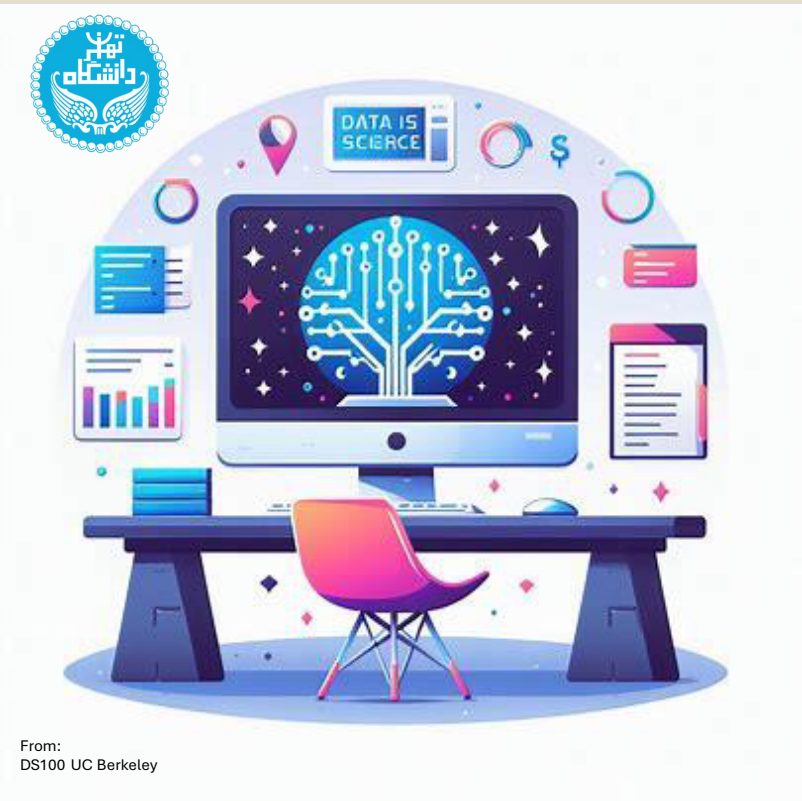

From:
DS100 UC Berkeley

Cross-validation and Regularization

Introduction to Data Science
Spring 1403

Yadollah Yaghoobzadeh

Goals for this Lecture

Circling back to two questions raised in the modeling lectures:

- How does model performance change on "seen" vs. "unseen" data?
- How do we control model complexity?

Agenda

Cross-Validation

- Training, Test, and Validation Sets
- K-Fold Cross-Validation

Regularization

- Constraining Model Parameters
- L2 Regularization (Ridge)
- L1 Regularization (LASSO)

Training, Test, and Validation Sets

Cross-Validation

- **Training, Test, and Validation Sets**
- K-Fold Cross-Validation

Regularization

- Constraining Model Parameters
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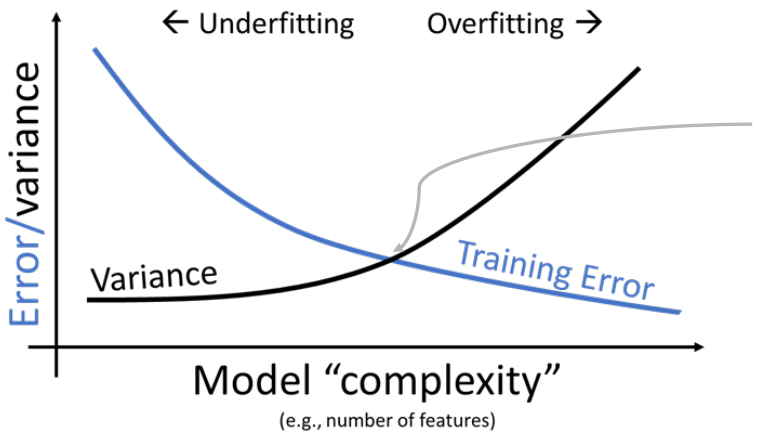
- L1 Regularization (LASSO)

Where We Left Things



Our goal: find this "sweet spot"

Stay tuned for ~30 min from now

Where We Left Things

First half of lecture: **Cross-Validation**

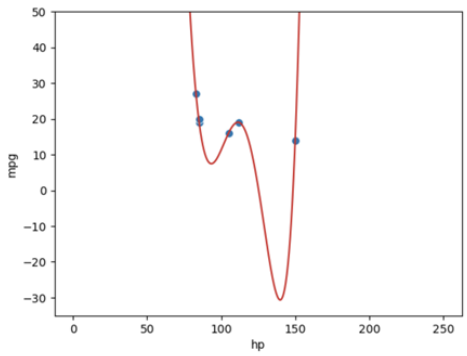
- Formalize the idea of training and test data.
- Introduce a method to "preview" how a model will perform on unseen data.

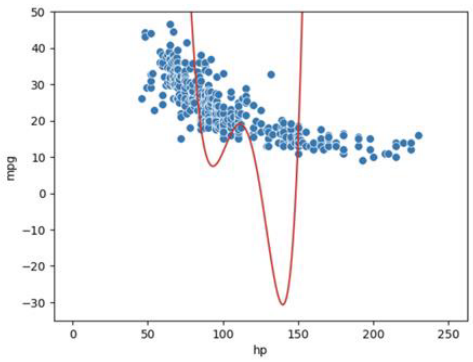
Second half of lecture: **Regularization**

- Introduce a method to finetune our model's complexity.

Where We Left Things

A complex model may not perform well on data it did not encounter during training.





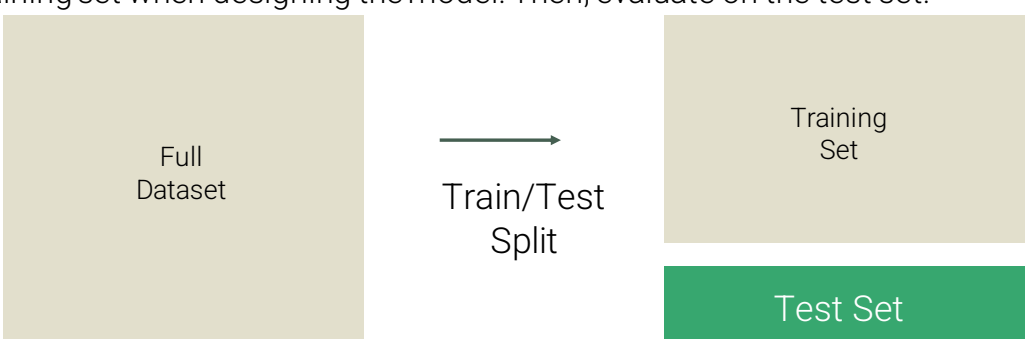
How to quantify performance on this "unseen" data? Introduce a **test set**.

Test Sets

A **test set** is a portion of our dataset that we set aside for testing purposes.

- We do *not* consider the test set when fitting/training the model.
- The test set is only ever touched once: to compute the performance (MSE, RMSE, etc) of the model *after* all fine-tuning has been completed.

Our new workflow for modeling: First, perform a **train-test split** (see documentation). Consider only the training set when designing the model. Then, evaluate on the test set.



Validation Sets

What if we were dissatisfied with our test set performance?

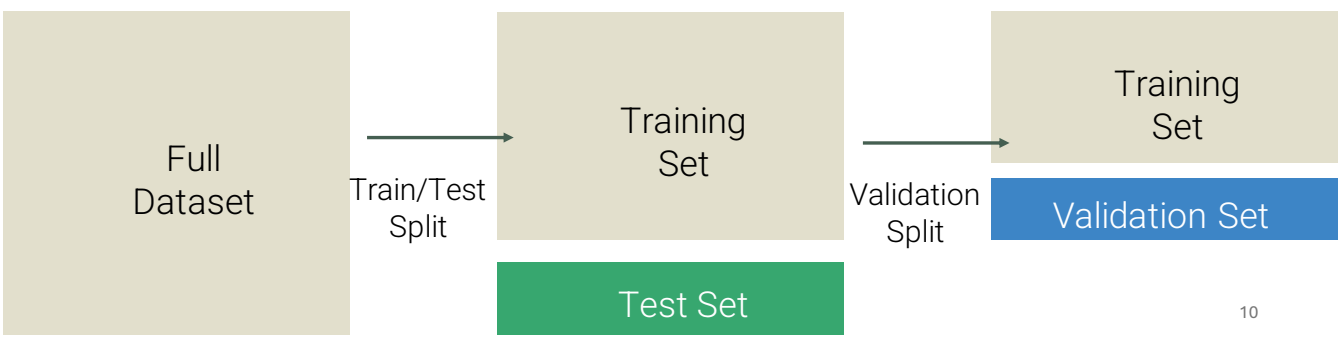
In our current framework, we'd be stuck – we can't then go back and adjust our model, because we'd be *factoring in information from the test set* to design our model. The test set would no longer represent performance on unseen data.

Solution: introduce a **validation set**.

Validation Sets

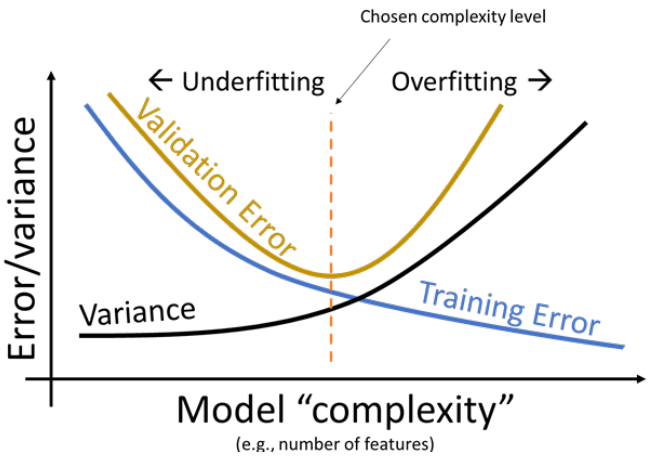
A **validation set** is a portion of our *training set* that we set aside for assessing model performance while it is *still being developed*.

- Train model on the training set. Assess performance on the validation set. Adjust the model, then repeat.
- After *all* model development is complete, assess final performance on the test set.

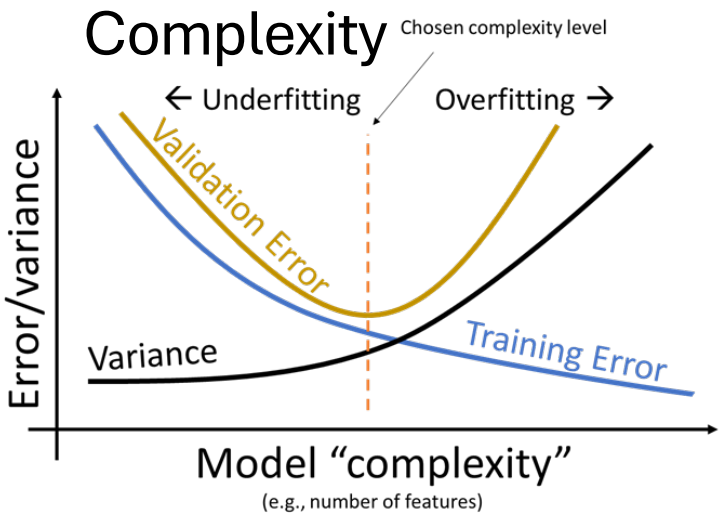


Updating Our Understanding of Model Complexity

Computing the validation error allows us to visualize under- and overfitting.



Updating Our Understanding of Model Complexity



In Lectures 17 and 18, we'll learn the mathematical origins of these relationships

Typically, as model complexity increases:

- Training error decreases
- Variance increases
- Error on validation set decreases, then increases

Our goal: Choose the model complexity that minimizes validation error.

We will discuss how in the second half of lecture.

K-Fold Cross-Validation

Cross-Validation

- Training, Test, and Validation Sets
- **K-Fold Cross-Validation**

Regularization

- Constraining Model Parameters
- L1 Regularization (LASSO)
- L2 Regularization (Ridge)

Another View of Validation

Introducing a validation set gave us one "extra" chance to assess model performance.

Specifically, now we understand how the model performs on *one* particular set of unseen data.

- It's possible that we may have, by random chance, selected a set of validation points that was *not* representative of other unseen data that the model might encounter.

Ideally: Assess model performance on *several* different validation sets before touching the test set.

```
Val error from train/validation split #1: 14.6104005581132
Val error from train/validation split #2: 24.755706579814404
Val error from train/validation split #3: 22.23208329959848
```

Validation Folds

In our original validation split, we set aside x% of the training data to use for validation.

- For example, 20% of the training data is used for validation

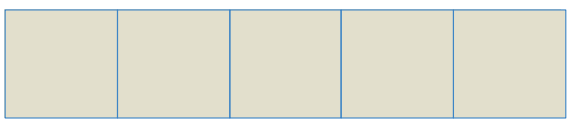
We could have selected *any* 20% portion of the training data for validation.

In total, there are 5 non-overlapping "chunks" of datapoints we could set aside for validation.

Validation Folds

The common term for one of these chunks is a "fold".

- Our training data has 5 folds, each containing 20% of the datapoints.



Another perspective: we actually have 5 validation sets "hidden" in our training set.

In **cross-validation**, we perform validation splits for *each* of these folds.

K-Fold Cross-Validation

For a dataset with K folds:

- Pick one fold to be the validation fold.
- Train model on data from every fold *other* than the validation fold.
- Compute the model's error on the validation fold and record it.
- Repeat for all K folds.

The **cross-validation error** is the average error across all K validation fo

Train model on all other folds

Compute MSE on V_1

Validation error #1

Validation error #2

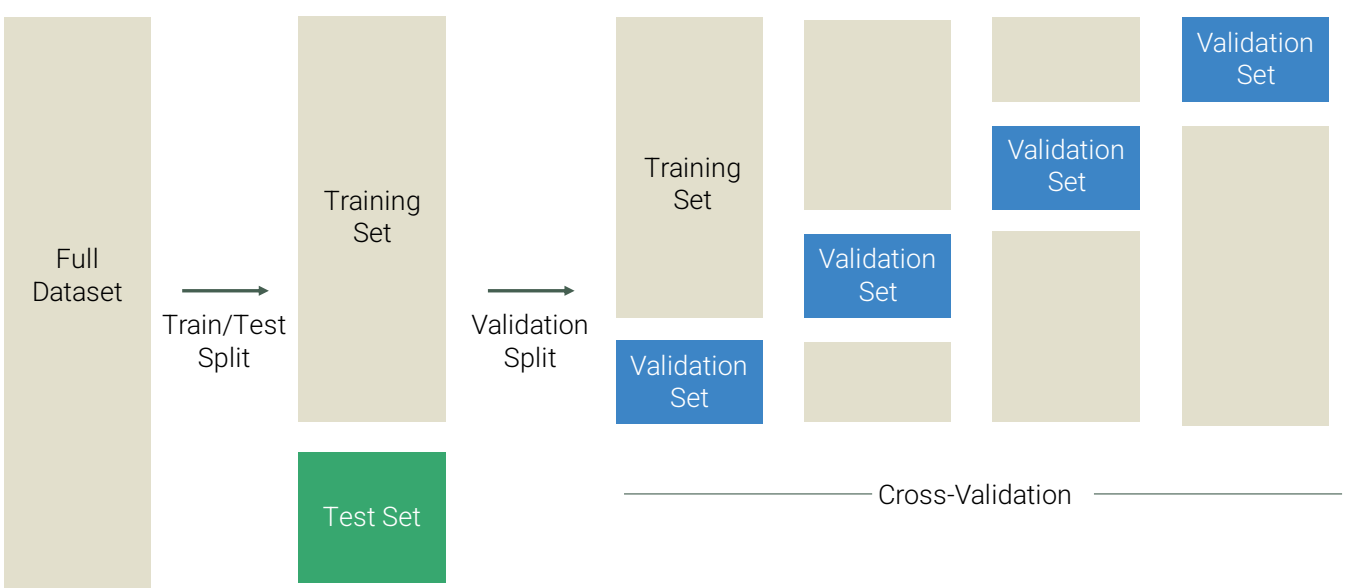
Validation error #3

Validation error #4

Validation error #5

Cross-validation error = mean of validation

Model Selection Workflow



Hyperparameters

Cross-validation is often used for **hyperparameter** selection.

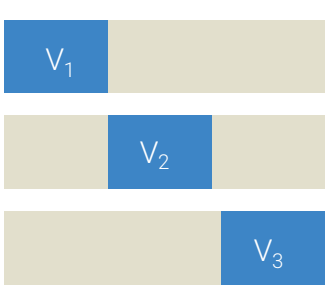
Hyperparameter: Value in a model chosen *before* the model is fit to data.

- Cannot solve for hyperparameters via calculus, OLS, gradient descent, etc – we must choose it ourselves.
- Examples
  - Degree of polynomial model
  - Gradient descent learning rate,
  - Regularization penalty, (to be introduced later this lecture)

Hyperparameter Tuning

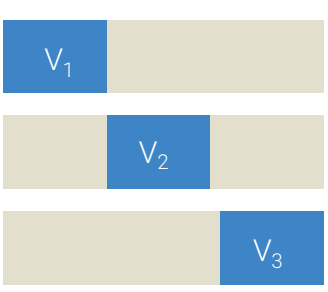
- To select a hyperparameter value via cross-validation:
- List out several different "guesses" for the best hyperparameter.
- For each guess, run cross-validation to compute the CV error for that choice of hyperparameter value.
- Select the hyperparameter value with lowest CV error.

$\alpha = 0.1$



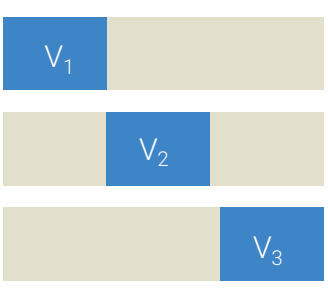
CV error: 4.67

$\alpha = 1$



CV error: 7.01

$\alpha = 10$



CV error: 10.22

Constraining Model Parameters

Cross-Validation

- Training, Test, and Validation Sets
- K-Fold Cross-Validation

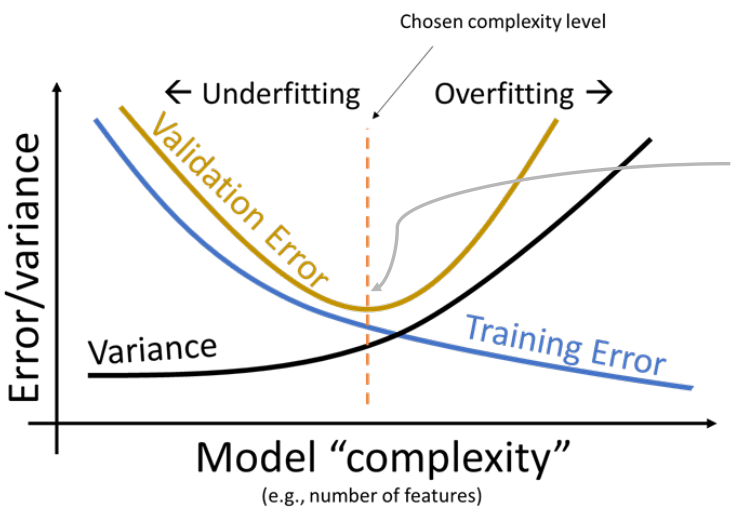
Regularization

- **Constraining Model Parameters**
- L2 Regularization (Ridge)
- L1 Regularization (LASSO)

Restricting Model Complexity

We've seen now that model complexity needs to be chosen carefully:

- Too complex: model overfits – "memorizes" training data too closely.
- Too simple: model underfits – does not take full advantage of the features available in the dataset.



Our goal: find this "sweet spot"

How do we control complexity?

Restricting Model Complexity

Idea: Only use each feature "a little" in the model.

$$\hat{\mathbb{Y}} = \theta_0 + \theta_1\phi_1 + \theta_2\phi_2 \ldots + \theta_p\phi_p$$

- If we restrict how large each parameter θ_i can be, we restrict how much each feature contributes to the model.
- When θ_i is close to or equal to 0, the model decreases in complexity because feature ϕ_i barely impacts the prediction.

In **regularization**, we restrict complexity by *putting a limit* on the magnitudes of the model parameters θ_i .

Restricting Model Complexity

In **regularization**, we restrict complexity by *putting a limit* on the magnitudes of the model parameters θ_i .

Example: Suppose we specify that the sum of all absolute parameters can be no larger than some number Q

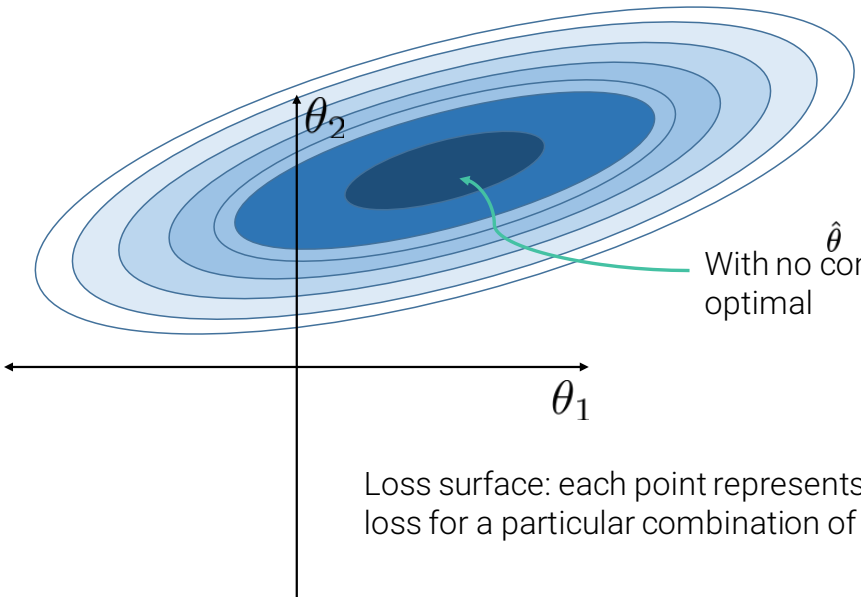
$$\sum_{i=1}^{p} |\theta_i| \leq Q$$

We've given the model a "budget" for how much weight to assign to each feature. Some parameters θ_i will need to be small in value so the sum remains below Q.

Note that the intercept term, θ_0, is typically excluded from this constraint.

Think Back to Gradient Descent

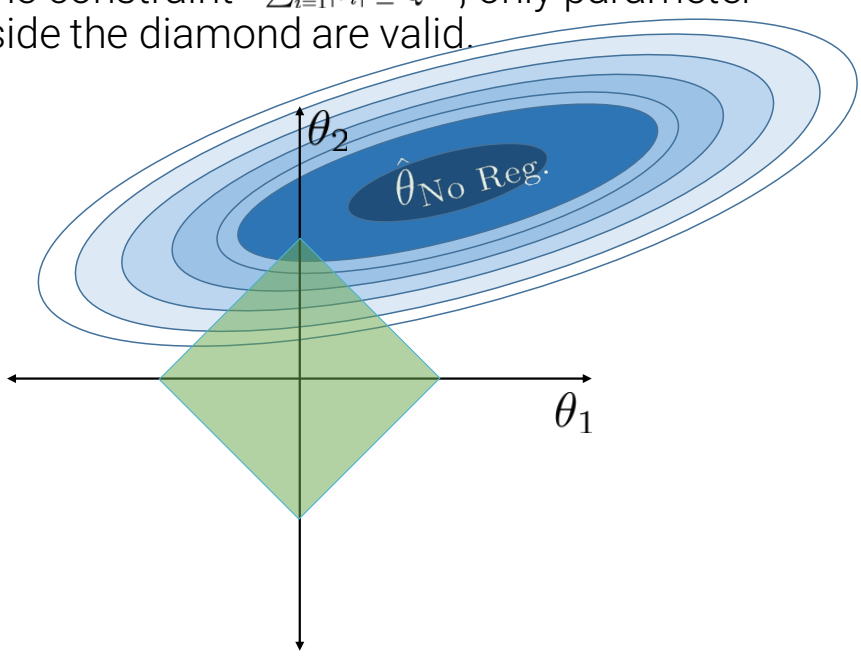
In gradient descent: visualize the loss surface as a contour map. Our goal is to find the combination of parameters that gives the lowest loss.



Loss surface: each point represents the model's loss for a particular combination of θ_1, θ_2.

Constraining Model Parameters

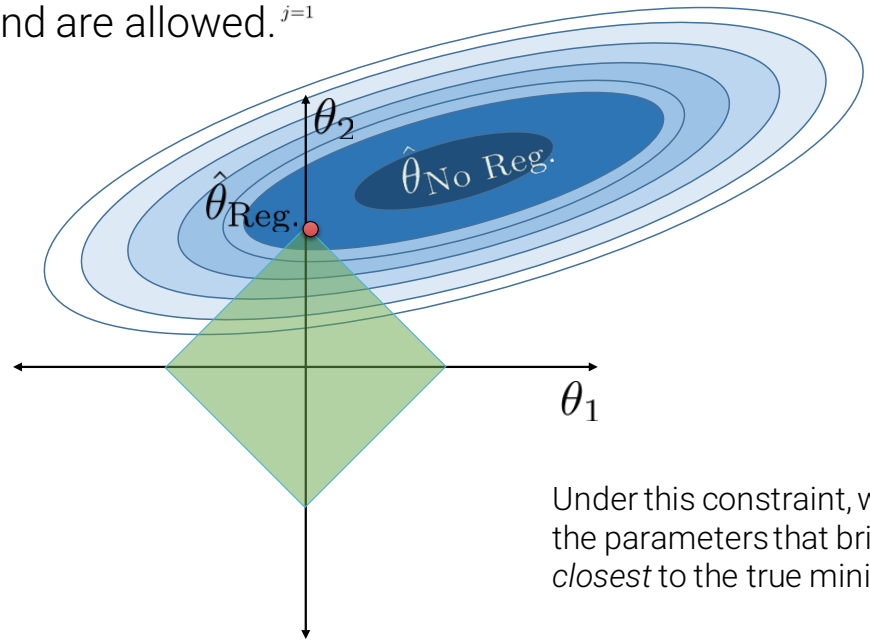
When we apply the constraint $\sum_{i=1}^{p} |\theta_i| \leq Q$, only parameter combinations inside the diamond are valid.



Q is some arbitrary number.

Constraining Model Parameters

When we apply the constraint $\sum_{j=1}^{d} |\theta_j| \leq Q$, only parameter combinations inside the diamond are allowed.

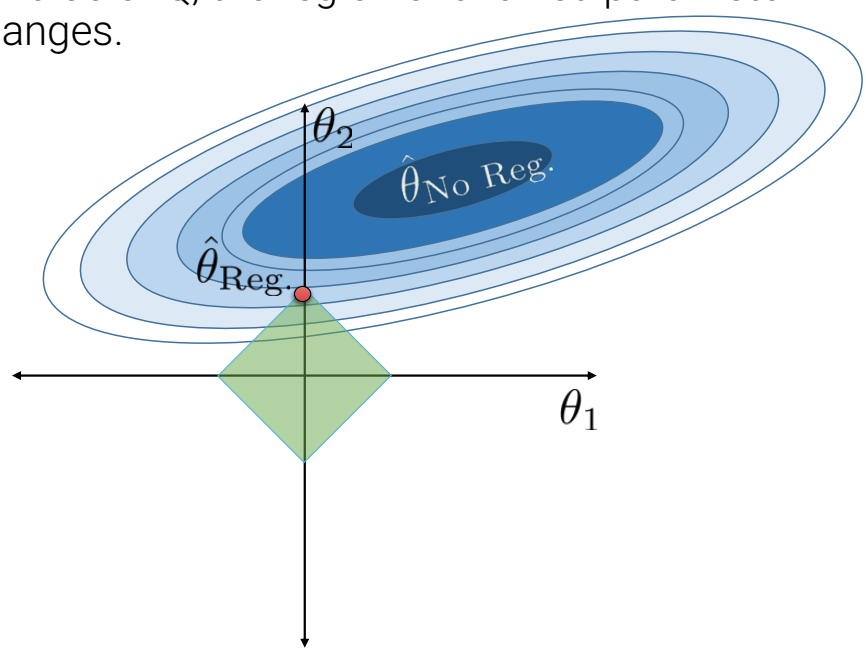


Under this constraint, we choose the parameters that bring us *closest* to the true minimum loss.

Q is some arbitrary number.

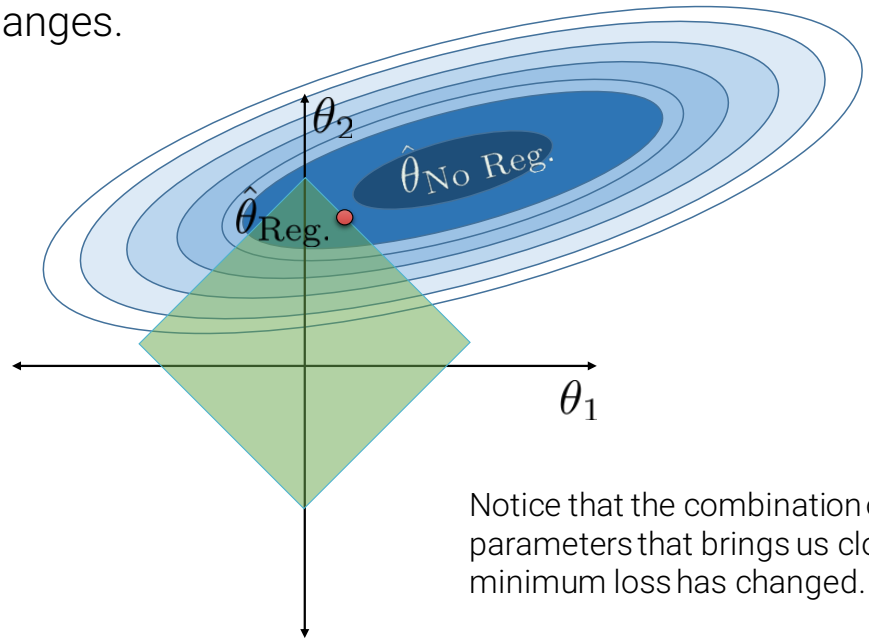
Smaller Q

If we change the value of Q, the region of allowed parameter combinations changes.



Larger Q

If we change the value of Q, the region of allowed parameter combinations changes.

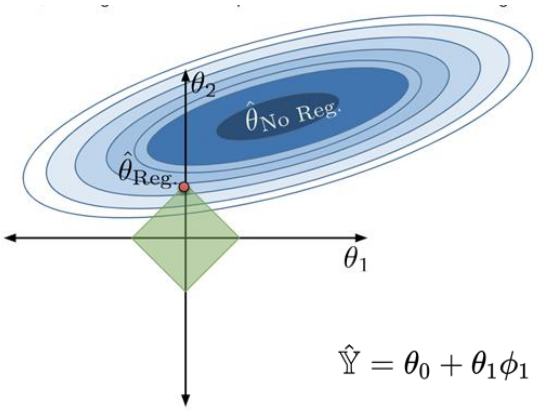


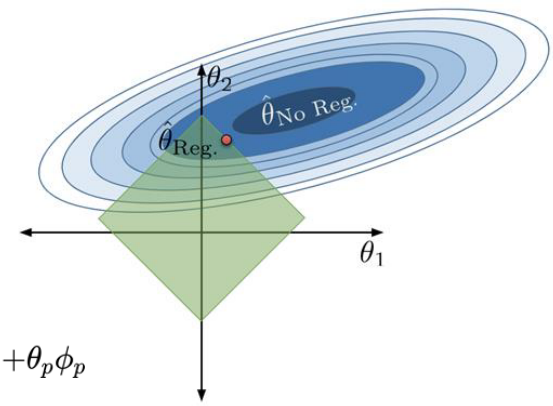
Notice that the combination of model parameters that brings us closest to minimum loss has changed.

How does the size of Q relate to model complexity?

Size of Q

If we change the value of Q, the region of allowed parameter combinations changes.





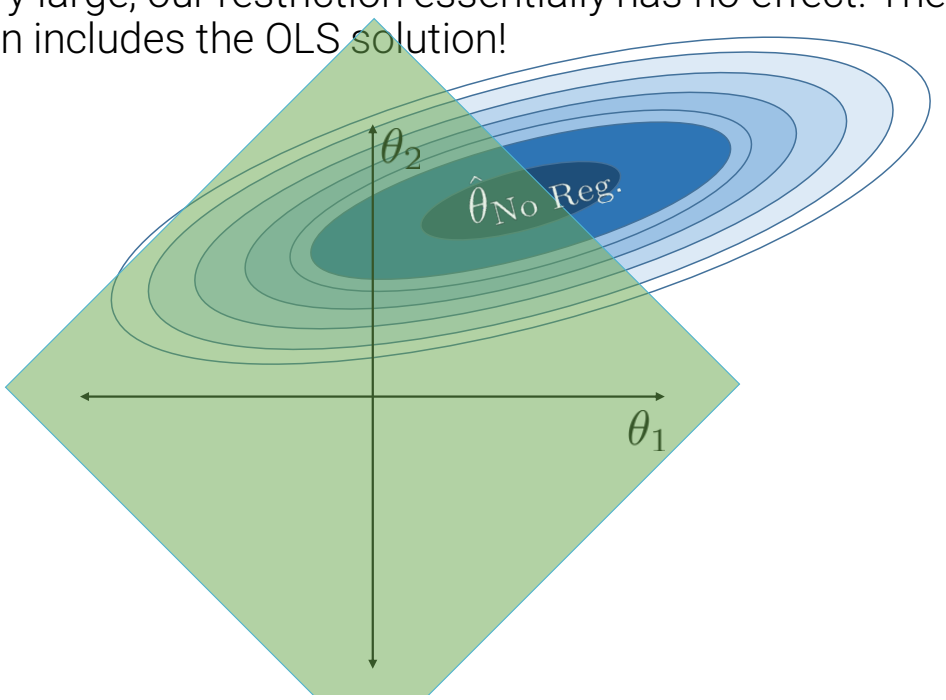
$$\hat{Y} = \theta_0 + \theta_1\phi_1 + \theta_2\phi_2 \ldots + \theta_p\phi_p$$

Small Q: θ_i are small in value; feature ϕ_i only contributes a little to the model → model becomes simpler.

Large Q: θ_i are large in value; feature ϕ_i contributes more to the model → model becomes more complex.

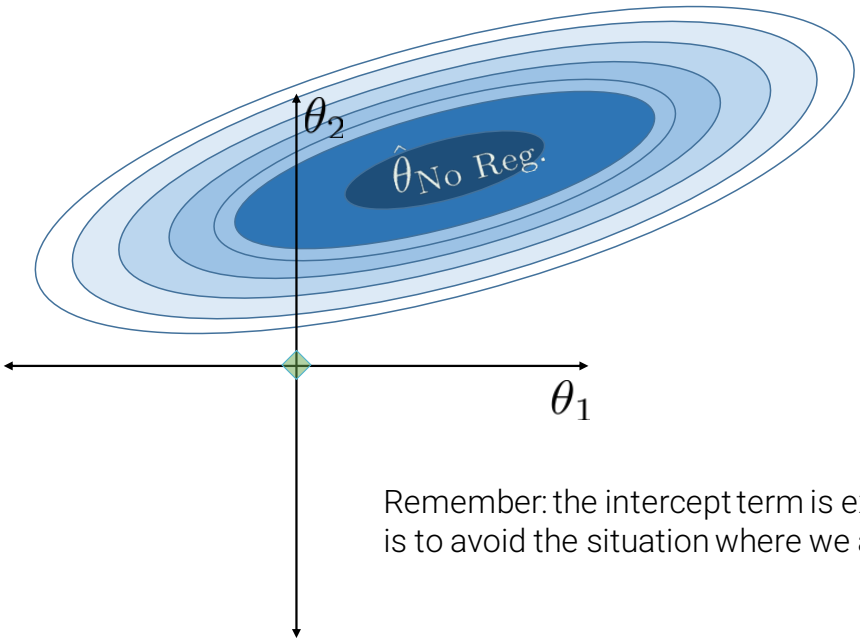
Size of Q

When Q is very large, our restriction essentially has no effect. The allowed region includes the OLS solution!



Size of Q

When Q is very small, parameters are set to (essentially) 0.



If the model has no intercept term:

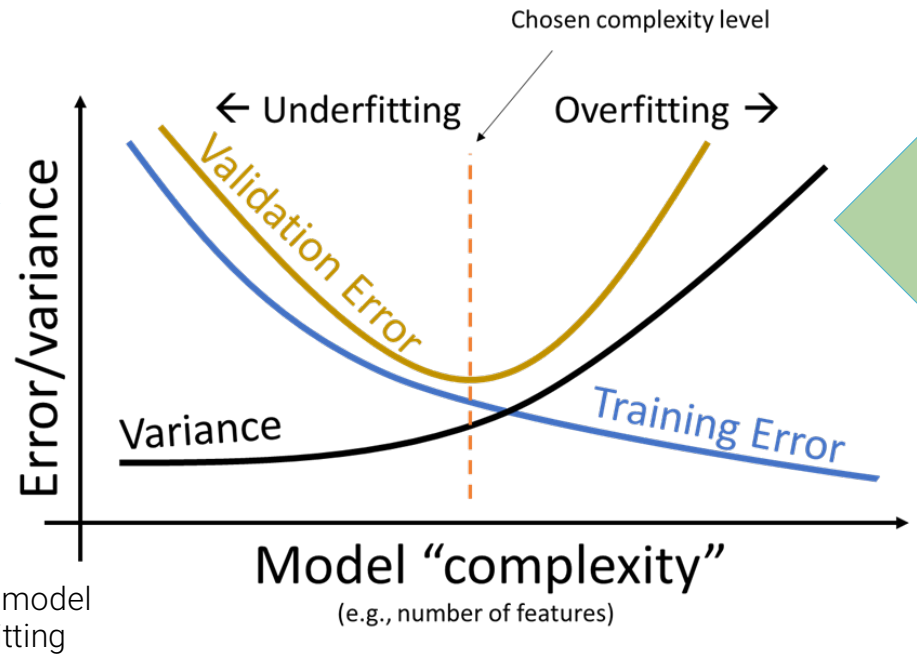
$$\hat{Y} = (0)\phi_1 + (0)\phi_2 + \ldots = 0$$

If the model has an intercept term:

$$\hat{Y} = \theta_0 + (0)\phi_1 + (0)\phi_2 + \ldots = \theta_0$$

Remember: the intercept term is excluded from the constraint – this is to avoid the situation where we always predict 0.

Complexity and Q



Small Q:

- Simple model
- Underfitting

Large Q:

- Complex model
- Overfitting

L1 Regularization (LASSO)

Cross-Validation

- Training, Test, and Validation Sets
- K-Fold Cross-Validation

Regularization

- Constraining Model Parameters
- **L1 Regularization (LASSO)**
- L2 Regularization (Ridge)

L1 Regularization

How do we actually apply our constraint $\sum_{i=1}^{p}|\theta_i| \leq Q$?

Recall our OLS framework: Find thetas that minimize the objective function:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_p\phi_{i,p}))^2$$

In **L1 regularization:** Find thetas that minimize the objective function:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_p\phi_{i,p}))^2 \quad \textbf{such that} \quad \sum_{i=1}^{p}|\theta_i| \leq Q$$

L1 Regularization

By the Lagrangian Duality*, these two problems are equivalent.

Our original problem: find thetas that minimize the objective function:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i-(\theta_0+\theta_1\phi_{i,1}+\ldots+\theta_p\phi_{i,p}))^2 \quad \textbf{such that} \quad \sum_{i=1}^{p}|\theta_i| \leq Q$$

Equivalent problem: find thetas that minimize the ***augmented*** **objective function:**

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-(\theta_0+\theta_1\phi_{i,1}+\ldots+\theta_p\phi_{i,p}))^2 + \lambda\sum_{i=1}^{p}|\theta_i|$$

L1 Regularization

In L1 regularization, we find thetas that minimize our **new objective function:**

$$\underbrace{\frac{1}{n}\sum_{i=1}^{n}(y_i-(\theta_0+\theta_1\phi_{i,1}+\ldots+\theta_p\phi_{i,p}))^2}_{\text{Keep MSE on the data low...}} + \underbrace{\lambda\sum_{i=1}^{p}|\theta_i|}_{\text{...while also keeping the size of parameters small}}$$

λ is the **regularization penalty hyperparameter**. When λ is large, our objective function is penalized more for choosing larger thetas → model will adjust by reducing thetas and decreasing complexity.

- How to choose the value for λ? Cross-validation!

L1 regularization is also called LASSO: "least absolute shrinkage and selection operator".

LASSO and Feature Selection

The optimal parameters for a LASSO model tend to include a lot of zeroes! In other words, LASSO effectively **selects only a subset** of the features.

- We often use L1 regularization for **feature selection** – the features with non-zero parameters are more informative for modeling than those with parameters set to zero.
- Intuition: We can get closer to the lowest loss contour at a corner of our constraint diamond.

LASSO: "least absolute **shrinkage** and **selection** operator"

Shrink parameter sizes

Select important features

One Issue With Our Approach

Our dataset has features with wildly different numerical scales!

	hp	hp^2	hp^3	hp^4	hp^5	hp^6	hp^7	hp^8
72	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
89	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
92	158.0	24964.0	3944312.0	6.232013e+08	9.846580e+10	1.555760e+13	2.458100e+15	3.883799e+17
124	180.0	32400.0	5832000.0	1.049760e+09	1.889568e+11	3.401222e+13	6.122200e+15	1.101996e+18
88	137.0	18769.0	2571353.0	3.522754e+08	4.826172e+10	6.611856e+12	9.058243e+14	1.240979e+17
...	...	...	...	...	...	...	...	...
2	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
104	167.0	27889.0	4657463.0	7.777963e+08	1.298920e+11	2.169196e+13	3.622558e+15	6.049671e+17
159	148.0	21904.0	3241792.0	4.797852e+08	7.100821e+10	1.050922e+13	1.555364e+15	2.301939e+17
180	115.0	13225.0	1520875.0	1.749006e+08	2.011357e+10	2.313061e+12	2.660020e+14	3.059023e+16
394	52.0	2704.0	140608.0	7.311616e+06	3.802040e+08	1.977061e+10	1.028072e+12	5.345973e+13

Coefficients From Earlier

	hp	hp^2	hp^3	hp^4	hp^5	hp^6	hp^7	hp^8
72	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
89	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
92	158.0	24964.0	3944312.0	6.232013e+08	9.846580e+10	1.555760e+13	2.458100e+15	3.883799e+17
124	180.0	32400.0	5832000.0	1.049760e+09	1.889568e+11	3.401222e+13	6.122200e+15	1.101996e+18
88	137.0	18769.0	2571353.0	3.522754e+08	4.826172e+10	6.611856e+12	9.058243e+14	1.240979e+17
...	...	...	...	...	...	...	...	...
2	150.0	22500.0	3375000.0	5.062500e+08	7.593750e+10	1.139062e+13	1.708594e+15	2.562891e+17
104	167.0	27889.0	4657463.0	7.777963e+08	1.298920e+11	2.169196e+13	3.622558e+15	6.049671e+17
159	148.0	21904.0	3241792.0	4.797852e+08	7.100821e+10	1.050922e+13	1.555364e+15	2.301939e+17
180	115.0	13225.0	1520875.0	1.749006e+08	2.011357e+10	2.313061e+12	2.660020e+14	3.059023e+16
394	52.0	2704.0	140608.0	7.311616e+06	3.802040e+08	1.977061e+10	1.028072e+12	5.345973e+13

```
lasso_model.coef_
```

```
array([-5.14100640e-01,  1.16422594e-03,  2.70209864e-06, -8.05153574e-10,
       -2.78280269e-11, -1.02040718e-13, -5.44295812e-17,  1.83589942e-18])
```


Pitfalls of Unscaled Data

Our model parameter for a feature with small numeric values (hp) is much, much larger than the parameter for a feature with large numeric values (hp^8).

- The feature with larger values will naturally contribute more to the predicted y_hat for each observation.
- The LASSO model needs to "spend" more of its parameter budget to allow hp to have much of an impact on each prediction.

First datapoint: $\hat{y}_i = \theta_0 + \theta_1(150) + \ldots + \theta_8\left(2.56 \times 10^{17}\right)$

The large values of hp^8 dominate the prediction.

$$\hat{y}_i = \theta_0 - 0.51(150) + \ldots + 1.84 \times 10^{-18}\left(2.56 \times 10^{17}\right)$$

The parameter for hp must be very large for hp to influence the prediction.

Making Things Fair

Ideally, our data should all be on the same scale.

- One approach: Standardize the data, i.e., replace everything with its Z-score.

$$z_k = \frac{x_k - \mu_k}{\sigma_k}$$

- Resulting features will be all on the same scale with mean 0 and SD 1.

L2 Regularization (Ridge)

Cross-Validation

- Training, Test, and Validation Sets
- K-Fold Cross-Validation

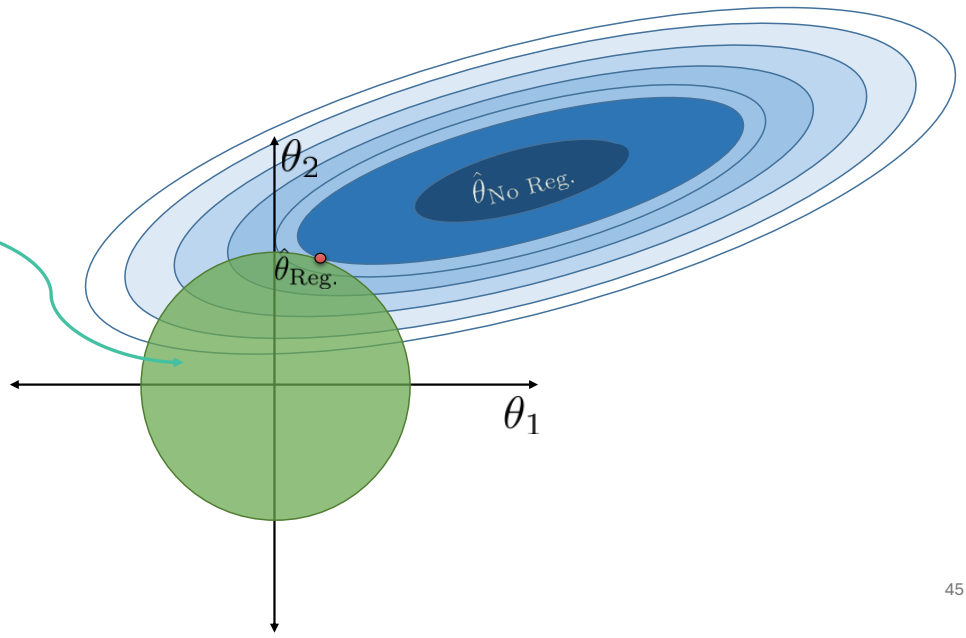
Regularization

- Constraining Model Parameters
- L1 Regularization (LASSO)
- **L2 Regularization (Ridge)**

Changing The Constraint

We could have applied a different constraint to our parameters: the sum of their *squares* must be less than some number Q.

$$\sum_{i=1}^{p} \theta_i^2 \leq Q$$



L2 Regularization

As with L1 regularization, we can express this constraint in two forms:

Original formulation:

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_p\phi_{i,p})\right)^2 \quad \textbf{such that} \quad \sum_{i=1}^{p}\theta_i^2 \leq Q$$

L2 objective function:

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_p\phi_{i,p})\right)^2 + \lambda\sum_{i=1}^{p}\theta_i^2$$

L2 Regularization

In L2 regularization, we find thetas that minimize our **new objective function:**

$$\underbrace{\frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_p\phi_{i,p})\right)^2}_{\text{Keep MSE on the data low...}} + \underbrace{\lambda\sum_{i=1}^{p}\theta_i^2}_{\text{...while also keeping the size of parameters small}}$$

L2 regularization is commonly called **ridge regression**.

Regularization for other models

- We can add the same L1 and L2 regularizations any loss function
  - Logistic regression
  - Neural networks