Regularization Hyperparameters

Model Selection

Model selection is the application of a principled method to determine the complexity of the model, e.g., choosing a subset of predictors, choosing the degree of the polynomial model, etc.

A strong motivation for performing model selection is to avoid **overfitting,** which we saw can happen when:there are too many predictors, because:

1. there are too many predictors, because:
    - the feature space has high dimensionality
    - the polynomial degree is too high
    - too many interaction terms are considered
2. the coefficients' values are too **extreme**

We've already seen ways to address the problem of choosing predictors and polynomial degree using greedy algorithms and cross-validation. But what about the second potential source of overfitting? How do we discourage extreme coefficient values in the model parameters?

Regularization

What we want is low model error. We've been using mean squared error for our model's loss function:

$$\frac{1}{n}\sum_{i=1}^{n}|y_i - \beta^T x_i|^2$$

We also want to discourage extreme parameter values. We could also create a loss which is a function of the magnitudes of the model's parameters. We'll call this L_{reg}. We could do this in several ways. For example, we could sum the squares of the parameters or their absolute values.

$$L_{reg} = \begin{cases} \sum_{j=1}^{J} \beta^2 j \\ \sum_{j=1}^{J} |\beta_j| \end{cases}$$

Not that the summation index starts at 1. The model is not penalized for its β_0 which can be interpreted as the intercept.

Now we can combine these two loss functions into a single loss function for our model using **regularization**.

$$L = \frac{1}{n}\sum_{i=1}^{n}|y_i - \beta^T x_i|^2 + \lambda L_{reg}$$

λ is the **regularization parameter**. It controls the relative importance between model error and the regularization term.

$\lambda = 0$: equivalent to regression model using no regularization. $\lambda = \infty$: yields a model where all βs are 0.

But how do we determine which value of λ to use? The answer is with cross-validation! We will try many different values of λ and pick the one that gives us the best cross-validation loss scores

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Regularization: LASSO Regression

LASSO regression: minimize L_{LASSO} with respect to βs.

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

Note that $\sum_{j=1}^{J}|\beta_j|$ is the $L1$ norm of the β vector.

There's no need to regularize the bias, β_0, since it is not connected to the predictors.

Regularization: Ridge Regression

Ridge regression: minimize L_{RIDGE} with respect to βs.

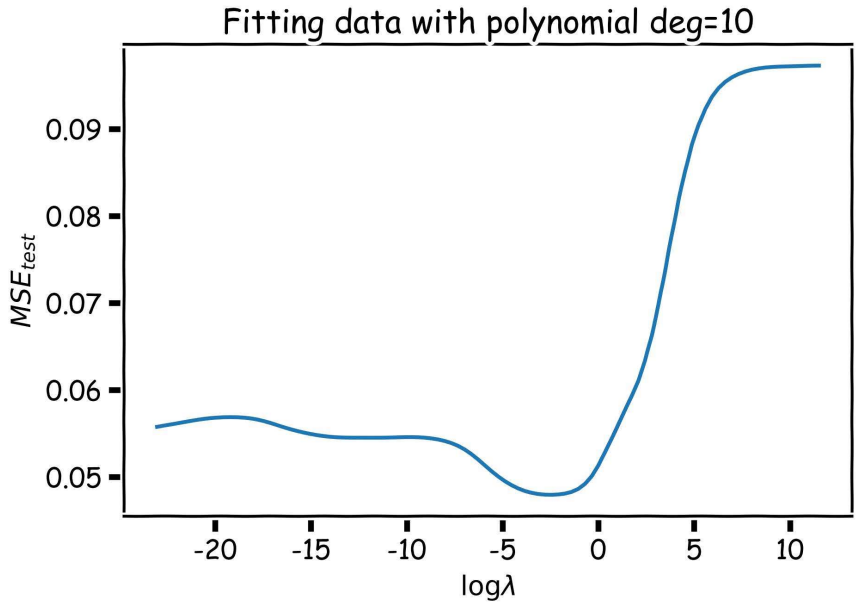
$$L_{RIDGE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \beta^T x_i|^2 + \lambda\sum_{j=1}^{J}\beta_j^2$$

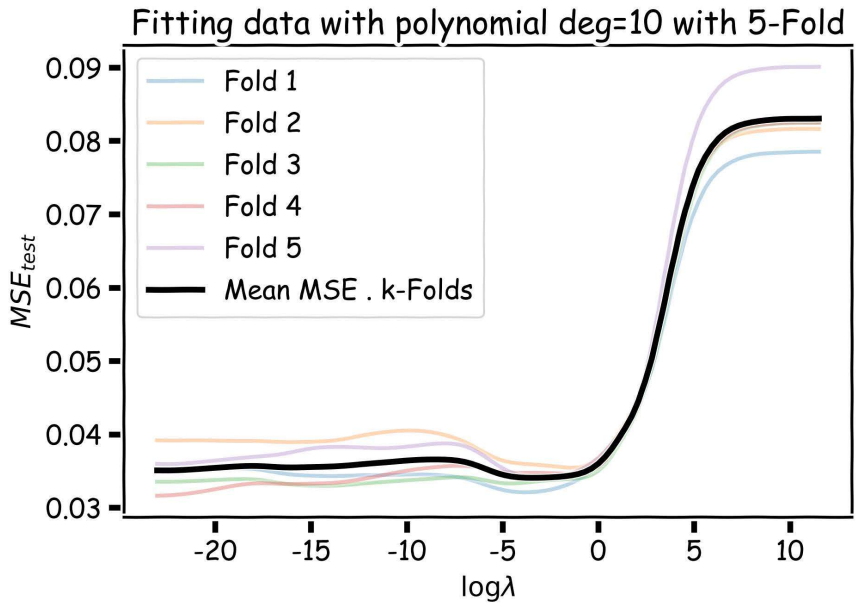
Note that $\sum_{j=1}^{J}\beta_j^2$ is the $L2$ norm of the β vetor.

Again we do not regularize the bias, β_0.

Ridge regularization with single validation set vs with cross-validation

To emphasize the usefulness of cross-validation, compare these two plots demonstrating ridge regularization using a single validation set and using cross-validation. Note how by taking the average of the 5 folds we can get more reliable results than relying on just one single validation split.





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