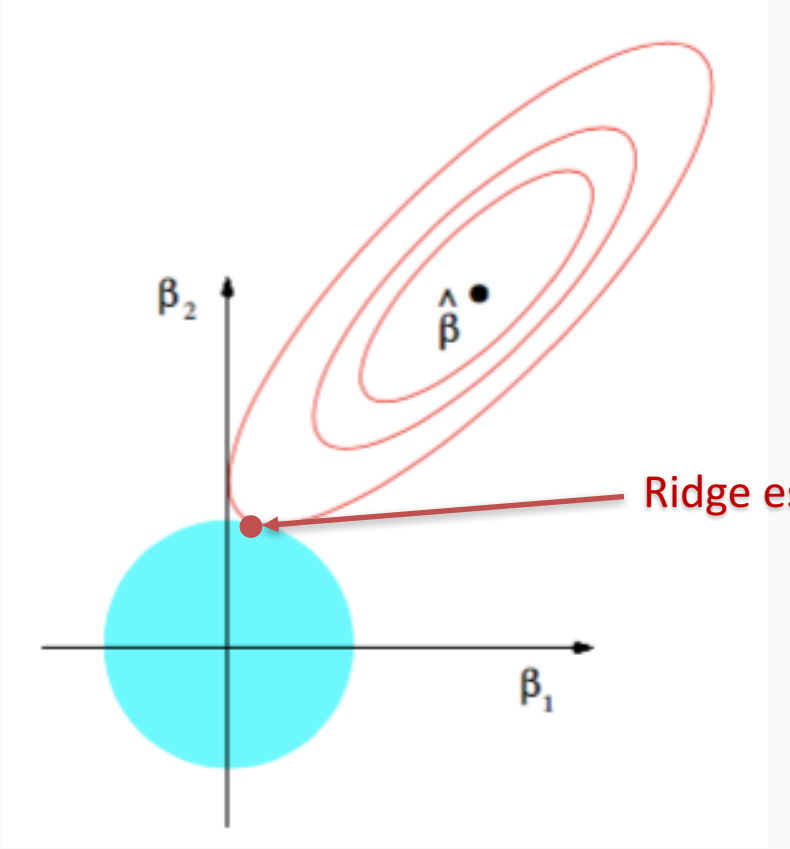
```
Lasso regression model:
 10.424895873901445 + [ 0.24482603  3.48164594  1.84836859 -0.06864603 -0.         -0.
 -0.02249766 -0.          0.          0.          0.          ]^T . x
```

In [ ]:
```
from sklearn.linear_model import Ridge
```

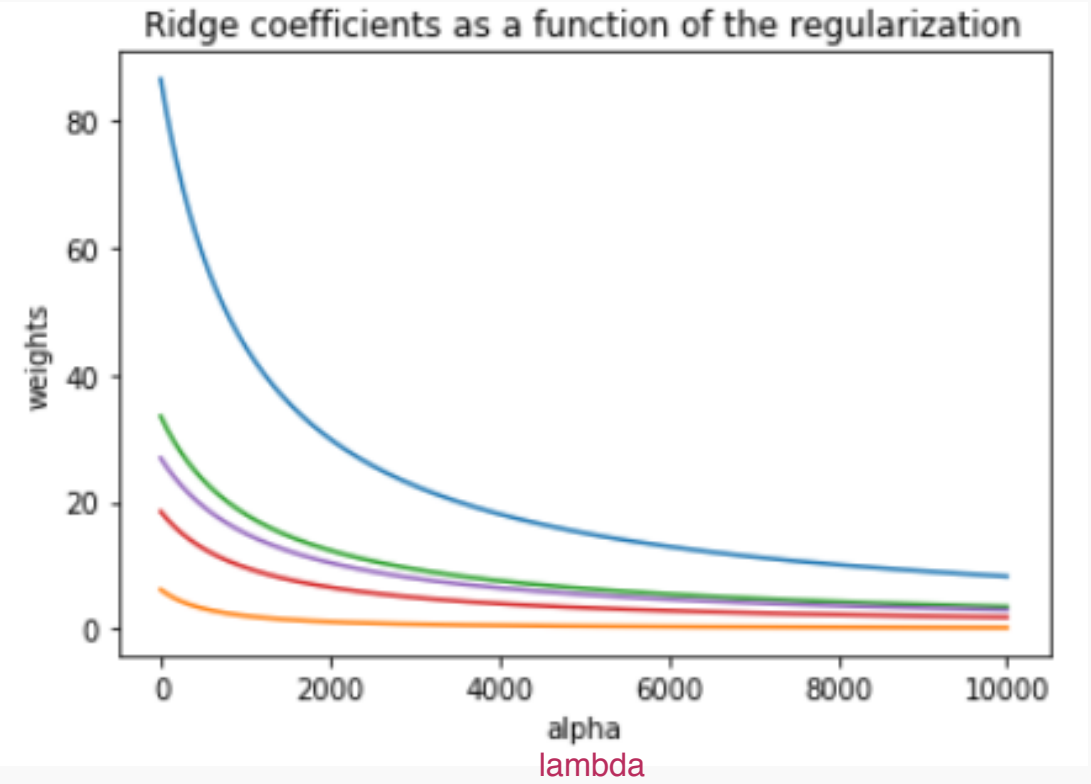
In [20]:
```
X_train = train[all_predictors].values
X_val = validation[all_predictors].values
X_test = test[all_predictors].values

ridge_regression = Ridge(alpha=1.0, fit_intercept=True)
ridge_regression.fit(np.vstack((X_train, X_val)), np.hstack((y_train, y_val)))

print('Ridge regression model:\n {} + {}^T . x'.format(ridge_regression.intercept_, ridge_regression.coe
```

```
Ridge regression model:
 -525.7662550875951 + [ 0.24007312  8.42566029  2.04098593 -0.04449172 -0.01227935  0.41902475
 -0.50397312 -4.47065168  4.99834262  0.          0.          0.29892679]^T . x
```

Ridge visualized

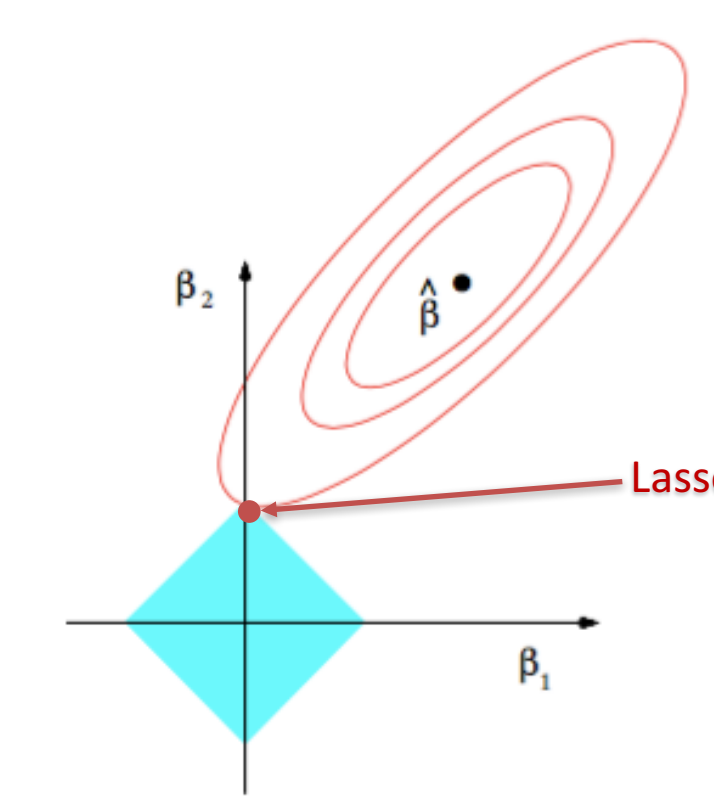


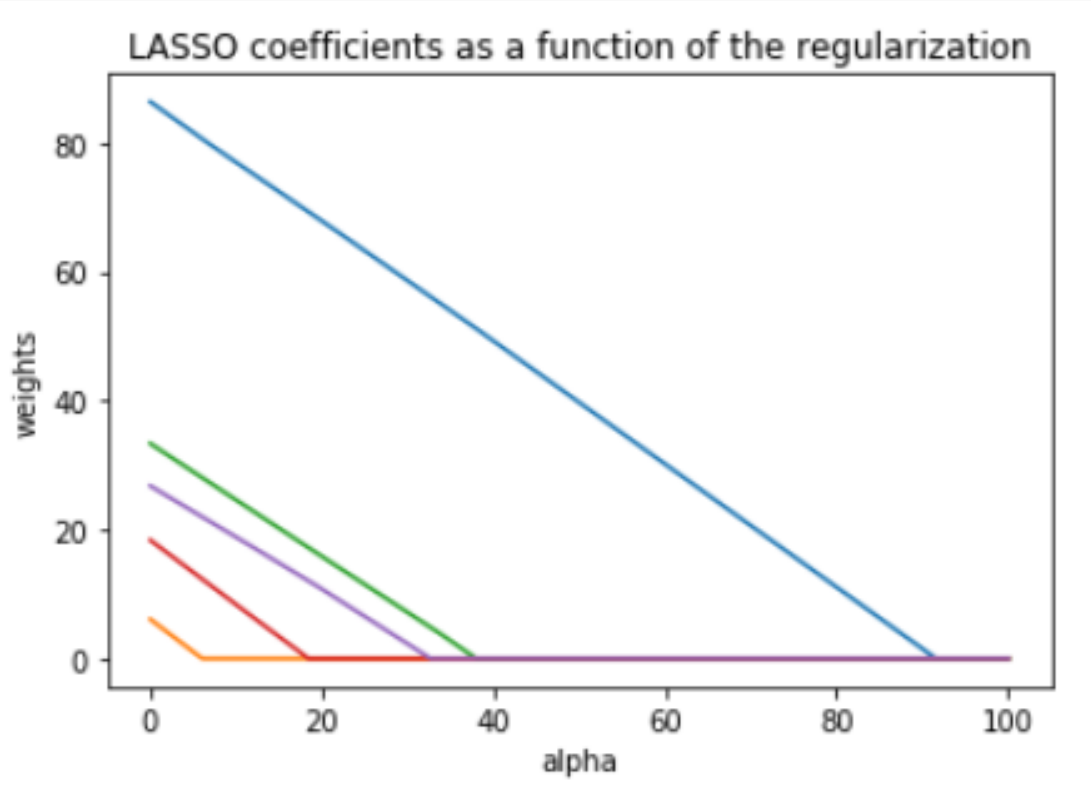
The ridge estimator is where the constraint and the loss intersect.



The values of the coefficients decrease as lambda increases, but they are not nullified.

LASSO visualized





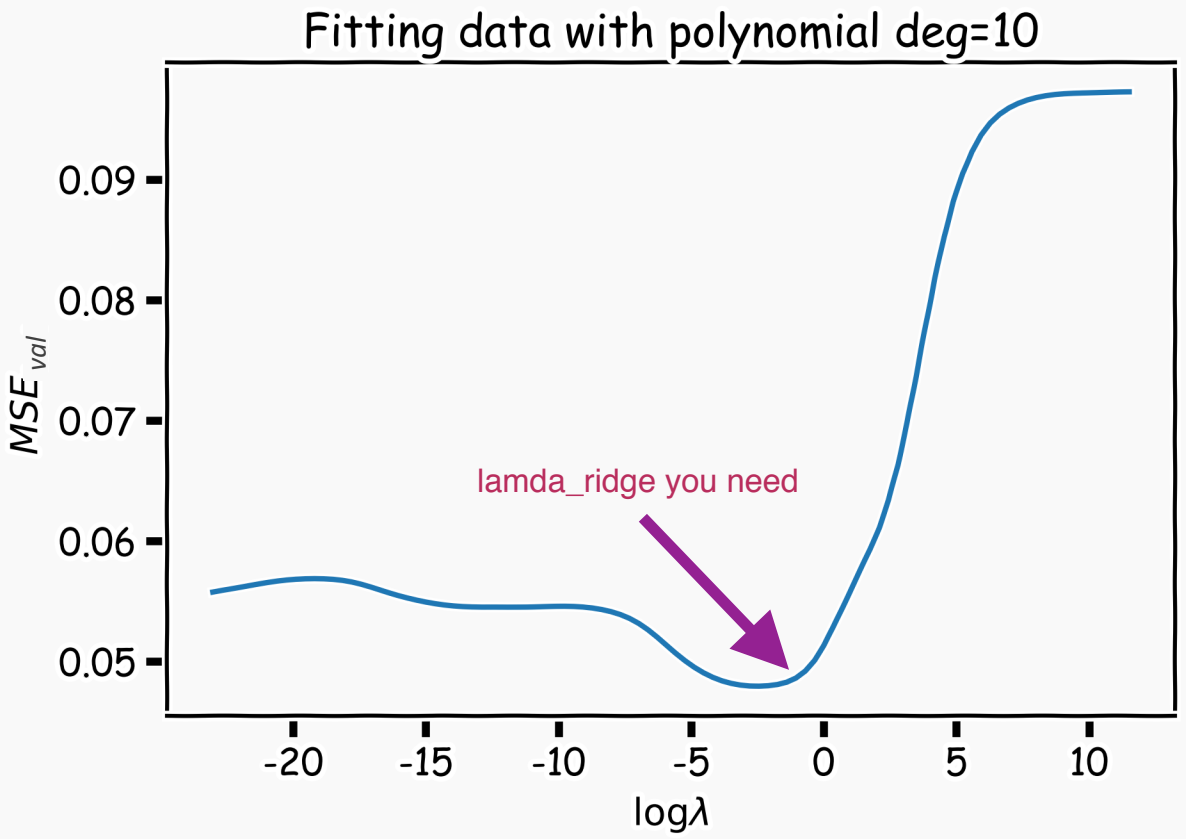
The Lasso estimator tends to zero out parameters as the OLS loss can easily intersect with the constraint on one of the axis.

The values of the coefficients decrease as lambda increases, and are nullified fast.

Ridge regularization with only **validation** : step by step

1. split data into $\{\{X,Y\}_{train}, \{X,Y\}_{validation}, \{X,Y\}_{test}\}$
2. for λ in $\{\lambda_{min}, \dots \lambda_{max}\}$: choose your min and max and go in log scale
    1. determine the β that minimizes the L_{ridge}, $\hat{\beta}_{Ridge}(\lambda) = \left(\mathrm{X}^{\mathrm{T}}\mathrm{X} + \lambda I\right)^{-1} X^T Y$, using the train data.
    2. record $L_{MSE}(\lambda)$ using validation data.
3. select the λ that minimizes the loss on the validation data,
$$\lambda_{ridge} = \mathrm{argmin}_{\lambda}\, L_{MSE}(\lambda)$$
4. Refit the model using both train and validation data, stick them together! $\{\{X,Y\}_{train}, \{X,Y\}_{validation}\}$, resulting to $\hat{\beta}_{ridge}(\lambda_{ridge})$
5. report MSE or R^2 on $\{X,Y\}_{test}$ given the $\hat{\beta}_{ridge}(\lambda_{ridge})$

Ridge regularization with **validation** only: step by step



Lasso regularization with **validation** only: step by step

1. split data into $\{\{X,Y\}_{train}, \{X,Y\}_{validation}, \{X,Y\}_{test}\}$
2. for λ in $\{\lambda_{min}, \dots \lambda_{max}\}$:
    A. determine the β that minimizes the L_{lasso}, $\hat{\beta}_{lasso}(\lambda)$, using the train data. **This is done using a solver.**
    B. record $L_{MSE}(\lambda)$ using validation data
3. select the λ that minimizes the loss on the validation data,
    $\lambda_{lasso} = \text{argmin}_{\lambda}\, L_{MSE}(\lambda)$
4. Refit the model using both train and validation data, $\{\{X,Y\}_{train}, \{X,Y\}_{validation}\}$, resulting to $\hat{\beta}_{lasso}(\lambda_{lasso})$
5. report MSE or R^2 on $\{X,Y\}_{test}$ given the $\hat{\beta}_{lasso}(\lambda_{lasso})$

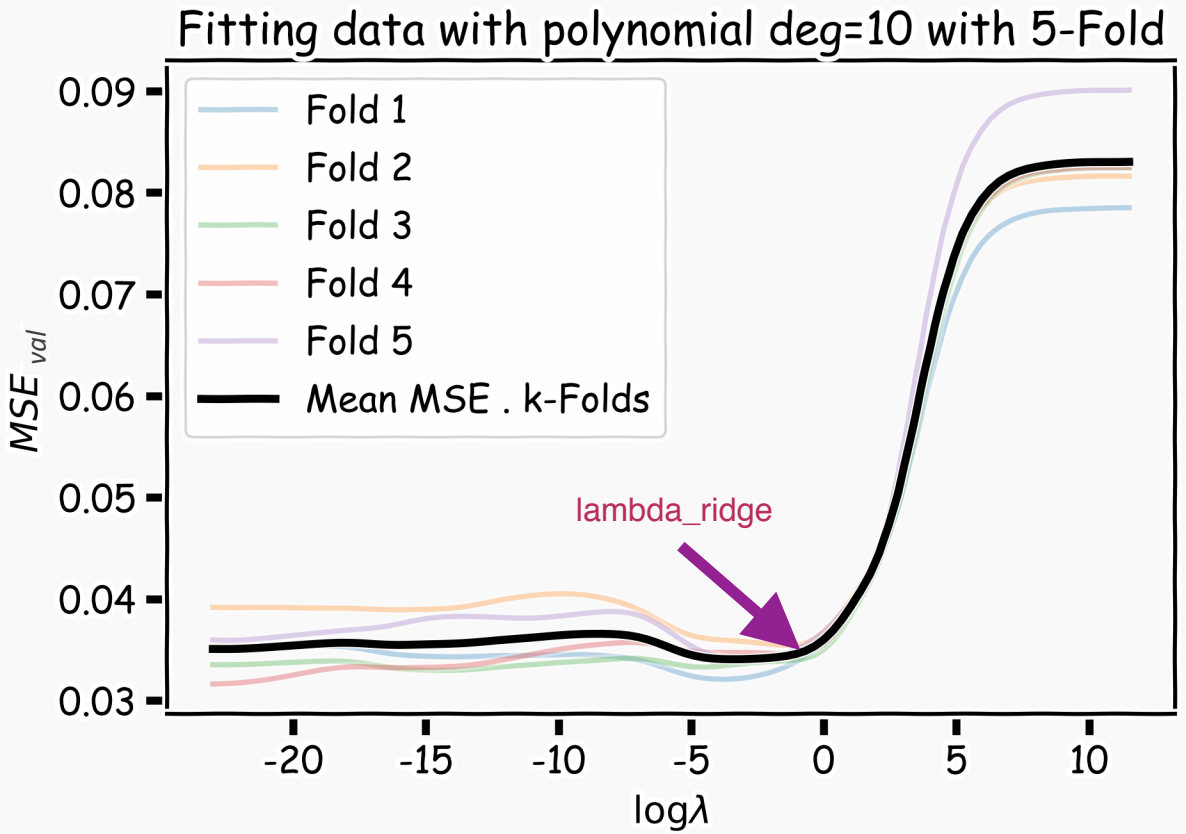
Ridge regularization with **CV**: step by step

	λ_1	λ_2	...	λ_n
k_1	L_{11}	L_{12}	..	...
k_2	L_{21}	...	..	...
...	..	...	..	...
k_n	...	...	...	...
E[]	$\bar{L}_1$	$\bar{L}_2$	...	$\bar{L}_n$

1. remove $\{X,Y\}_{test}$ from data
2. split the rest of data into K folds, $\{\{X,Y\}_{train}^{-k}, \{X,Y\}_{val}^{k}\}$
3. for k in $\{1,\ldots,K\}$ iterate over k folds
    1. for λ in $\{\lambda_0, \ldots, \lambda_n\}$: iterate over lambdas you chose
        A. determine the β that minimizes the L_{ridge}, $\hat{\beta}_{ridge}(\lambda,k) = \left(\mathrm{X}^{\mathrm{T}}\mathrm{X} + \lambda I\right)^{-1} X^T Y$, using the train data of the fold, $\{X,Y\}_{train}^{-k}$.
        B. record $L_{MSE}(\lambda,k)$ using the validation data of the fold $\{X,Y\}_{val}^{k}$

        At this point we have a 2-D matrix, rows are for different k, and columns are for different λ values.
4. Average the $L_{MSE}(\lambda,k)$ for each λ, $\bar{L}_{MSE}(\lambda)$.
5. Find the λ that minimizes the $\bar{L}_{MSE}(\lambda)$, resulting to λ_{ridge}.
6. Refit the model using the full training data, $\{\{X,Y\}_{train}, \{X,Y\}_{val}\}$, resulting to $\hat{\beta}_{ridge}(\lambda_{ridge})$
7. report MSE or R^2 on $\{X,Y\}_{test}$ given the $\hat{\beta}_{ridge}(\lambda_{ridge})$

Ridge regularization with **validation** only: step by step



Variable Selection as Regularization

Since LASSO regression tend to produce zero estimates for a number of model parameters - we say that LASSO solutions are **sparse** - we consider LASSO to be a method for variable selection.

Many prefer using LASSO for variable selection (as well as for suppressing extreme parameter values) rather than stepwise selection, as LASSO avoids the statistic problems that arises in stepwise selection.

Question: What are the pros and cons of the two approaches?

Quiz time: Lecture 8