Lecture 15

Cross Validation, Regularization

Different methods for ensuring the generalizability of our models to unseen data.

Today's Roadmap

Cross Validation

- **The Holdout Method**
- K-Fold Cross Validation
- Test Sets

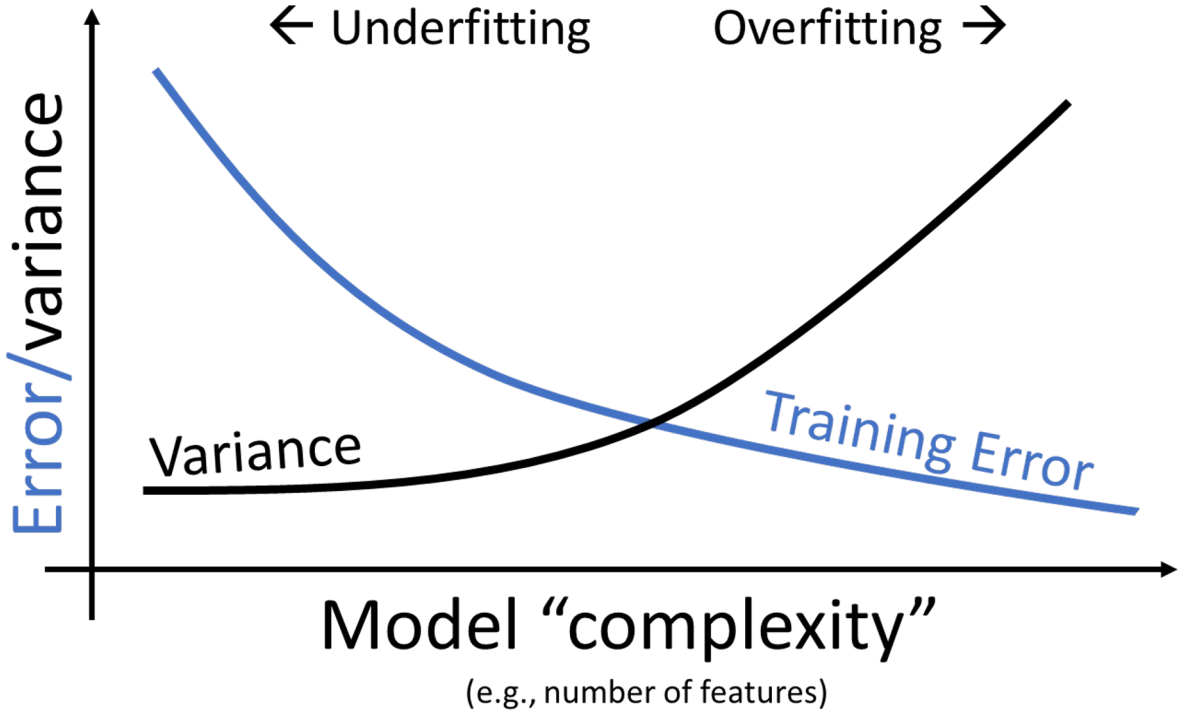
Regularization

- L2 Regularization (Ridge)
- Scaling Data for Regularization
- L1 Regularization (LASSO)

Review: Error vs. Complexity

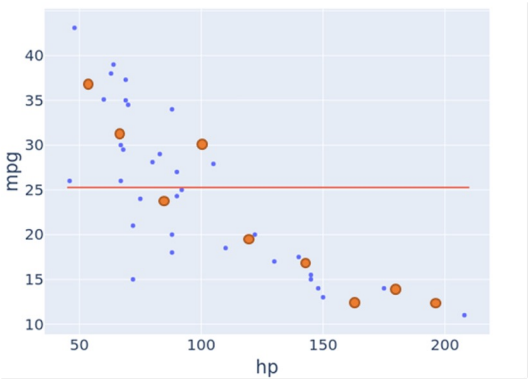
As we increase the complexity of our model:

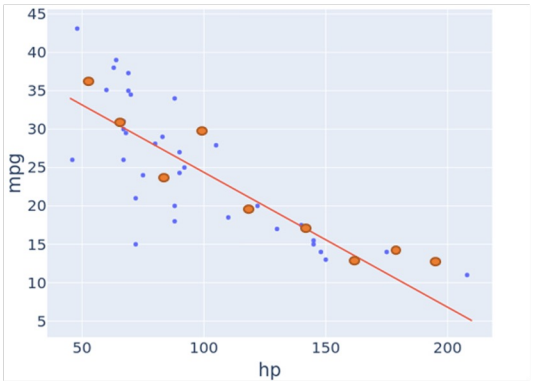
- Training error decreases.
- Variance increases.

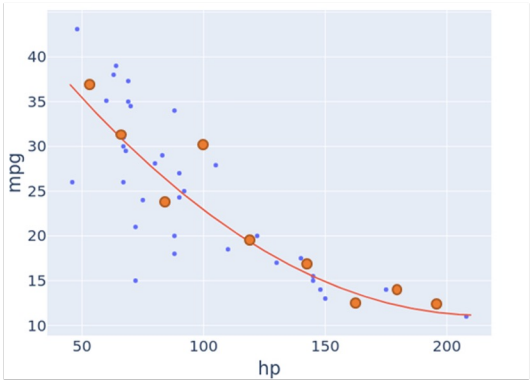


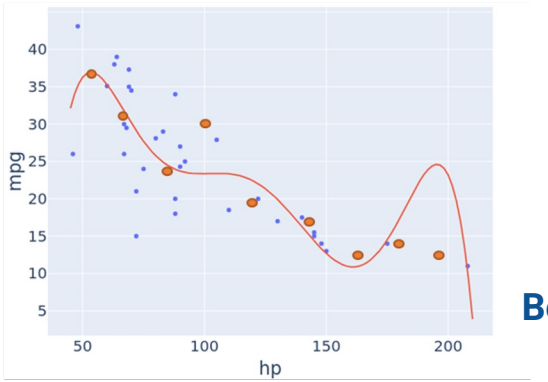
Review: Collecting More Data to Detect Overfitting

Suppose we collect the 9 new orange data points. Can compute MSE for our original models **without refitting using the new orange data points**.









Best?

k	MSE
0	72.091396
1	28.002727
2	25.835769
3	25.831592
4	25.763052
5	25.609403
6	23.269001

Original 35 data points

Best?

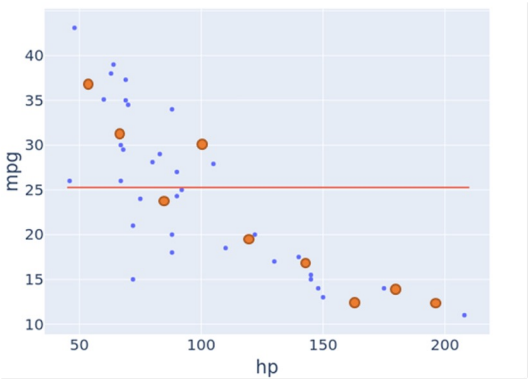
k	MSE
0	69.198210
1	31.189267
2	27.387612
3	29.127612
4	34.198272
5	37.182632
6	53.128712

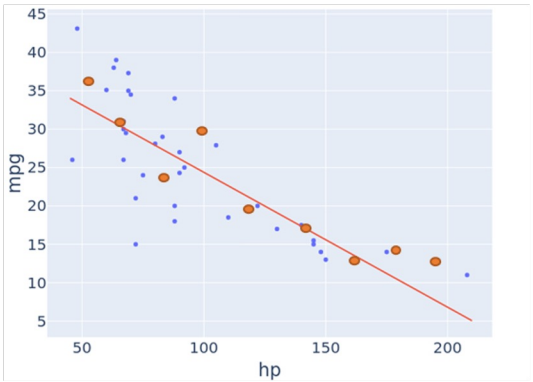
New 9 data points

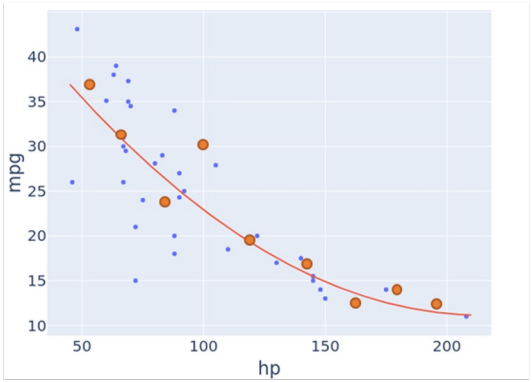
Review: Collecting More Data to Detect Overfitting

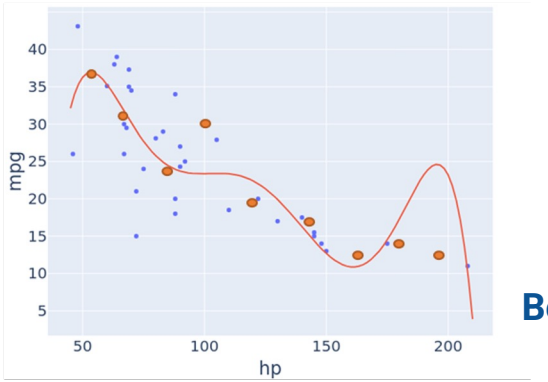
The order 2 model seems best to me.

- Performs best on data that has not yet been seen.









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New 9 data points

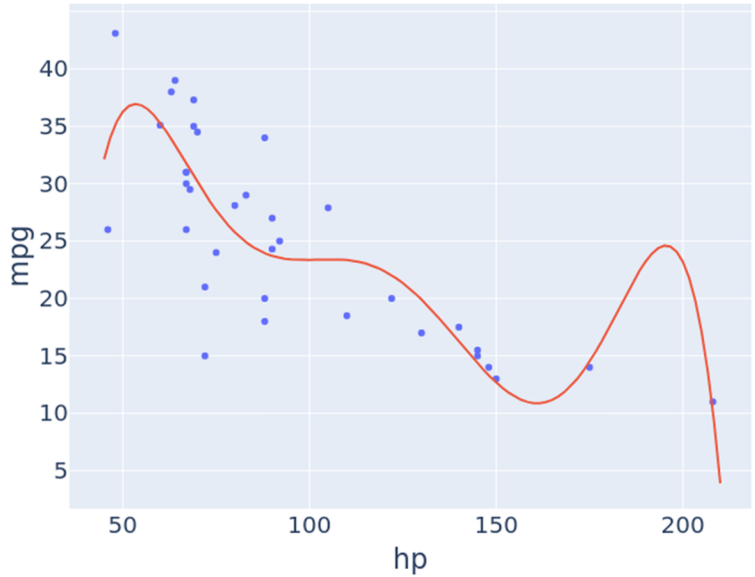
Review: Collecting More Data to Detect Overfitting

Suppose we have 7 models and don't know which is best.

- Can't necessarily trust the training error. We may have overfit!

We could wait for more data and see which of our 7 models does best on the new points.

- Unfortunately, that means we need to wait for more data. May be very expensive or time consuming.
- Will see an alternate approach in today's lecture

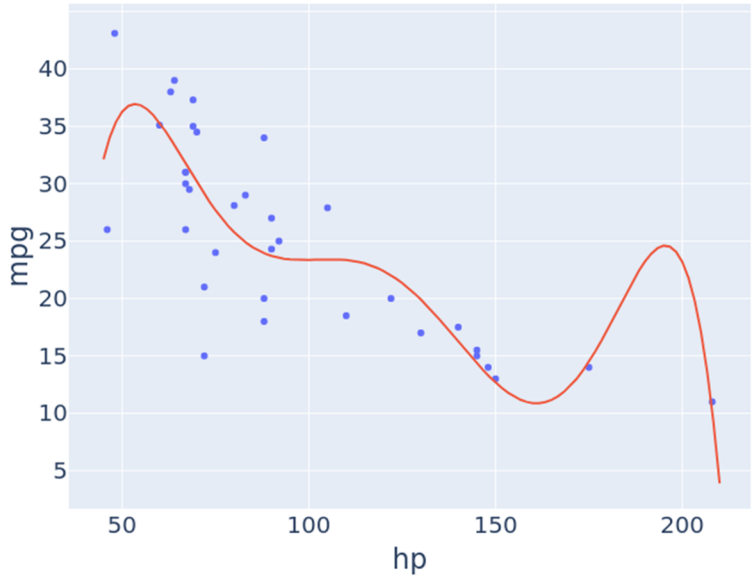


Idea 1: The Holdout Method

The simplest approach for avoiding overfitting is to keep some of our data secret from ourselves.

Example:

- Previous approach: We fit 7 models on all 35 of the available data points. Then waited for 9 new data points to decide which is best.
- Holdout Method: We **train** our models on all **25**/35 of the available data points. Then we **evaluate** the models' performance on the **remaining 10 data points**.
  - Data used to train is called the "**training set**".
  - **Held out data** is often called the "**validation set**" or "**development set**" or "**dev set**". These terms are all synonymous and used by different authors.



Holdout Set Demo

The code below splits our data into two sets of size 25 and 10.

```
from sklearn.utils import shuffle
training_set, dev_set = np.split(shuffle(vehicle_data_sample_35), [25])
```

	mpg	cylinders	displacement	hp
201	18.5	6	250.0	110.0
215	13.0	8	318.0	150.0
...	...	...	...	...
108	20.0	4	97.0	88.0
304	37.3	4	91.0	69.0

25 rows × 11 columns

Used for **Training**

	mpg	cylinders	displacement	hp
244	43.1	4	90.0	48.0
159	14.0	8	351.0	148.0
...	...	...	...	...
302	34.5	4	105.0	70.0
223	15.5	8	318.0	145.0

10 rows × 11 columns

Used for **Evaluation**

Reflection: Shuffling

Question: Why did I shuffle first?

```
from sklearn.utils import shuffle
training_set, dev_set = np.split(shuffle(vehicle_data_sample_35), [25])
```

Reflection: Shuffling

Question: Why did I shuffle first?

```
from sklearn.utils import shuffle
training_set, dev_set = np.split(shuffle(vehicle_data_sample_35), [25])
```

I'm using a large contiguous block of data as my validation set.

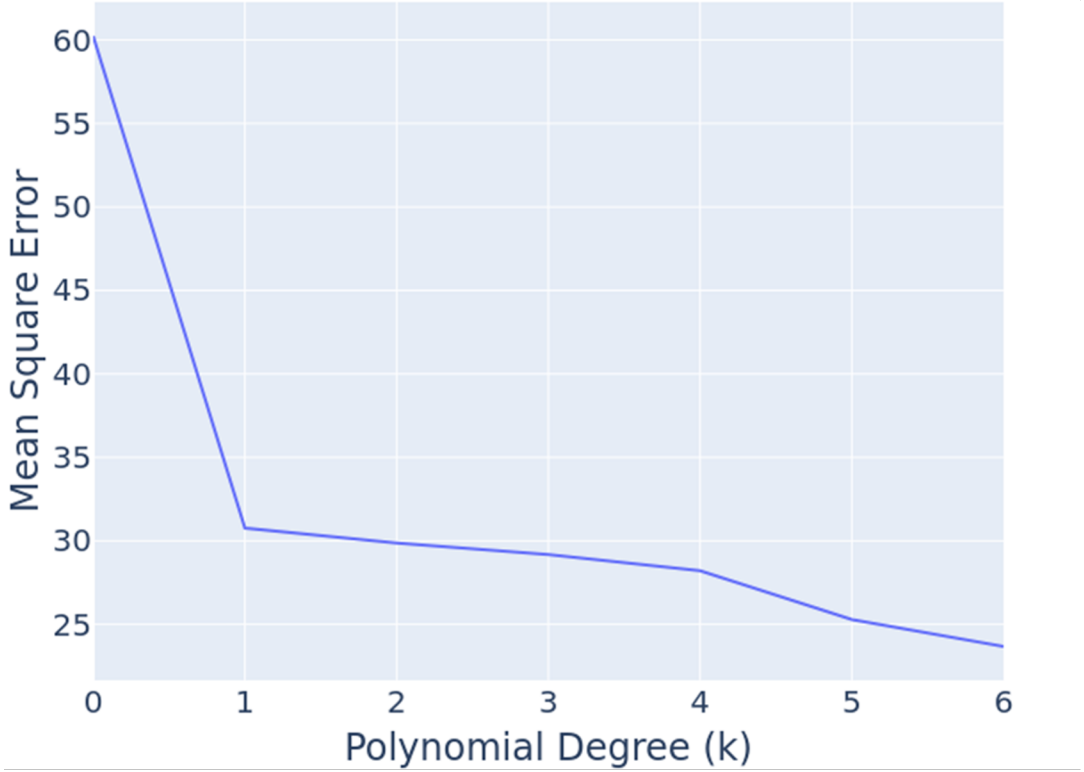
- If the set is sorted by something e.g. vehicle MPG, then my model will perform poorly on this unseen data.
  - Model will have never seen a high MPG vehicle.

Shuffling prevents this problem.

- Alternate mathematically equivalent approach: Picking 10 samples randomly.

Hold Out Method Demo Step 1: Generating Models of Various Orders

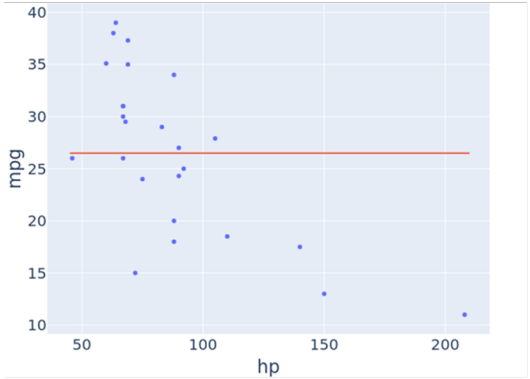
First we **train** 7 models the experiment now on our **training set of 25 points**, yielding the MSEs shown below. As before, MSE decrease monotonically with model order.

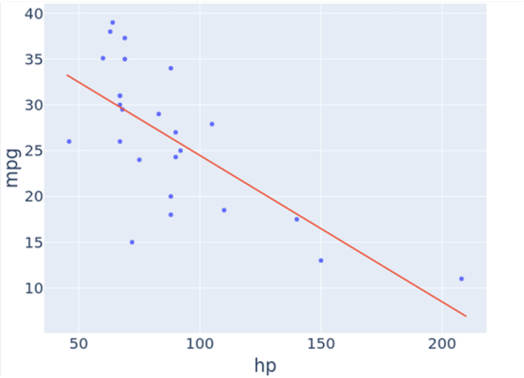


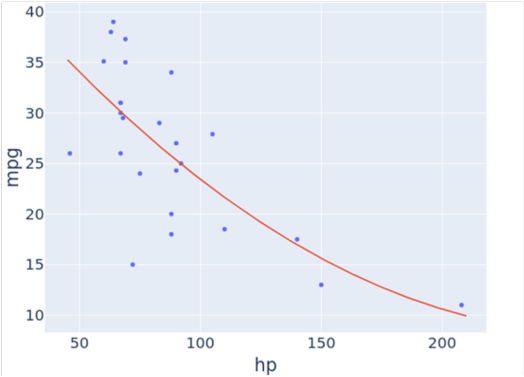
k	MSE
0	60.235744
1	30.756678
2	29.875269
3	29.180868
4	28.214850
5	25.290990
6	23.679651

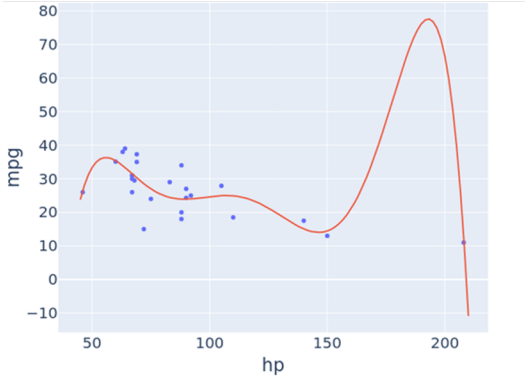
Hold Out Method Demo Step 1: Generating Models of Various Orders (visualization)

Below, we show the order 0, 1, 2, and 6 models trained on our **25 training points**.









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0	60.235744
1	30.756678
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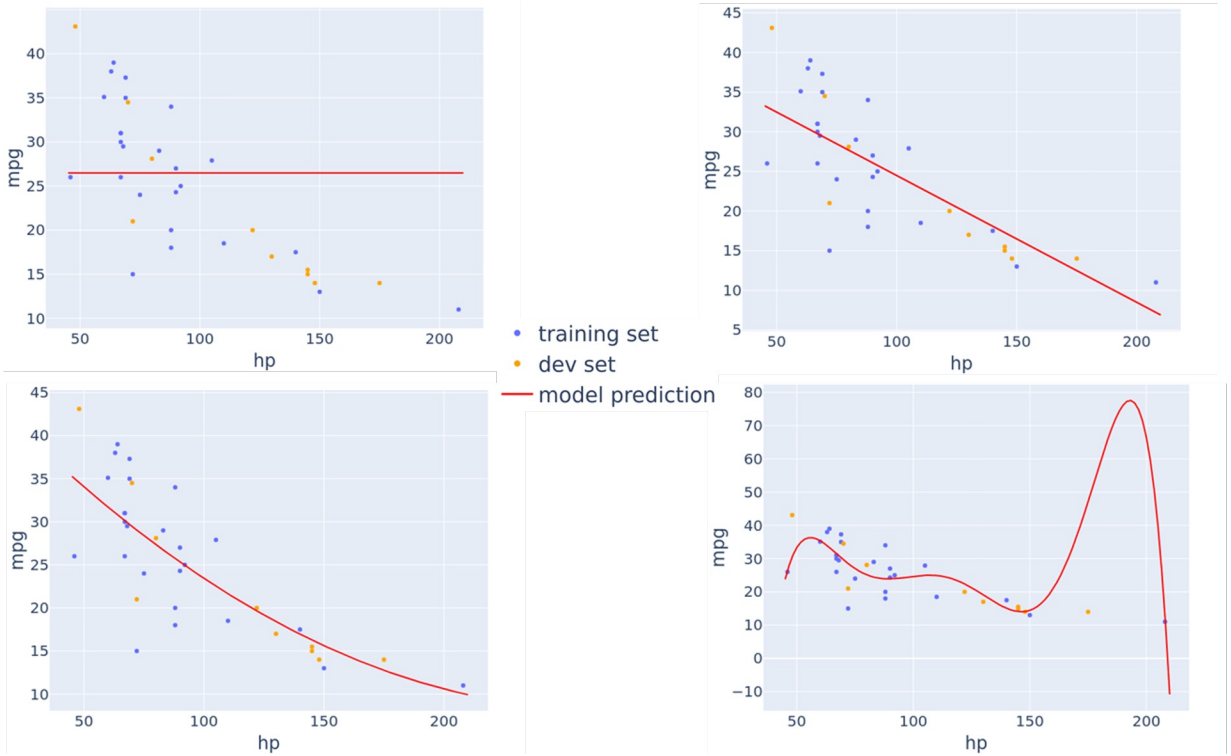
5	25.290990
6	23.679651

Note: Our degree 6 model looks different than before. No surprise since variance is high and we're using a different data set.

Hold Out Method Demo Step 2: Evaluating on the Validation Set (a.k.a. Dev Set)

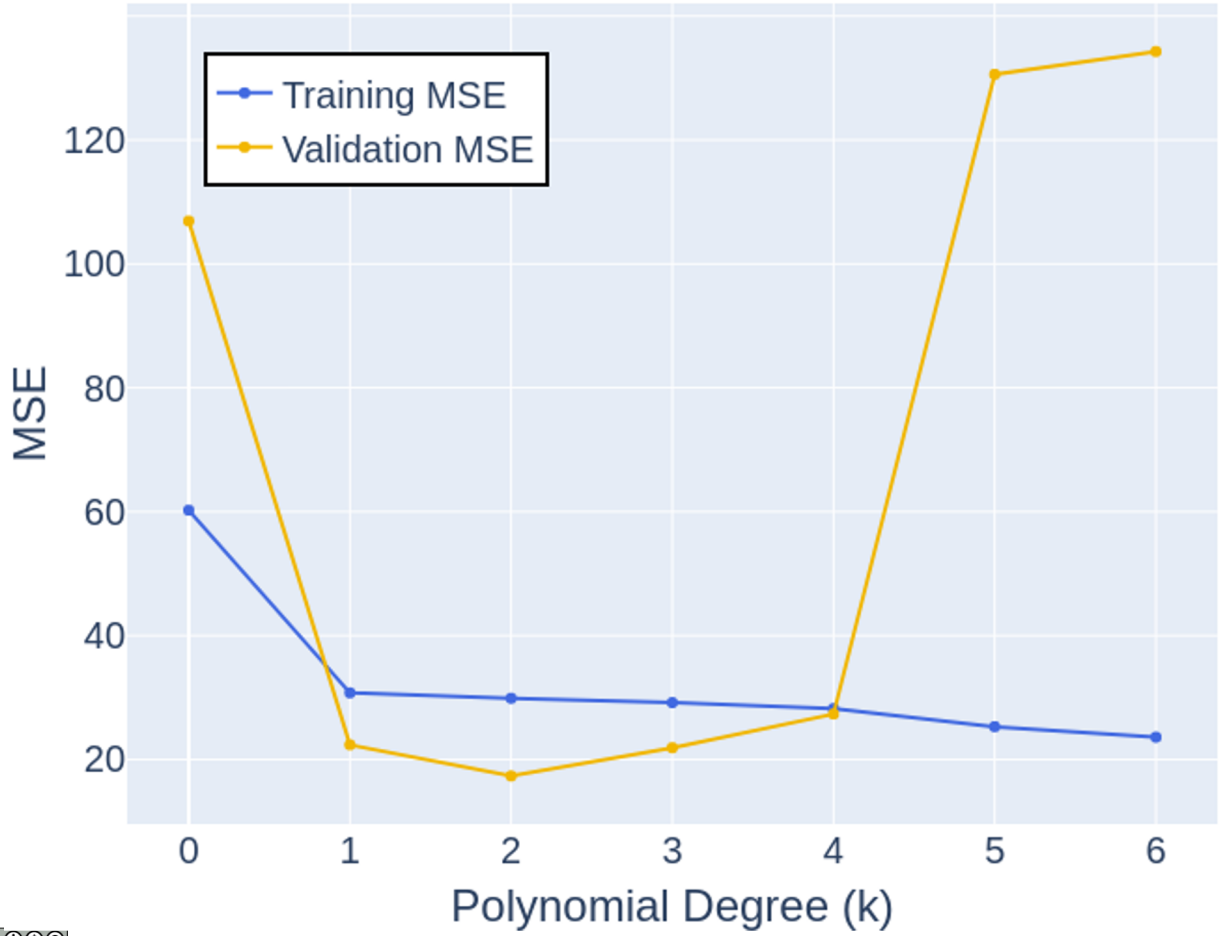
Then we compute MSE on our **10 dev set points** (in orange) for all 7 models **without refitting using these orange data points**. Models are only fit on the 25 training points.



k	Training MSE	Validation MSE
0	60.235744	106.925296
1	30.756678	22.363676
2	29.875269	17.331880
3	29.180868	21.889257
4	28.214850	27.340989
5	25.290990	130.597678
6	23.679651	135.787493

Evaluation: **Validation set MSE** is best for degree = 2!

Plotting Training and Validation MSE



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4	28.214850	27.340989
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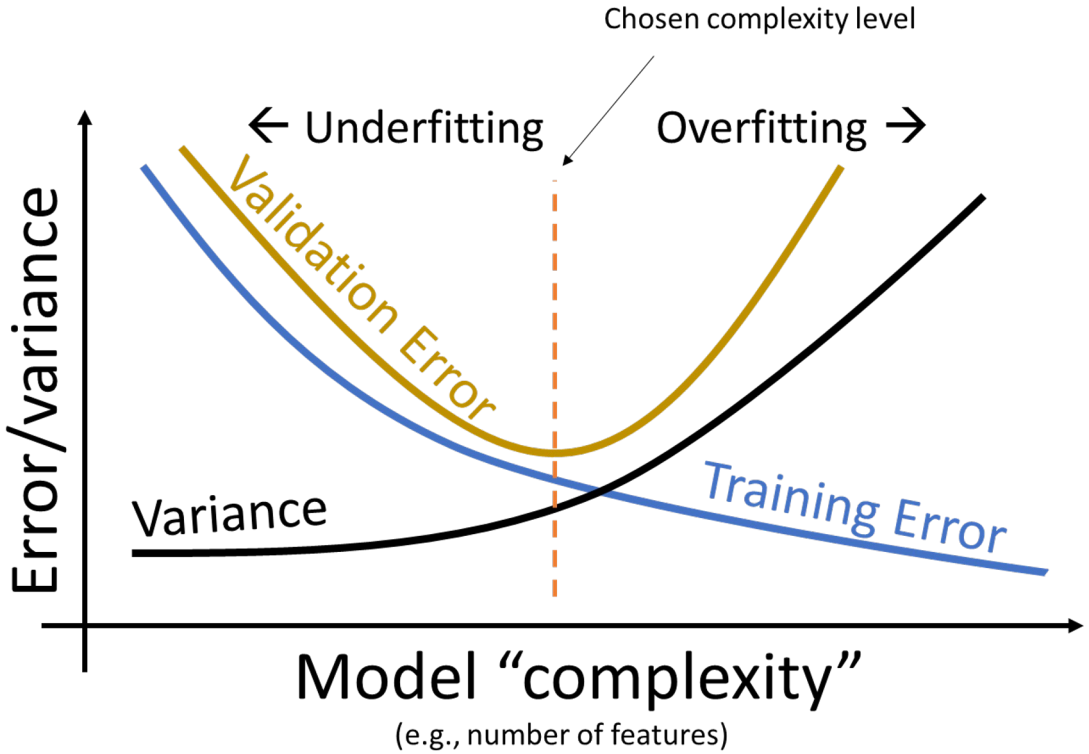
6	23.679651	135.787493

Idealized Picture of Training and Validation Error

As we increase the complexity of our model:

- **Training error** decreases.
- Variance increases.
- Typically, **error on validation data** decreases, then increases.

We pick the model complexity that minimizes **validation set error**.



Hyperparameter: Terminology

In machine learning, a **hyperparameter** is a value that controls the learning process itself.

- For our example today, we built seven models, each of which had a hyperparameter called degree or k that controlled the order of our polynomial.

We use:

- The training set to select parameters.
- The validation set (a.k.a. development set) (a.k.a. cross validation set) to select hyperparameters, or more generally, between different competing models.

K-Fold Cross Validation

Cross Validation

- The Holdout Method
- **K-Fold Cross Validation**
- Test Sets

Regularization

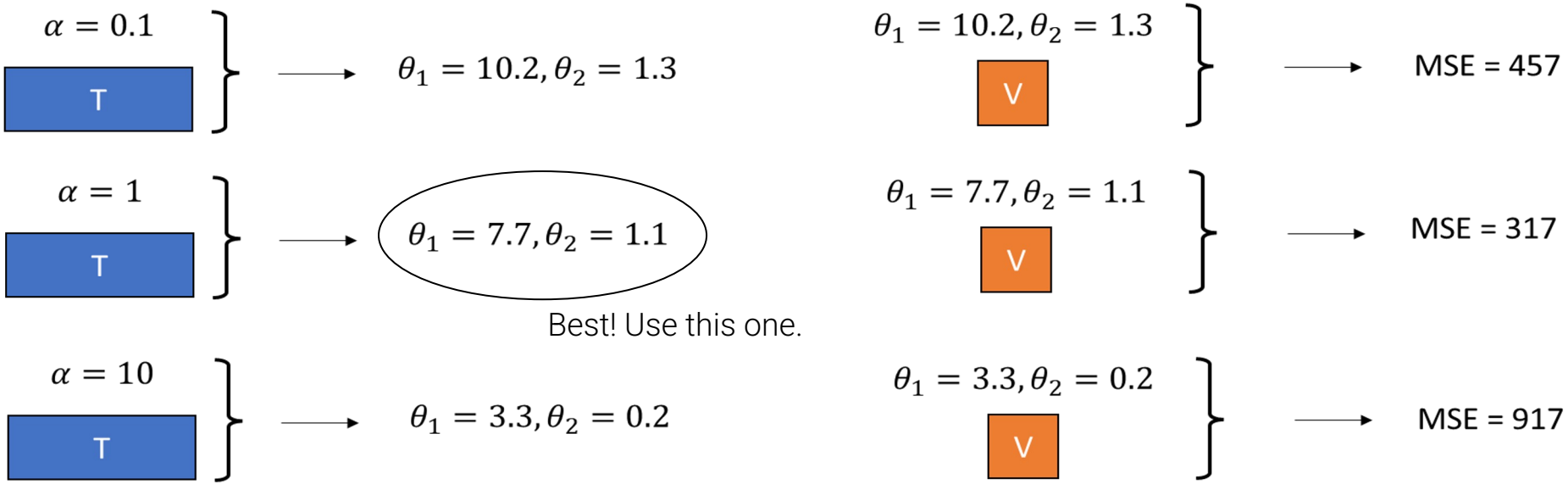
- L2 Regularization (Ridge)
- Scaling Data for Regularization
- L1 Regularization (LASSO)

Another View of The Holdout Method

To determine the quality of a particular hyperparameter:

- **Train model** on **ONLY** the **training set.** **Quality** is model's error on ONLY the **validation set**.

Example, imagine we are trying to pick between three values of a hyperparameter alpha.



Another View of The Holdout Method

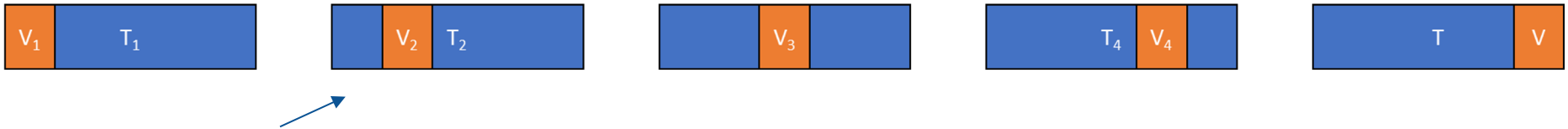
In the Holdout Method, we set aside the validation set at the beginning, and our choice is fixed.

- **Train model** on **ONLY** the **training set.** **Quality** is model's error on ONLY the **validation set**.

Example below where the last 20% is used as the validation set.

Thought Experiment

If we decided (arbitrarily) to use non-overlapping contiguous chunks of 20% of the data, there are 5 possible “chunks” of data we could use as our validation set, as shown below.

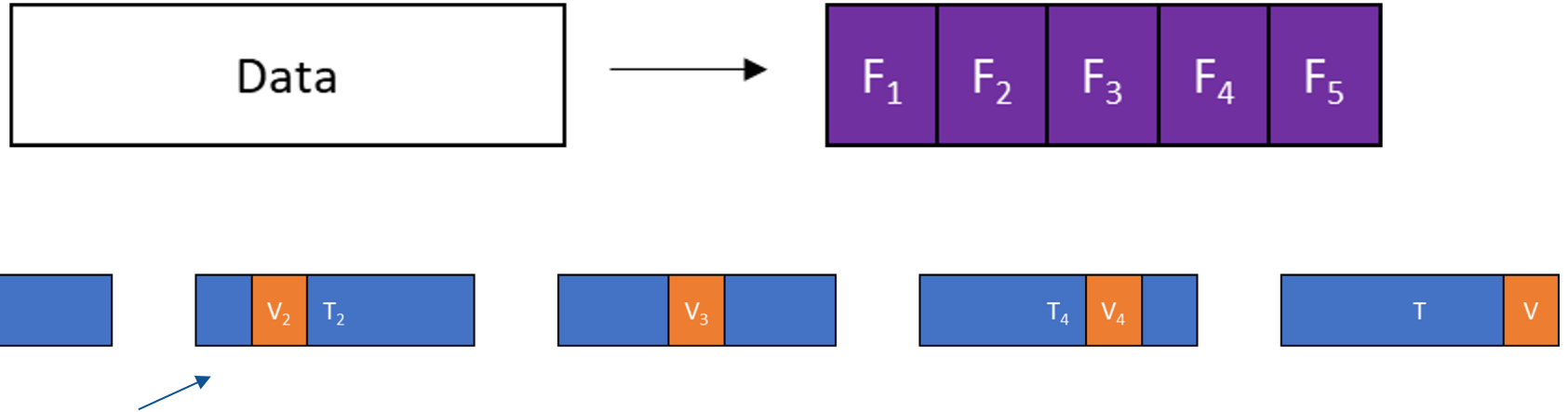


Use first 20% and last 60% to train, remaining 20% as validation set.

Thought Experiment

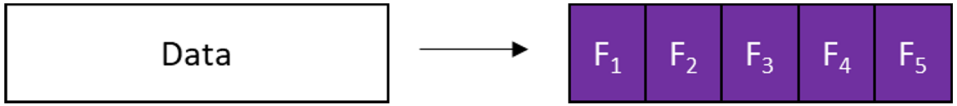
If we decided (arbitrarily) to use non-overlapping contiguous chunks of 20% of the data, there are 5 possible “chunks” of data we could use as our validation set, as shown below.

- The common term for these chunks is a “fold”.
  - For example, for chunks of size 20%, we have 5 folds.



K-Fold Cross Validation

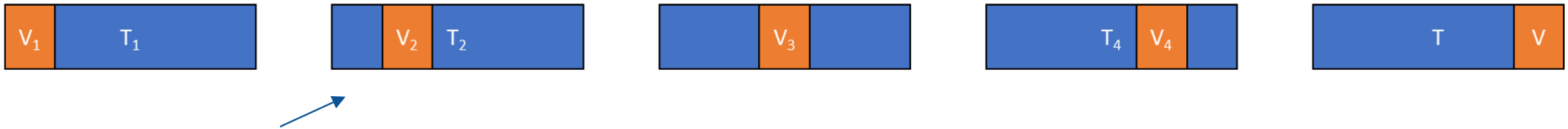
In the k-fold cross-validation approach, we split our data into k equally sized groups (often called folds).



Given k folds, to determine the quality of a particular hyperparameter:

- Pick a fold, which we'll call the validation fold. Train model on all but this fold. Compute error on the validation fold.
- Repeat the step above for all k possible choices of validation fold.
- Quality is the average of the k validation fold errors.

Example for k = 5:

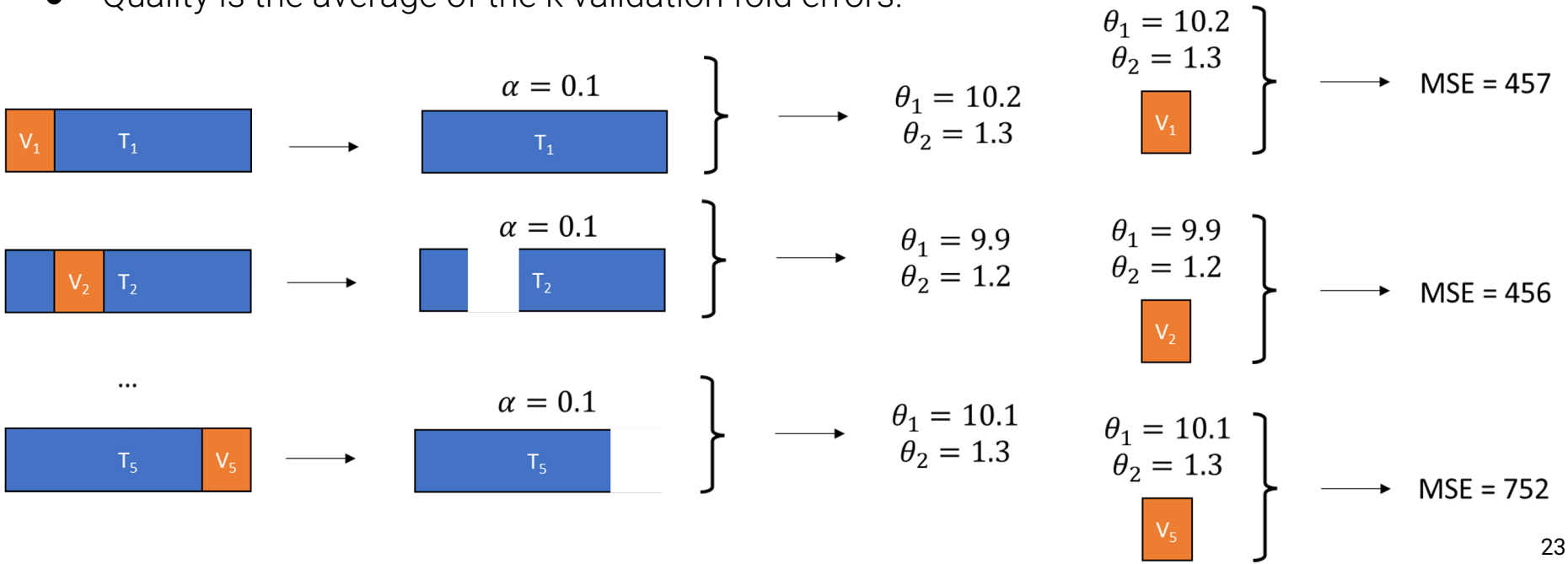


Use folds 1, 3, 4, and 5 to train, and use fold 2 as validation set.

5-Fold Cross Validation Demo

Given k folds, to determine the quality of a particular hyperparameter, e.g. alpha = 0.1:

- Pick a fold, which we'll call the validation fold. Train model on all but this fold. Compute error on the validation fold.
- Repeat the step above for all k possible choices of validation fold.
- Quality is the average of the k validation fold errors.



5-Fold Cross Validation Demo

Given k folds, to determine the quality of a particular hyperparameter, e.g. alpha = 0.1:

- Pick a fold, which we'll call the validation fold. Train model on all but this fold. Compute error on the validation fold.
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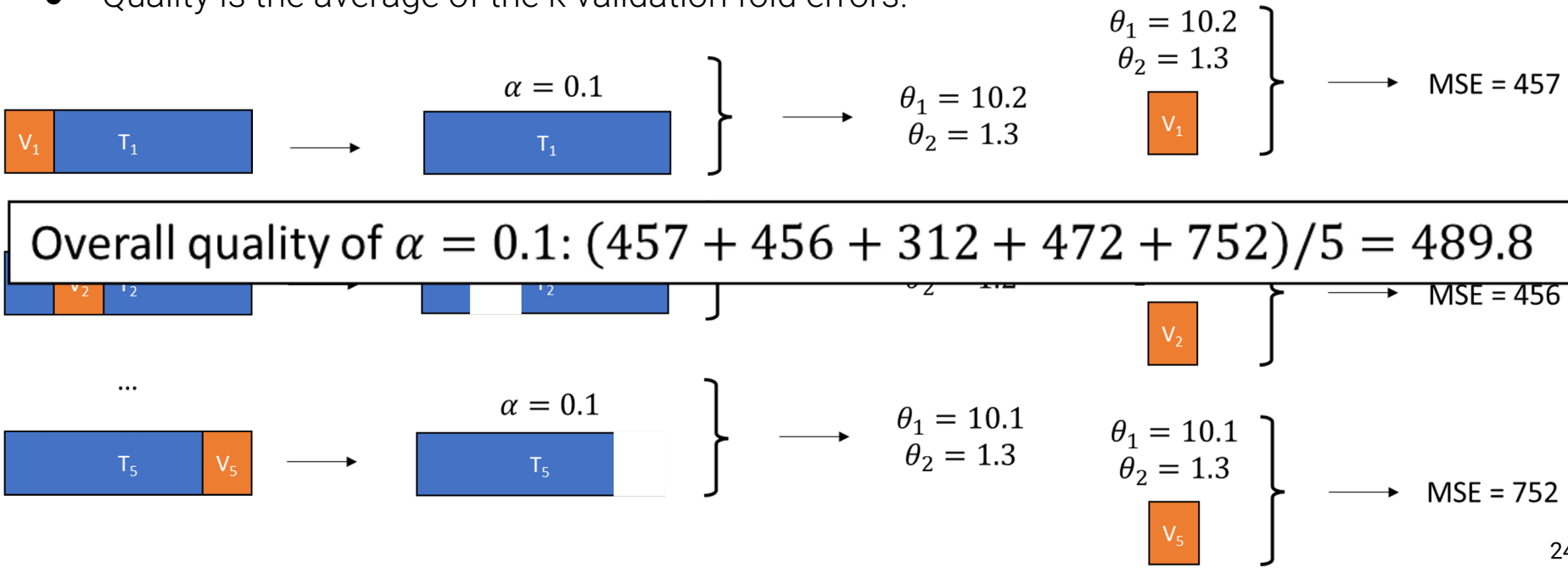


Test Your Understanding: How Many MSEs?

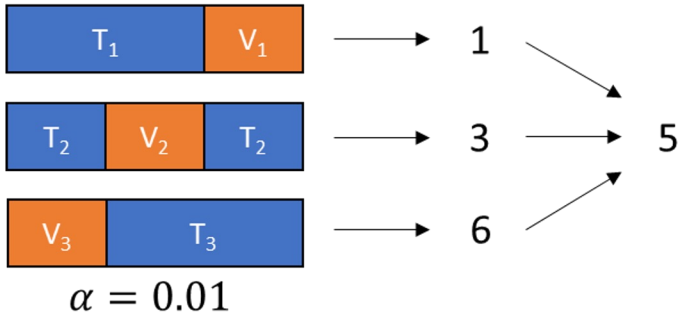
Suppose we pick k = 3 and we have 4 possible hyperparameter values α=[0.01, 0.1, 1, 10].

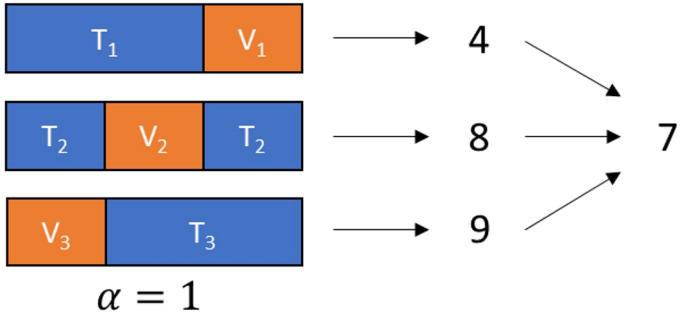
- How many total MSE values will we compute to get the quality of α=10?
- How many total MSE values will we compute to find the best α?

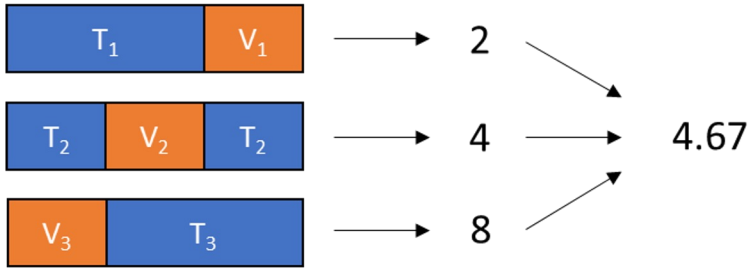
Test Your Understanding: How Many MSEs?

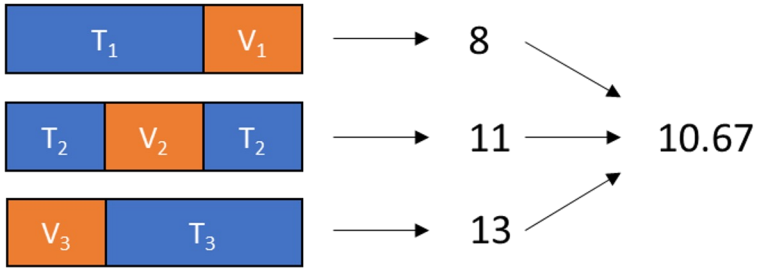
Suppose we pick k = 3 and we have 4 possible hyperparameter values α=[0.01, 0.1, 1, 10].

- How many total MSE values will we compute to get the quality of α=10? 3
- How many total MSE values will we compute to find the best α? 12





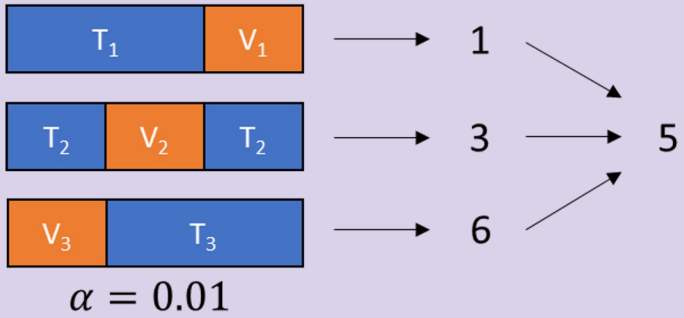




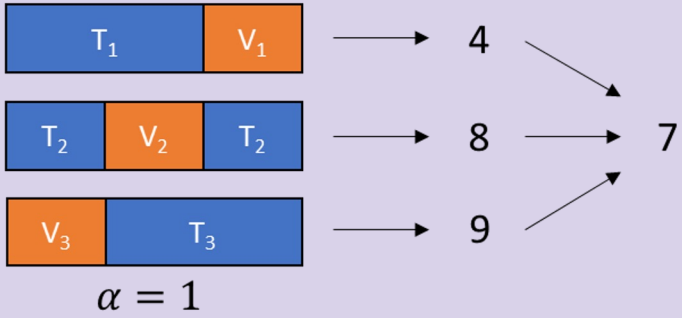
Test Your Understanding: Selecting Alpha

Which α should we pick?

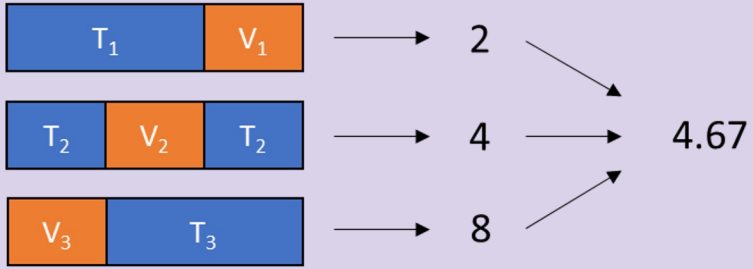
What fold (or folds) should we use as our training set for computing our final model parameters θ?

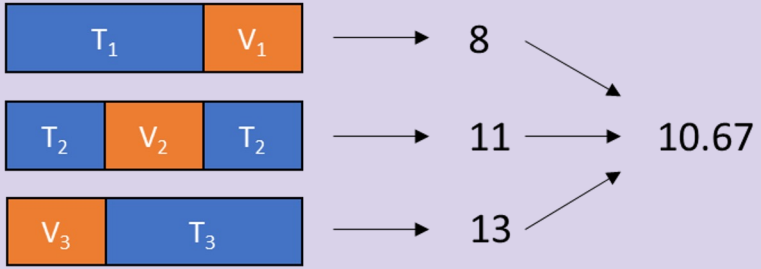


$\alpha = 0.01$



$\alpha = 1$



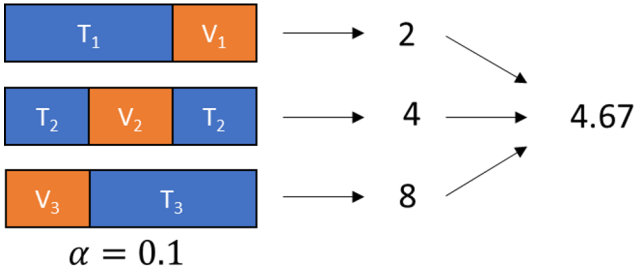


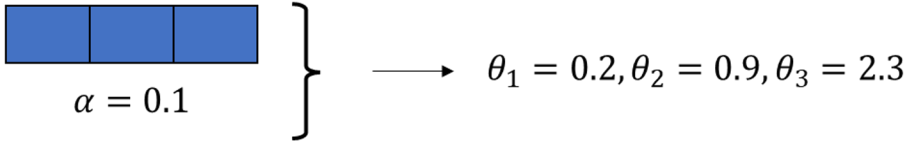
Test Your Understanding: Selecting Alpha

Which α should we pick? 0.1

What fold (or folds) should we use as our training set for computing our final model parameters θ?

- There's no reason to prefer any fold over any other. In practice, best to train all model on all of the data, i.e. use all 3 folds.





Picking K

Typical choices of k are 5, 10, and N, where N is the amount of data.

- K=N is also known as “leave one out cross validation”, and will typically give you the best results.
  - In this approach, each validation set is only one point.
  - Every point gets a chance to get used as the validation set.
- k=N is also very expensive, require you to fit a huge number of models.

Ultimately, the tradeoff is between k and computation time.

K-Fold Cross Validation and Hold Out Method in sklearn

As an example, the code below performs a GridSearchCV uses 5 fold cross validation to find the optimal parameters for a model called “scaled_ridge_model”.

- The hyperparameters to try are stored in a dictionary called “parameters_to_try”.
- The loss function is given by the “scoring” parameter.
- The number of folds is given by “cv = 5”.

```
model_finder = GridSearchCV(estimator = scaled_ridge_model,
                            param_grid = parameters_to_try,
                            scoring = "neg_mean_squared_error",
                            cv = 5)
```

Can also do the Hold Out method in sklearn:

```
model_finder = GridSearchCV(estimator = scaled_ridge_model,
                            param_grid = parameters_to_try,
                            scoring = "neg_mean_squared_error",
                            cv=[[training_indices, dev_indices]])
```

Cross Validation Summary

When selecting between models, we want to pick the one that we believe would generalize best on unseen data. Generalization is estimated with a "**cross validation score**"*.

- When selecting between models, keep the model with the best **score**.

Two techniques to compute a "**cross validation score**":

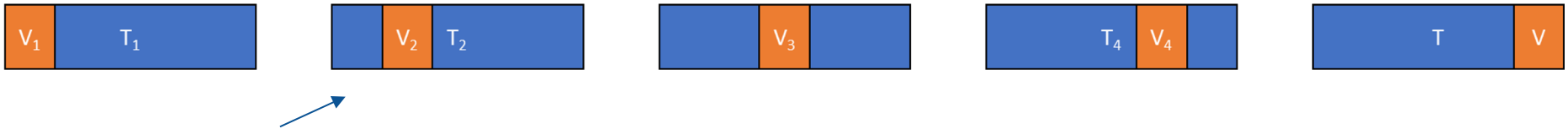
- The Holdout Method: Break data into a separate **training set** and **validation set**.
  - Use **training set** to **fit** parameters (thetas) for the model.
  - Use **validation set** to **score** the model.
  - Also called "Simple Cross Validation" in some sources.
- K-Fold Cross Validation: Break data into K contiguous non-overlapping "folds".
  - Perform K rounds of Simple Cross Validation, except:
    - Each fold gets to be the **validation set** exactly once.
    - The final **score** of a model is the **average validation score** across the K trials.

Extra: Exhaustive Cross Validation

We don't have to use non-overlapping contiguous chunks! Could use

- Every 5th data point as validation set.
- Data in positions 0-2%, 20-22%, 40-42%, 60-62%, 80-82% as validation set.
- Etc.

Iterating over ALL possible such permutations is known as "exhaustive cross validation."



Use first 20% and last 60% to train, remaining 20% as validation set.

Test Sets

Cross Validation

- The Holdout Method
- K-Fold Cross Validation
- **Test Sets**

Regularization

- L2 Regularization (Ridge)
- Scaling Data for Regularization
- L1 Regularization (LASSO)

Providing an Estimate of Model Generalization to the World

Suppose we're researchers building a state of the art regression model.

- After months of work and after comparing billions of candidate models, we find the model with the best **validation set loss**.

Now we want to report this model out to the world so it can be compared to other models.

- Our **validation set loss** is not an unbiased estimator of its performance!
- Instead, we'll run our model just one more time on a special **test set**, that we've never seen or used for any purpose whatsoever.

Test Sets

Test sets can be something that we generate ourselves. Or they can be a common data set whose solution is unknown.

In real world machine learning competitions, competing teams share a **common test set**.

- To avoid accidental or intentional overfitting, the **correct predictions for the test set are never seen by the competitors**.

Creating a Test Set Ourselves

We can do this easily in code. As before, we shuffle using scikit-learn then split using numpy.

```
diamond_data = shuffle(diamond_data)
diamond_data.head()
```

```
#split our 2000 rows into 1500 for training, 300 for validation, 200 for test
diamond_training_data, diamond_validation_data, diamond_test_data = np.split(diamond_data, [1500, 1800])
```

Then we use np.split, now providing two numbers instead of one. For example, the code above splits the data into a **Training**, **Validation**, and **Test** set.

- Recall that a **validation set** is just another name for a **development set**.
- **Training set** used to pick parameters.
- **Validation set** used to pick hyperparameters (or **pick between different models**).
- **Test set** used to provide an **unbiased MSE at the end**.

Validation Sets and Test Sets in Real World Practice

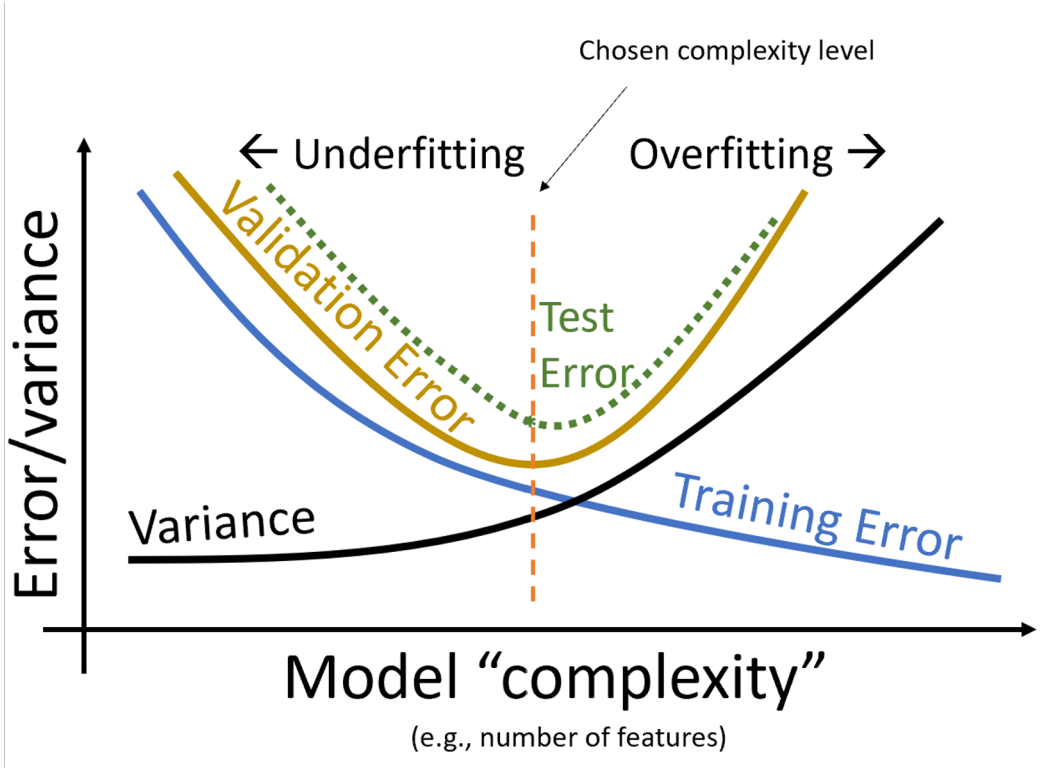
Standard **validation sets** and **test sets** are used as standard benchmarks to compare ML algorithms.

- Example: ImageNet is a dataset / competition used to compare to different image classification algorithms (e.g. this image is of a “Dog”).
  - 1,281,167 **training images**. Images and correct label provided.
  - 50,000 **validation images**. Images and correct label provided.
  - 100,000 **test images**. Images provided, but no correct label.
- When writing papers, researchers report their performance on the **validation images**.
  - This set is a “**validation set**” with respect to the entire global research community.
  - Research groups cannot report the **test error** because they cannot compute it!
- When ImageNet was a competition, the **test set** was used to rank different algorithms.
  - Researchers provide their predictions for the **test set** to a central server.
  - Server (which knows the labels) reports back a **test set score**.
  - Best **test set score** wins.

Idealized Training, Validation, and Test Error

As we increase the complexity of our model:

- **Training error** decreases.
- Variance increases.
- Typically, **validation error** decreases, then increases.
- The **test error** is the essentially the same thing as the **validation error**! Only difference is that we are much restrictive about computing the **test error**
  - Don't get to see the whole curve!



Recipe for Successful Generalization

1. Split your data into **training** and **test** sets (90%, 10%)
2. Use **only the training data** when designing, training, and tuning the model

   Use **cross validation** to test *generalization* during this phase

   Do not look at the test data!
3. Commit to your final model and train once more using **only the training data.**
4. Test the final model using the **test data**.
5. Train on **all available data** and ship it!

Regularization

Cross Validation

- The Holdout Method
- K-Fold Cross Validation
- Test Sets

Regularization

- L2 Regularization (Ridge)
- Scaling Data for Regularization
- L1 Regularization (LASSO)

Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Controlling the *Model Complexity*

Such that:

f_θ does not “overfit”

Can we make this more formal?

Basic Idea

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Controlling the *Model Complexity*

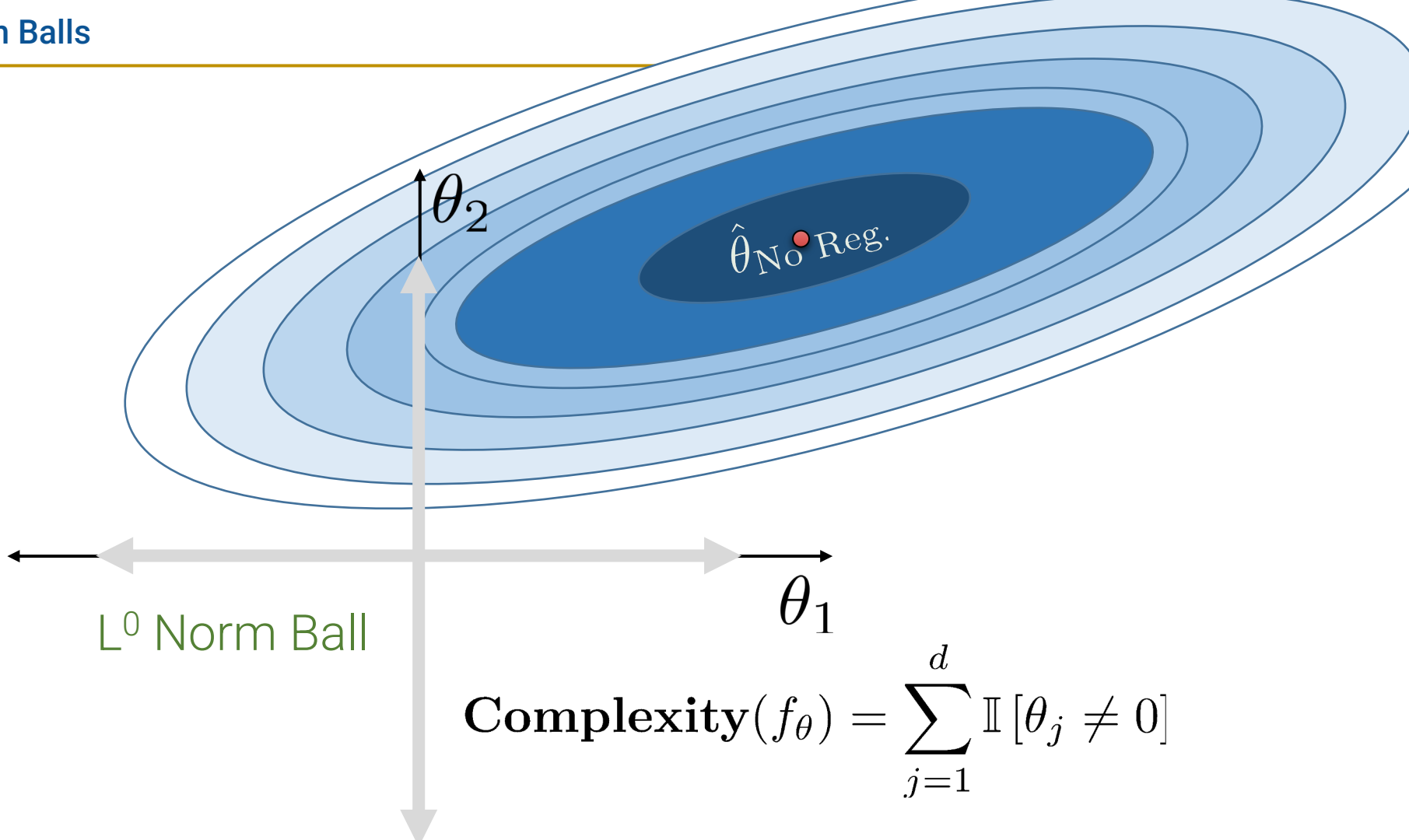
Such that:

$$\text{Complexity}(f_\theta) \leq \beta$$

Regularization Hyperparameter

How do we define this?

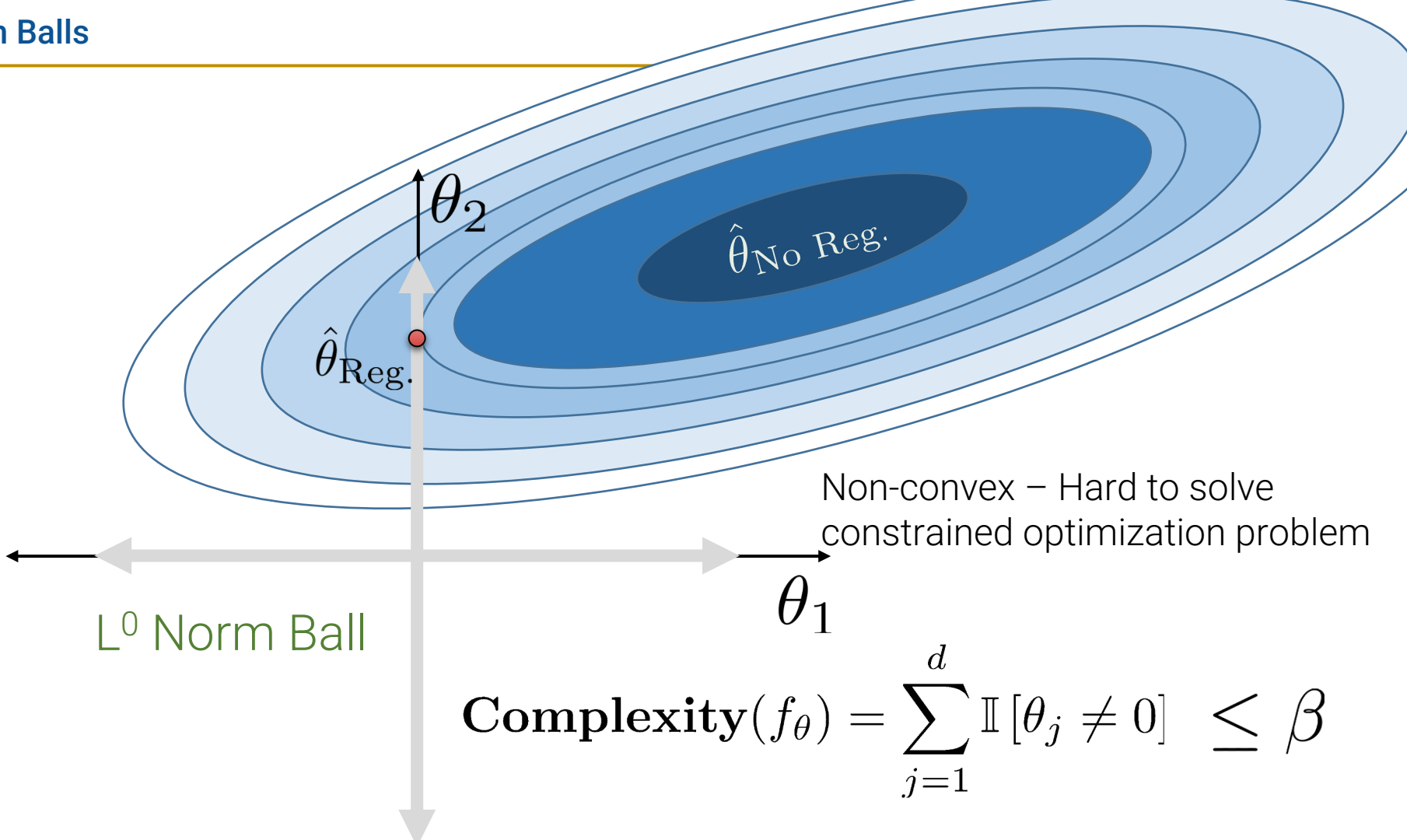
Norm Balls



L^0 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right]$$

Norm Balls



Non-convex – Hard to solve constrained optimization problem

L^0 Norm Ball

$$\textbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Ideal “Regularization”

Find the best value of θ which uses fewer than β features.

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathbf{Loss}\left(y_i, f_\theta(x_i)\right)$$

Such that:

Need an approximation!

$$\mathbf{Complexity}(f_\theta) = \sum_{j=1}^{d} \mathbb{I}\left[\theta_j \neq 0\right] \leq \beta$$

Combinatorial search problem – NP-hard to solve in general.

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.

L2 Regularization (Ridge)

Cross Validation

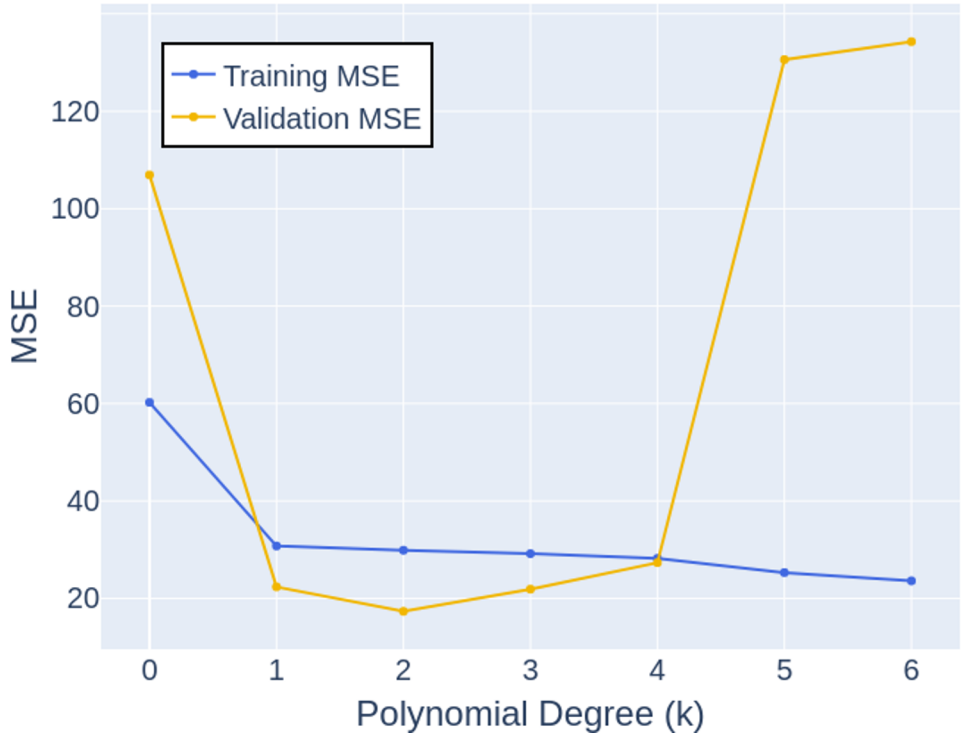
- The Holdout Method
- K-Fold Cross Validation
- Test Sets

Regularization

- **L2 Regularization (Ridge)**
- Scaling Data for Regularization
- L1 Regularization (LASSO)

Earlier

We saw how we can select model complexity by choosing the hyperparameter that minimizes **validation error**. This **validation error** can be computed using the **Holdout Method** or **K-Fold Cross Validation**.

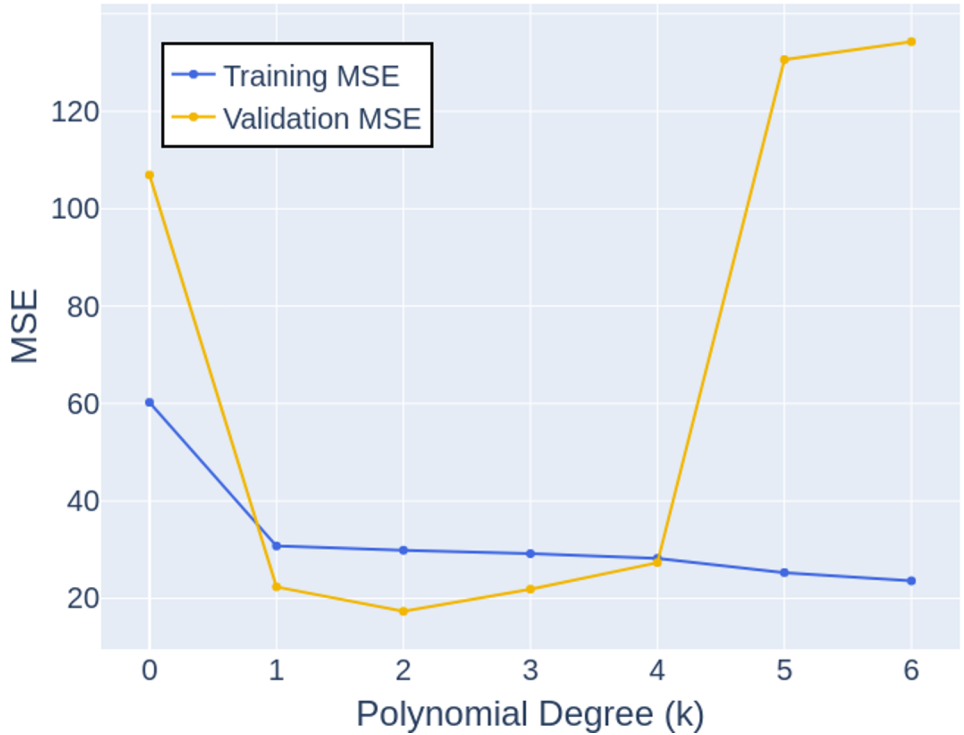


k	Training MSE	Validation MSE
0	60.235744	106.925296
1	30.756678	22.363676
2	29.875269	17.331880
3	29.180868	21.889257
4	28.214850	27.340989
5	25.290990	130.597678
6	23.679651	135.787493

Earlier

For the example below, our hyperparameter was the polynomial degree.

- Tweaking the “complexity” is simple, just increase or decrease the degree.



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5	25.290990	130.597678
6	23.679651	135.787493

A More Complex Example

Suppose we have a dataset with 9 features.

- We want to decide which of the 9 features to include in our linear regression.

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
150.0	3433.0	304.0	22500.0	514950.0	45600.0	11785489.0	1043632.0	92416.0
140.0	3449.0	302.0	19600.0	482860.0	42280.0	11895601.0	1041598.0	91204.0
...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
82.0	2720.0	119.0	6724.0	223040.0	9758.0	7398400.0	323680.0	14161.0

Tweaking Complexity via Feature Selection

With 9 features, there are 2^9 different models.One approach:

- For each of the 2^9 linear regression models, compute the **validation MSE**.
- Pick the model that has the lowest **validation MSE**.

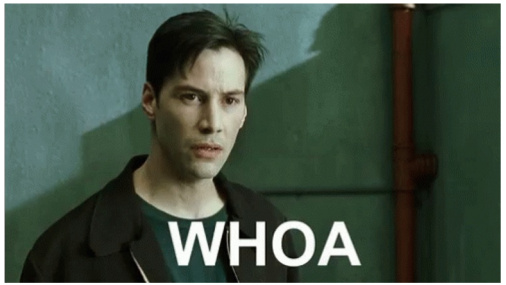
Runtime is exponential in the number of parameters!

	hp	w	dis	hp^2	hp w	hp dis	w^2	w dis	dis^2	MSE
Least complex model	no	no	no	no	no	no	no	no	no	172.2
	no	no	no	no	no	no	no	no	yes	77.3
	no	no	no	no	no	no	no	yes	no	85.3
	no	no	no	no	no	no	no	yes	yes	77.2
	no	no	no	no	no	no	yes	no	no	81.1
	no	no	no	no	no	no	yes	no	yes	74.6
						...				
Most complex model	yes	yes	yes	yes	yes	yes	yes	yes	yes	195.3

Tweaking Complexity via Feature Selection

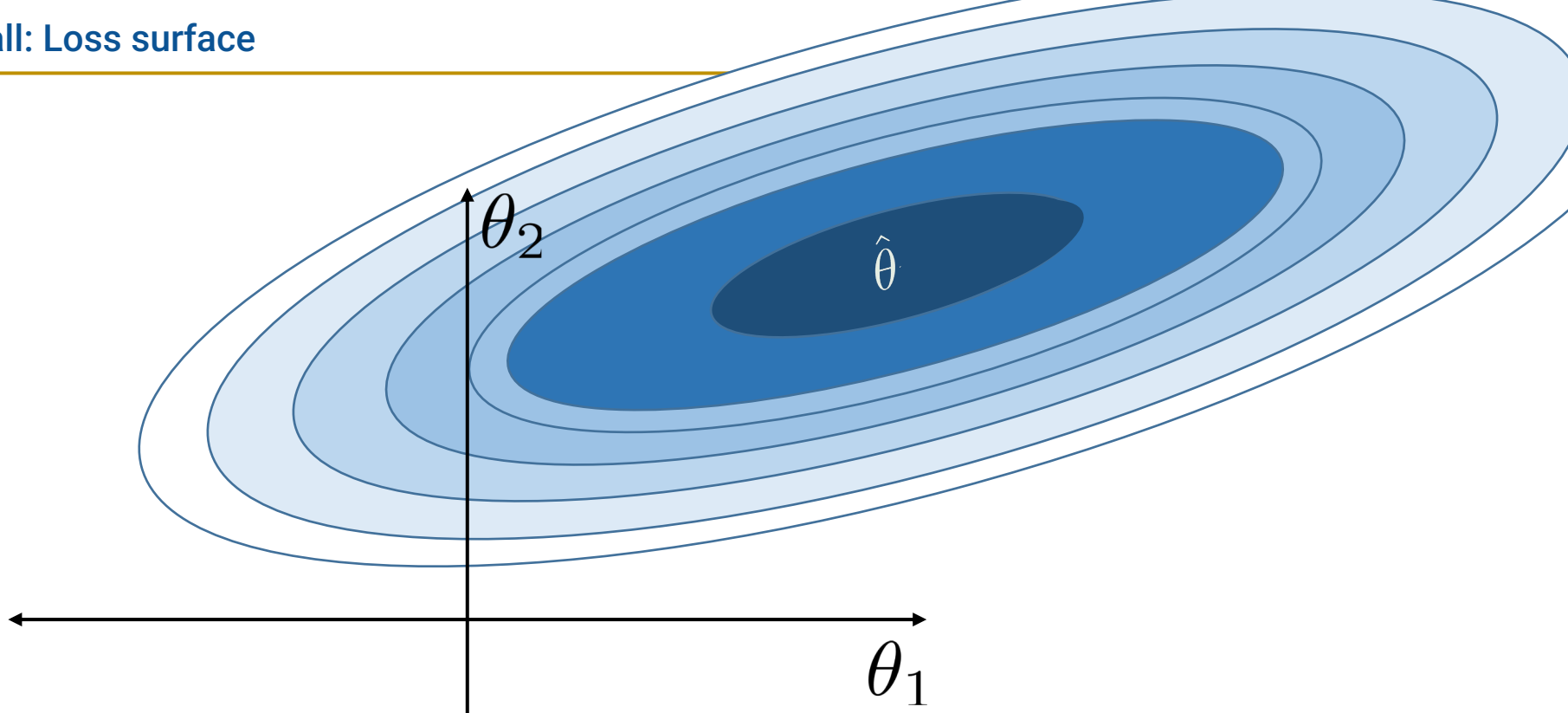
Alternate Idea: What if we use all of the features, but only a little bit?

- Let's see a simple example for a 2 feature model.
- Will return to this 9 feature model later.



	hp	w	dis	hp^2	hp w	hp dis	w^2	w dis	dis^2	MSE
Least complex model	no	no	no	no	no	no	no	no	no	172.2
	no	no	no	no	no	no	no	no	yes	77.3
	no	no	no	no	no	no	no	yes	no	85.3
	no	no	no	no	no	no	no	yes	yes	77.2
	no	no	no	no	no	no	yes	no	no	81.1
	no	no	no	no	no	no	yes	no	yes	74.6
						...				
Most complex model	yes	yes	yes	yes	yes	yes	yes	yes	yes	195.3

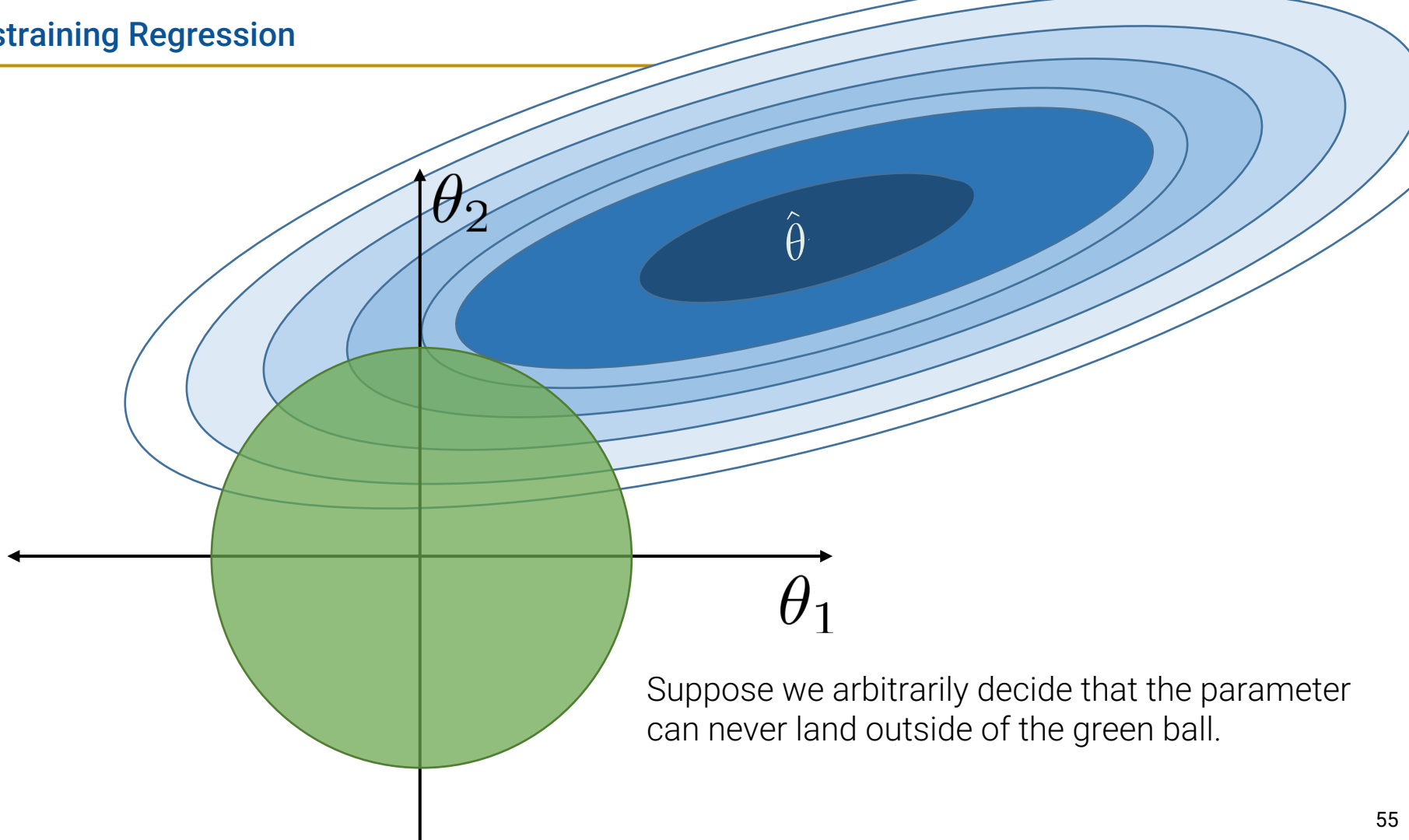
Recall: Loss surface



Imagine we have a two parameter model.

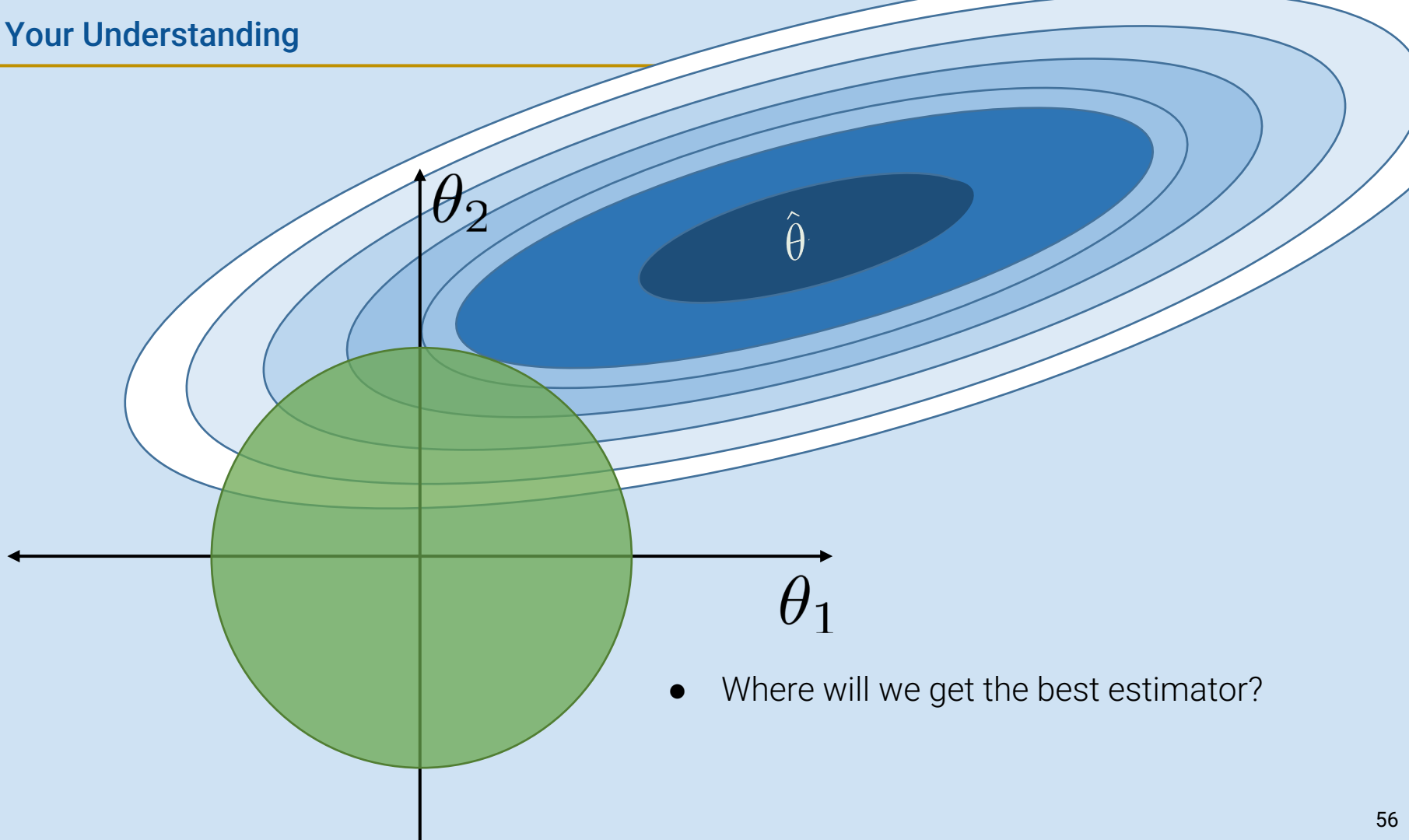
- Optimal parameters are given by theta hat.

Constraining Regression



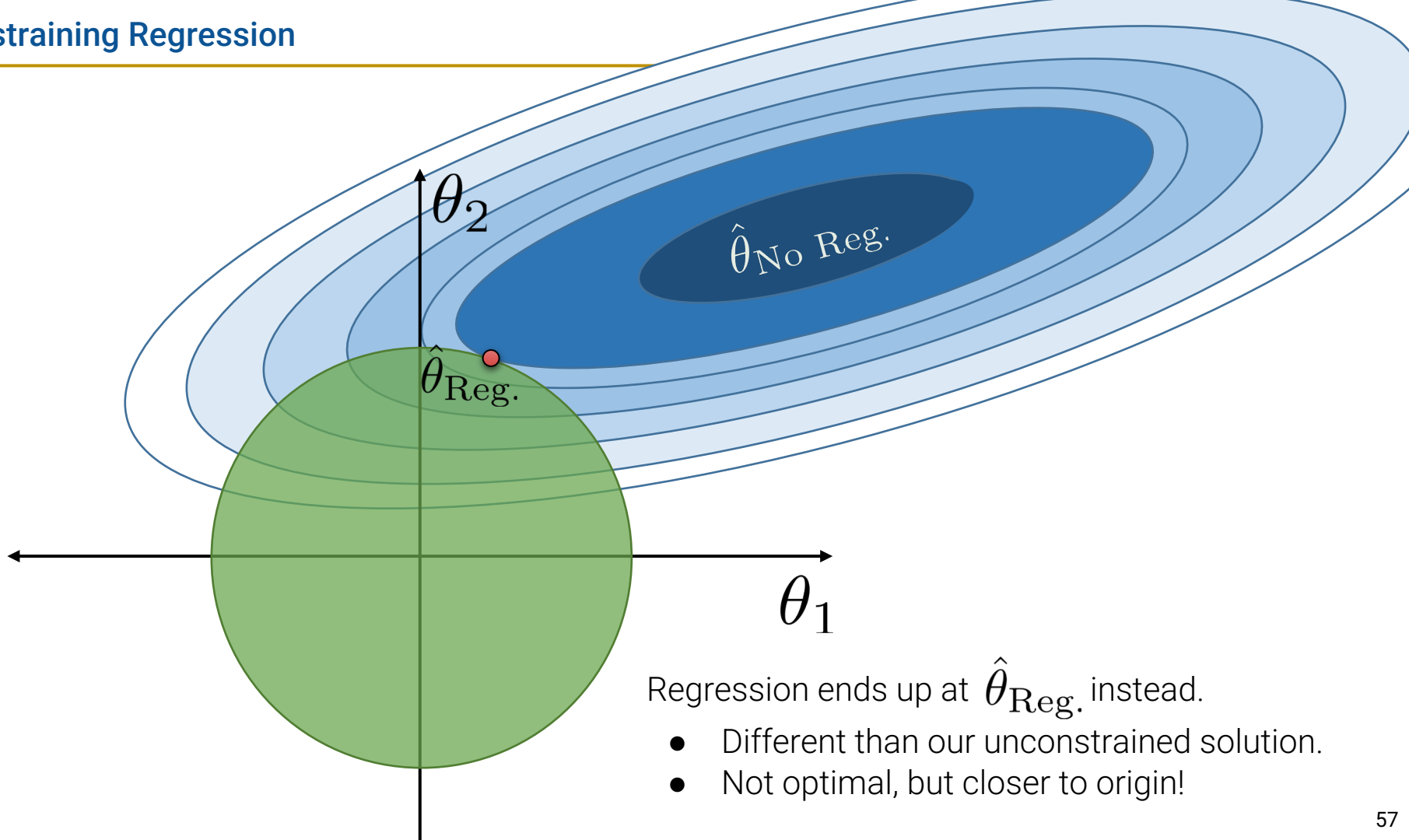
Suppose we arbitrarily decide that the parameter can never land outside of the green ball.

Test Your Understanding



- Where will we get the best estimator?

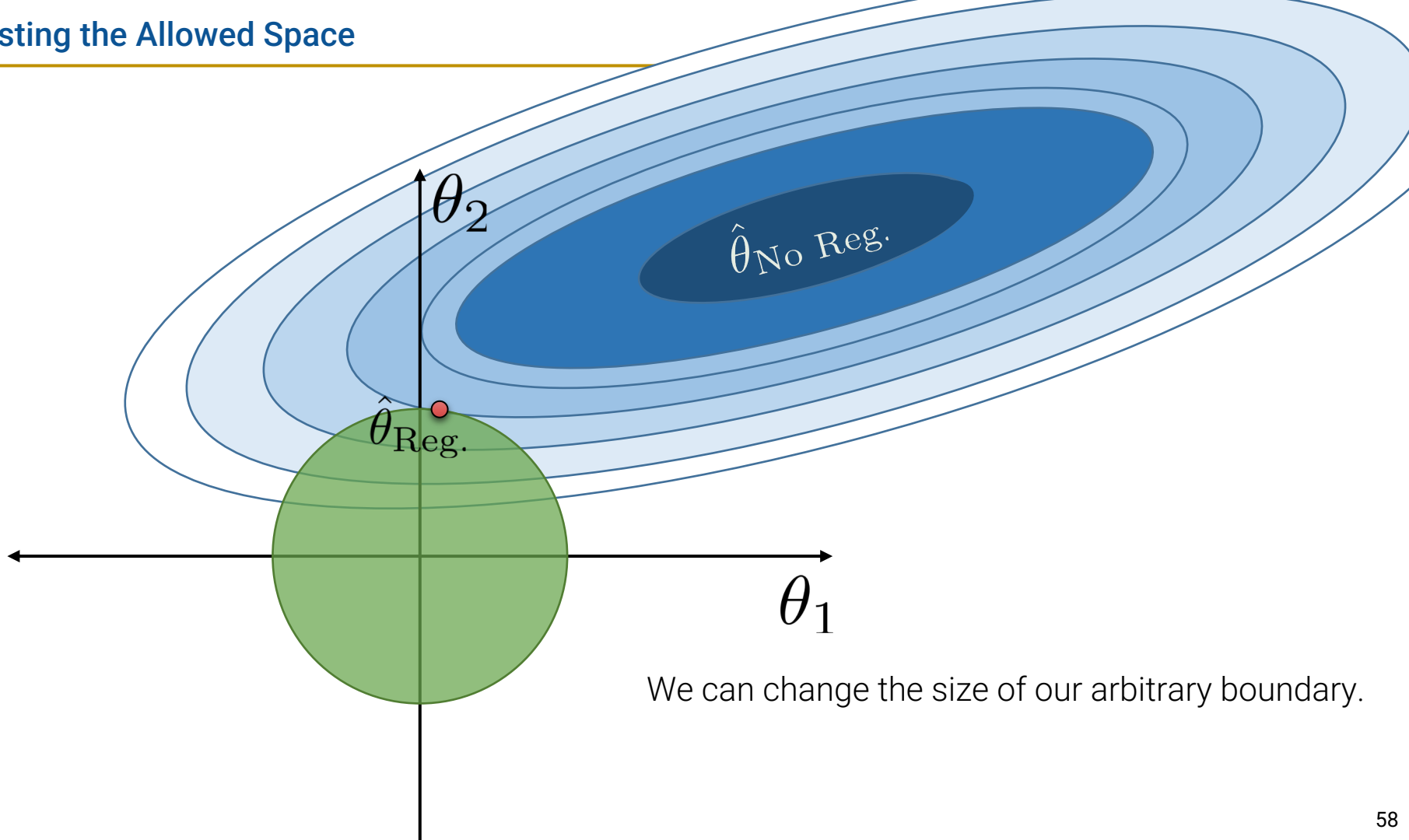
Constraining Regression



Regression ends up at $\hat{\theta}_{\text{Reg.}}$ instead.

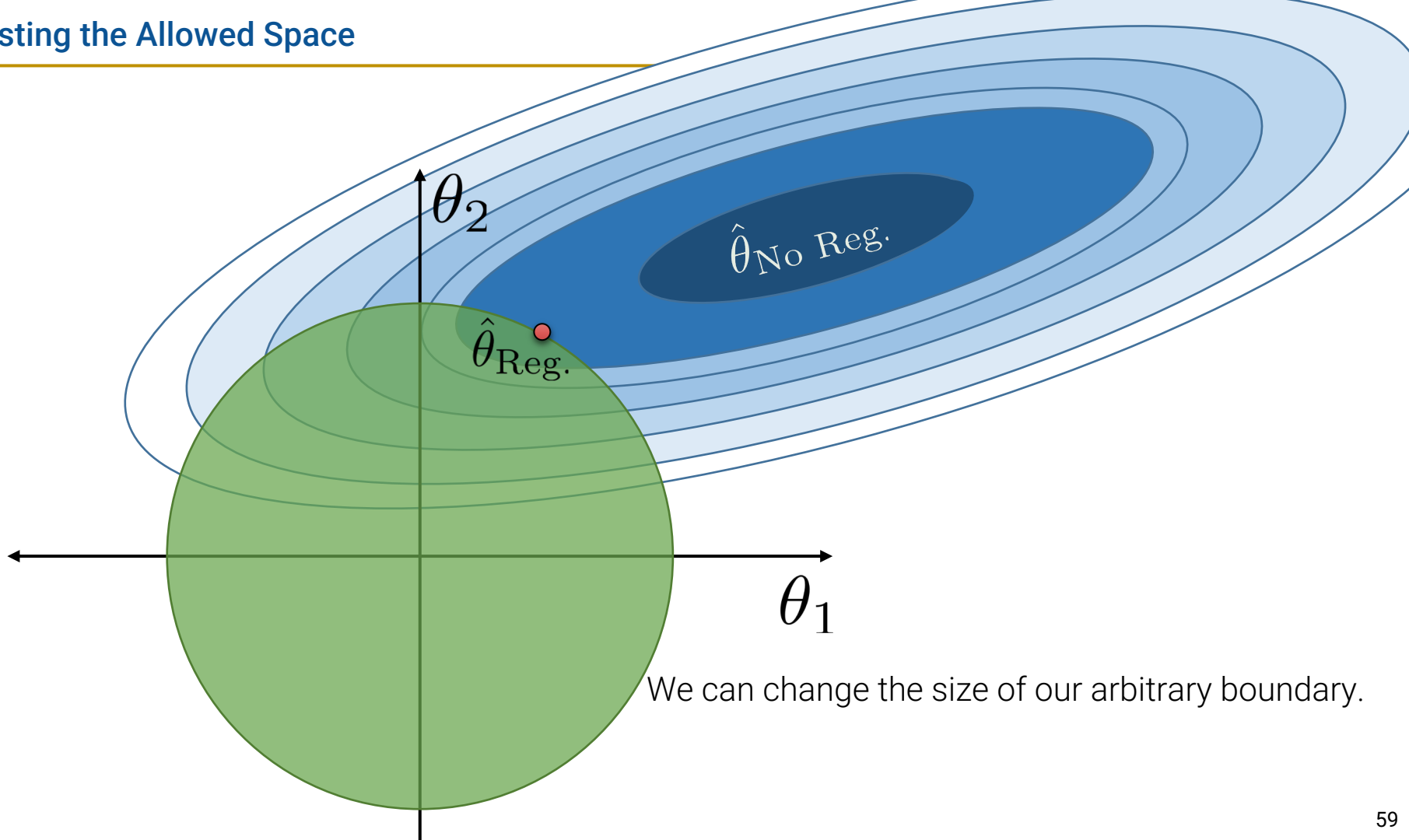
- Different than our unconstrained solution.
- Not optimal, but closer to origin!

Adjusting the Allowed Space



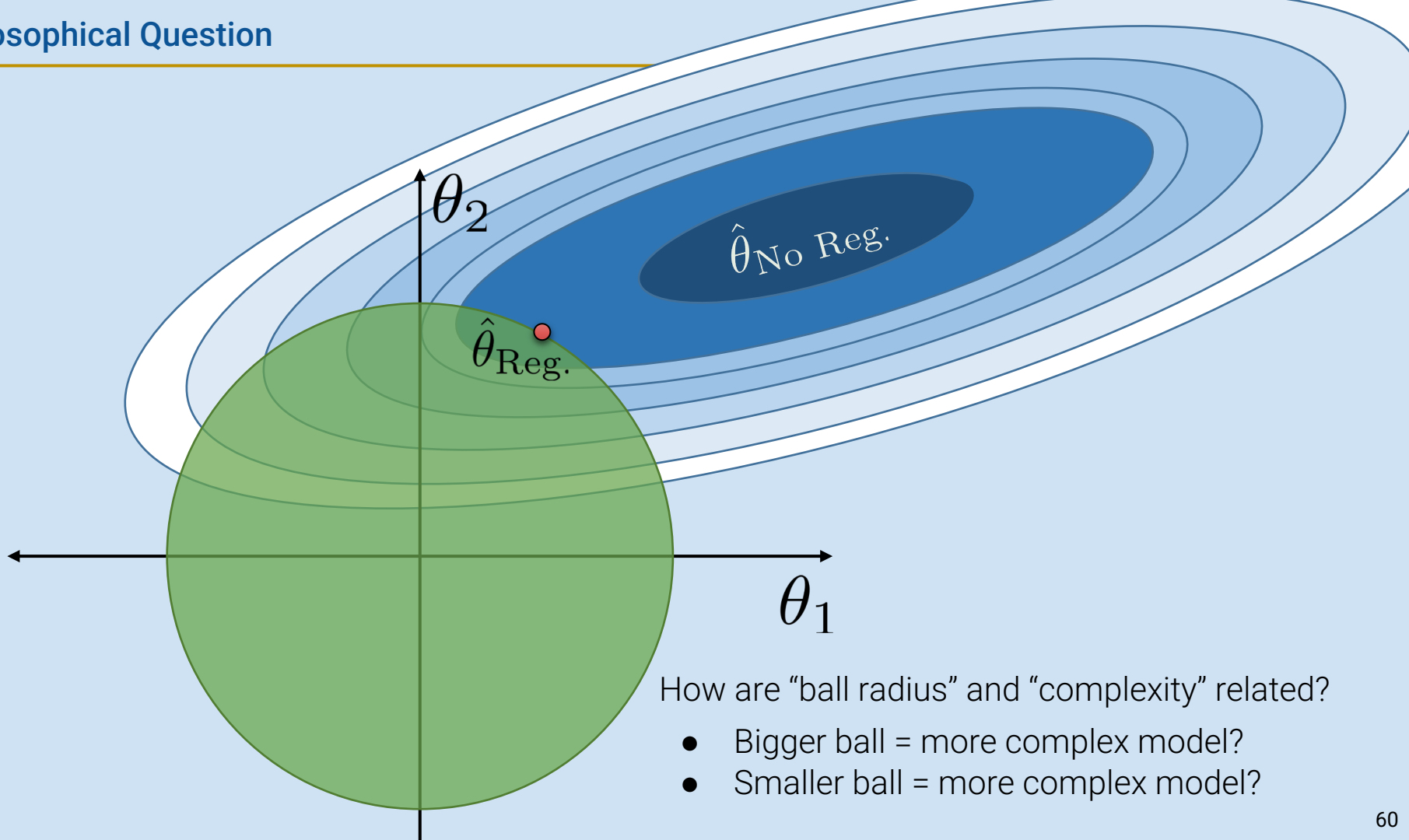
We can change the size of our arbitrary boundary.

Adjusting the Allowed Space



We can change the size of our arbitrary boundary.

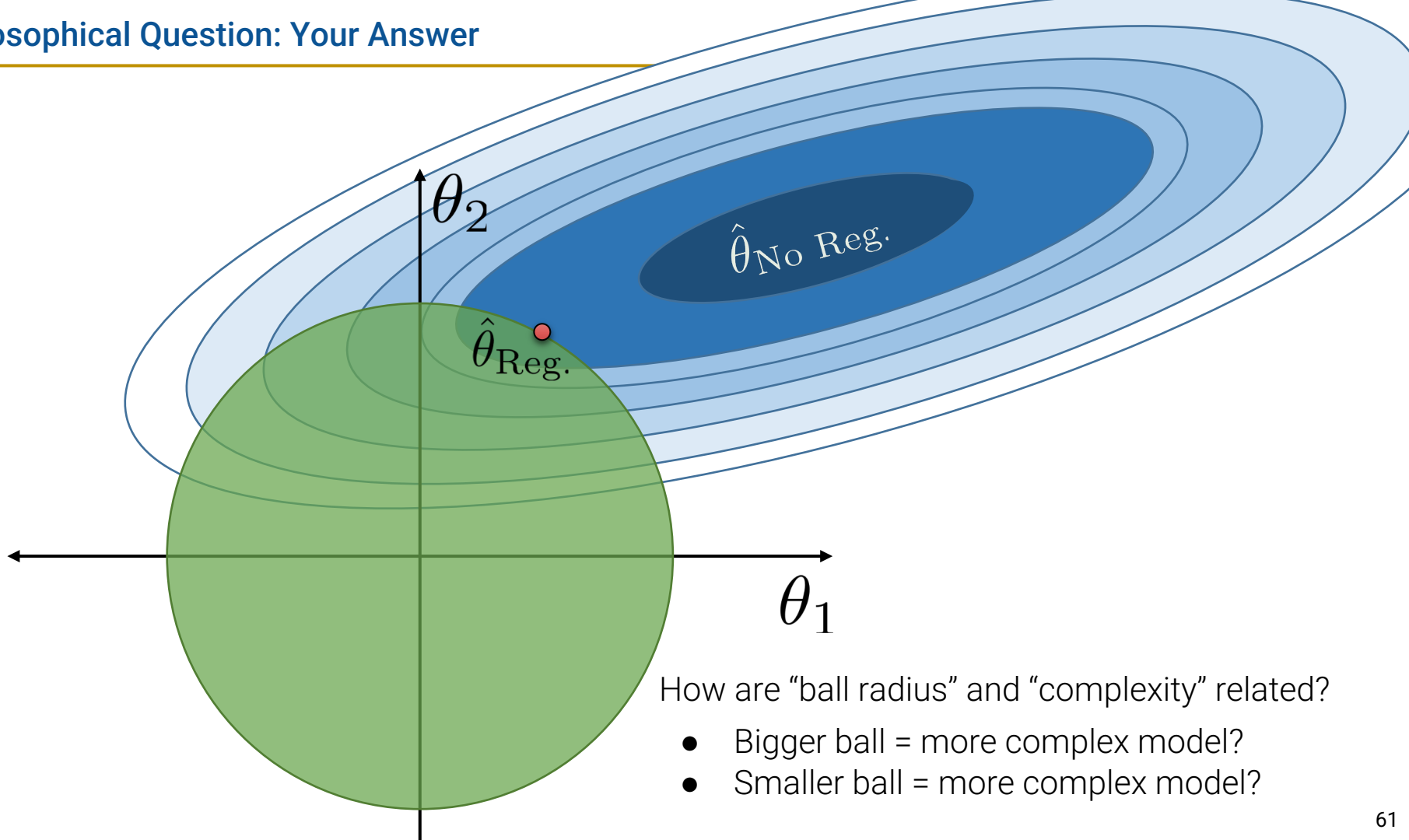
Philosophical Question



How are “ball radius” and “complexity” related?

- Bigger ball = more complex model?
- Smaller ball = more complex model?

Philosophical Question: Your Answer



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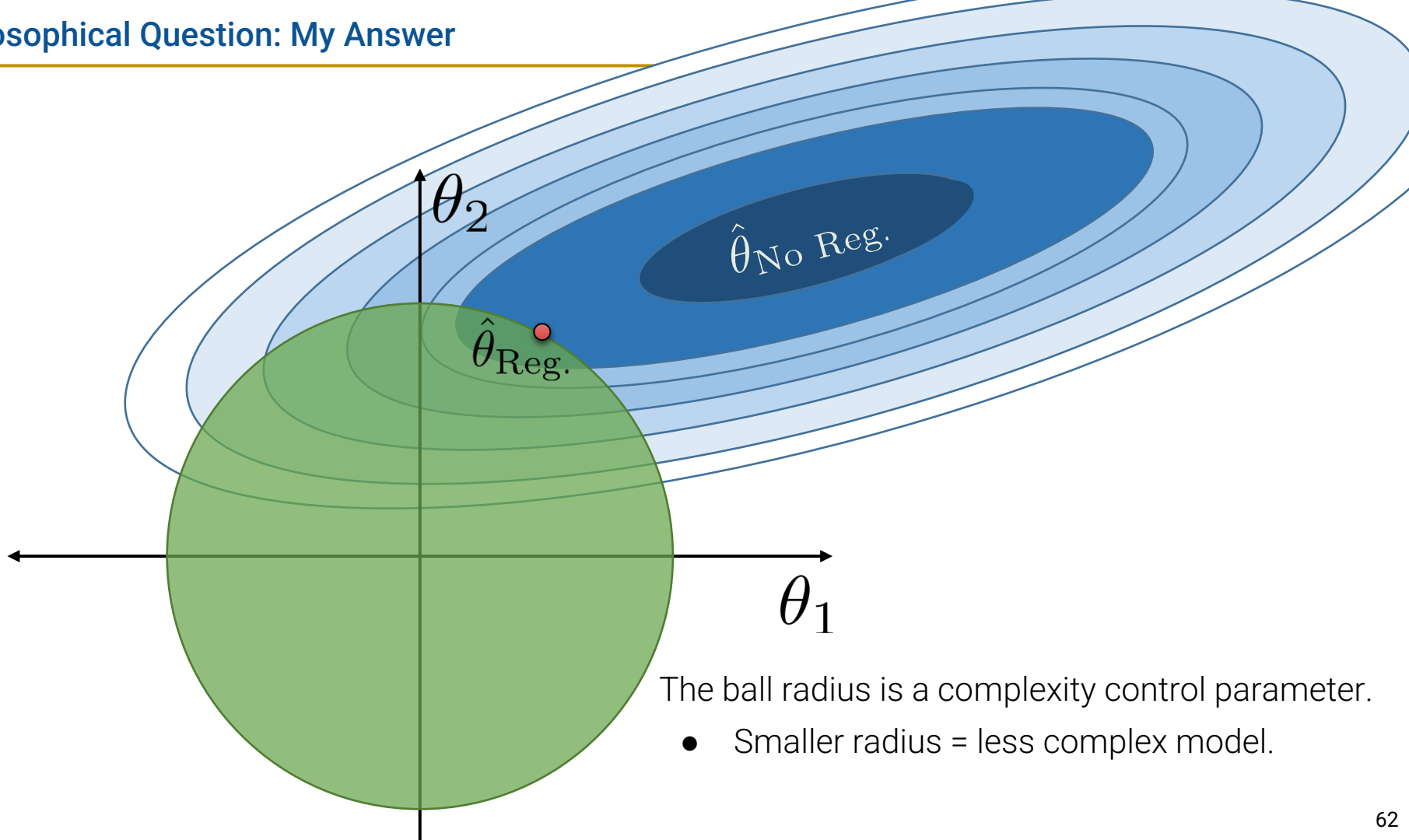
Philosophical Question: My Answer



The ball radius is a complexity control parameter.

- Smaller radius = less complex model.

Test Your Understanding

Let's return to our 9 feature model from before (d = 9).

- If we pick a very small ball radius, what kind of model will we have?

a. A model that only returns zero.
b. A constant model.
c. Ordinary least squares.
d. Something else.

$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
150.0	3433.0	304.0	22500.0	514950.0	45600.0	11785489.0	1043632.0	92416.0
140.0	3449.0	302.0	19600.0	482860.0	42280.0	11895601.0	1041598.0	91204.0
...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
82.0	2720.0	119.0	6724.0	223040.0	9758.0	7398400.0	323680.0	14161.0

Test Your Understanding Answer

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b. A constant model.
c. Ordinary least squares.
d. Something else.

$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

Answer: It depends!

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
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150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
150.0	3433.0	304.0	22500.0	514950.0	45600.0	11785489.0	1043632.0	92416.0
140.0	3449.0	302.0	19600.0	482860.0	42280.0	11895601.0	1041598.0	91204.0
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86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
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84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
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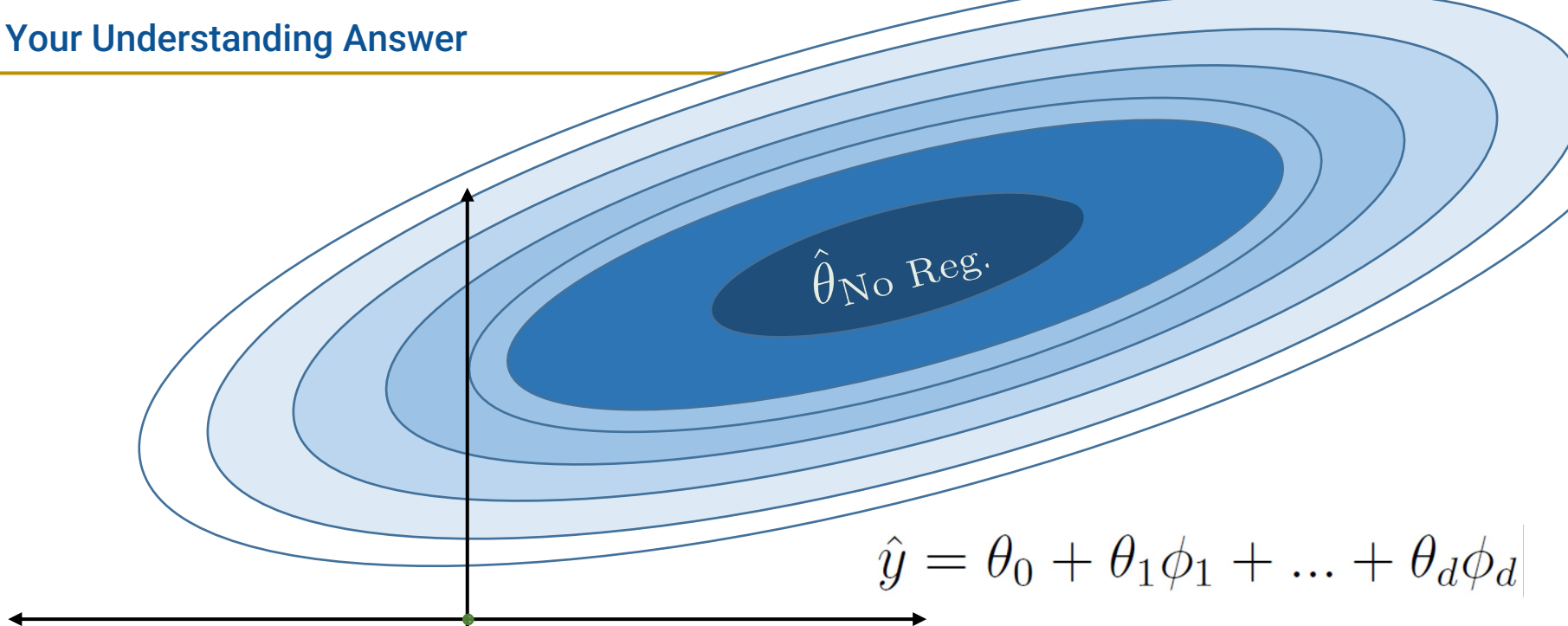
82.0	2720.0	119.0	6724.0	223040.0	9758.0	7398400.0	323680.0	14161.0

Test Your Understanding Answer

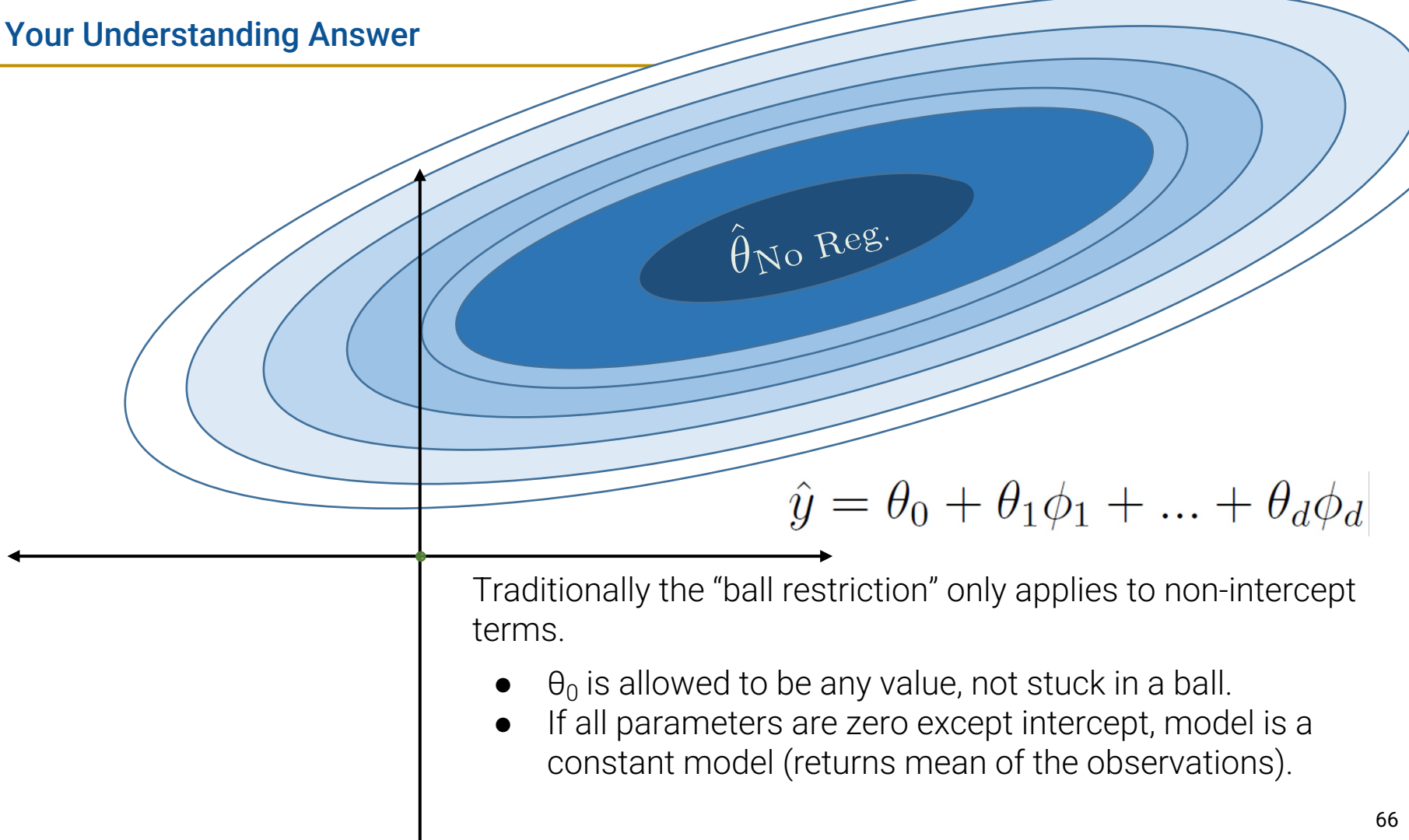


$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

If the ball is very tiny, our gradient descent is stuck near the origin.

- If all parameters are zero including intercept, model always outputs zero.
- If all parameters are zero except intercept, model is a constant model (returns mean of the observations).

Test Your Understanding Answer



$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

Traditionally the “ball restriction” only applies to non-intercept terms.

- θ_0 is allowed to be any value, not stuck in a ball.
- If all parameters are zero except intercept, model is a constant model (returns mean of the observations).

Test Your Understanding

Back to our 9 feature model from before (d = 9).

- If we pick a very large ball radius, what kind of model will we have?

a. A model that only returns zero.
b. A constant model.
c. Ordinary least squares.
d. Something else.

$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
150.0	3433.0	304.0	22500.0	514950.0	45600.0	11785489.0	1043632.0	92416.0
140.0	3449.0	302.0	19600.0	482860.0	42280.0	11895601.0	1041598.0	91204.0
...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
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Test Your Understanding Answer

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...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
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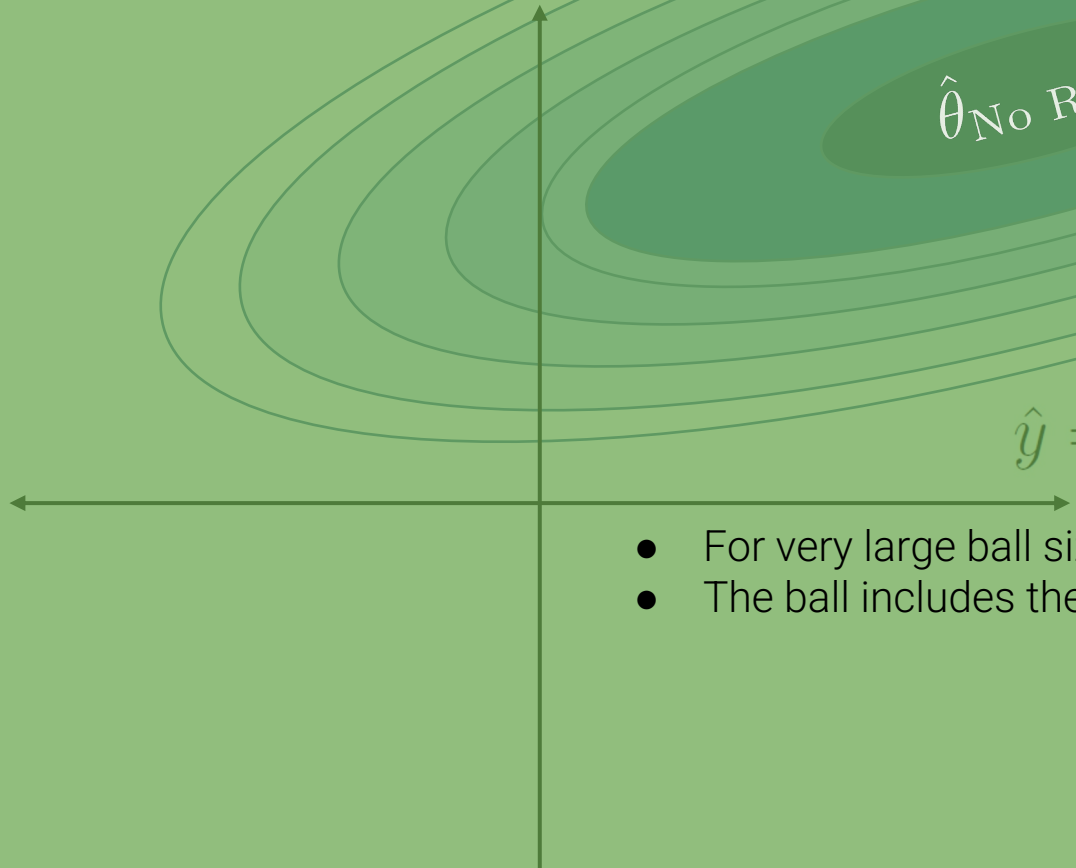
Test Your Understanding Answer



$$\hat{y} = \theta_0 + \theta_1\phi_1 + \ldots + \theta_d\phi_d$$

- For very large ball sizes, the restriction has no effect.
- The ball includes the OLS solution!

Training and Validation Errors vs. Ball Size for Our 9D Model

For very small ball size:

- Model behaves like a constant model. Can't actually use our 9 features!
- High **training error**, low variance, high **validation error**.

For very large ball size:

- Model behaves like OLS.
- **If we have tons of features**, results in overfitting. Low **training error**, high variance, high **validation error**.

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
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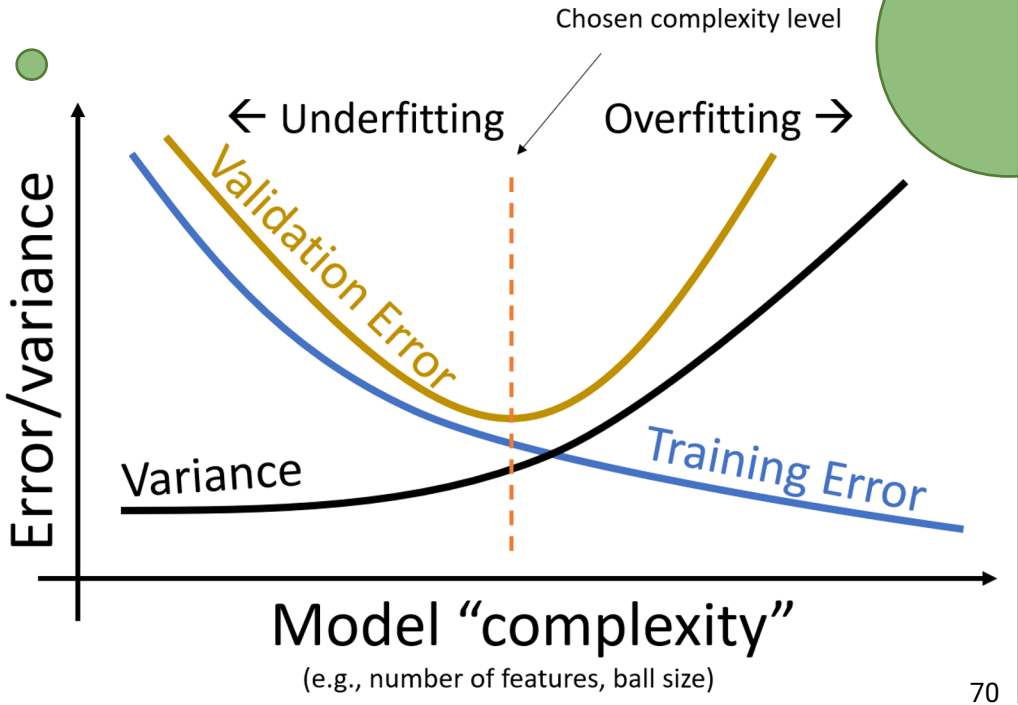
...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
82.0	2720.0	119.0	6724.0	223040.0	9758.0	7398400.0	323680.0	14161.0



L2 Regularization

Constraining our model's parameters to a ball around the origin is called **L2 Regularization**.

- The smaller the ball, the simpler the model.

Ordinary least squares. Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2$$

Ordinary least squares with **L2 regularization**. Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2$$

Such that θ_1 through θ_d live inside a ball of radius Q.

L2 Regularization

Constraining our model's parameters to a ball around the origin is called **L2 Regularization**.

- The smaller the ball, the simpler the model.

Ordinary least squares. Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2$$

Ordinary least squares with **L2 regularization**. Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2 \quad \textbf{such that} \quad \sum_{j=1}^{d}\theta_j^2 \leq Q$$

Note, intercept term not included!

L2 Regularized Least Squares in sklearn

We can run least squares with an **L2 regularization term** by using the “Ridge” class.

```
from sklearn.linear_model import Ridge
ridge_model = Ridge(alpha = 10000)
ridge_model.fit(vehicle_data_with_squared_features, vehicle_data["mpg"])
```

Coefficients we get back:

```
ridge_model.coef_
```

```
array([-5.56414449e-02, -7.93804083e-03, -8.22081425e-02, -6.18785466e-04,
       -2.55492157e-05,  9.47353944e-04,  7.58061062e-07,  1.07439477e-05,
       -1.64344898e-04])
```

Note: sklearn’s “alpha” parameter is proportional to the inverse of the ball radius!

- Large alpha means small ball.

L2 Regularized Least Squares in sklearn

We can run least squares with an **L2 regularization term** by using the “Ridge” class.

```
from sklearn.linear_model import Ridge
ridge_model = Ridge(alpha = 10**-5)
ridge_model.fit(vehicle_data_with_squared_features, vehicle_data["mpg"])
```

For a tiny alpha, the coefficients are larger:

```
ridge_model.coef_
```

```
array([-1.35872588e-01, -1.46864458e-04, -1.18230336e-01, -4.03590098e-04,
       -1.12862371e-05,  8.25179864e-04, -1.17645881e-06,  2.69757832e-05,
       -1.72888463e-04])
```

Note: sklearn’s “alpha” parameter is proportional to the inverse of the ball radius!

- Small alpha means large ball.

L2 Regularized Least Squares in sklearn

We can run least squares with an **L2 regularization term** by using the "Ridge" class. For a tiny alpha, the coefficients are also about the same as a standard OLS model's coefficients!

```
ridge_model.coef_
```

```
array([-1.35872588e-01, -1.46864458e-04, -1.18230336e-01, -4.03590098e-04,
       -1.12862371e-05,  8.25179864e-04, -1.17645881e-06,  2.69757832e-05,
       -1.72888463e-04])
```

```
from sklearn.linear_model import LinearRegression
linear_model = LinearRegression()
linear_model.fit(vehicle_data_with_squared_features, vehicle_data["mpg"])
linear_model.coef_
```

```
array([-1.35872588e-01, -1.46864447e-04, -1.18230336e-01, -4.03590097e-04,
       -1.12862370e-05,  8.25179863e-04, -1.17645882e-06,  2.69757832e-05,
       -1.72888463e-04])
```

Green ball includes the OLS solution!

Terminology Note

Why does sklearn use the word “Ridge”?

Because least squares with an **L2 regularization term** is also called “**Ridge Regression**”.

- Term is historical. Doesn’t really matter.

Lagrangian Duality

Problem 1: Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2 \quad \textbf{such that} \quad \sum_{j=1}^{d}\theta_j^2 \leq Q$$

Problem 2: Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_{i,1} + \ldots + \theta_d\phi_{i,d}))^2 + \alpha\sum_{j=1}^{d}\theta_j^2$$

The “objective function” that gradient descent is minimizing now has an extra term.

Intuitively, this extra **right term penalizes large thetas**.

Mathematical Note

Ridge Regression has a closed form solution which we will not derive.

- Note: The solution exists even if the feature matrix has collinearity between its columns.

$$\hat{\theta}_{ridge} = (\mathbb{X}^T\mathbb{X} + n\alpha I)^{-1}\mathbb{X}^T\mathbb{Y}$$

Identity matrix

- This solution exists **even if** $\mathbb{X}$ is not full rank – an important reason why we often prefer L2 regularization.

Scaling Data for Regularization

Cross Validation

- The Holdout Method
- K-Fold Cross Validation
- Test Sets

Regularization

- L2 Regularization (Ridge)
- **Scaling Data for Regularization**
- L1 Regularization (LASSO)

One Issue With Our Approach

Our data from before has features of quite different numerical scale!

- Optimal theta for hp will probably be much further from origin than theta for weight^2.

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
150.0	3436.0	318.0	22500.0	515400.0	47700.0	11806096.0	1092648.0	101124.0
150.0	3433.0	304.0	22500.0	514950.0	45600.0	11785489.0	1043632.0	92416.0
140.0	3449.0	302.0	19600.0	482860.0	42280.0	11895601.0	1041598.0	91204.0
...	...	...	...	...	...	...	...	...
86.0	2790.0	140.0	7396.0	239940.0	12040.0	7784100.0	390600.0	19600.0
52.0	2130.0	97.0	2704.0	110760.0	5044.0	4536900.0	206610.0	9409.0
84.0	2295.0	135.0	7056.0	192780.0	11340.0	5267025.0	309825.0	18225.0
79.0	2625.0	120.0	6241.0	207375.0	9480.0	6890625.0	315000.0	14400.0
82.0	2720.0	119.0	6724.0	223040.0	9758.0	7398400.0	323680.0	14161.0

Theta will tend to be smaller for weight^2 than other parameters

Coefficients from Earlier

hp	weight	displacement	hp^2	hp weight	hp displacement	weight^2	weight displacement	displacement^2
130.0	3504.0	307.0	16900.0	455520.0	39910.0	12278016.0	1075728.0	94249.0
165.0	3693.0	350.0	27225.0	609345.0	57750.0	13638249.0	1292550.0	122500.0
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```
ridge_model.coef_
```

```
array([-1.35872588e-01, -1.46864458e-04, -1.18230336e-01, -4.03590098e-04,
       -1.12862371e-05,  8.25179864e-04, -1.17645881e-06,  2.69757832e-05,
       -1.72888463e-04])
```

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.

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

L1 Regularization (LASSO)

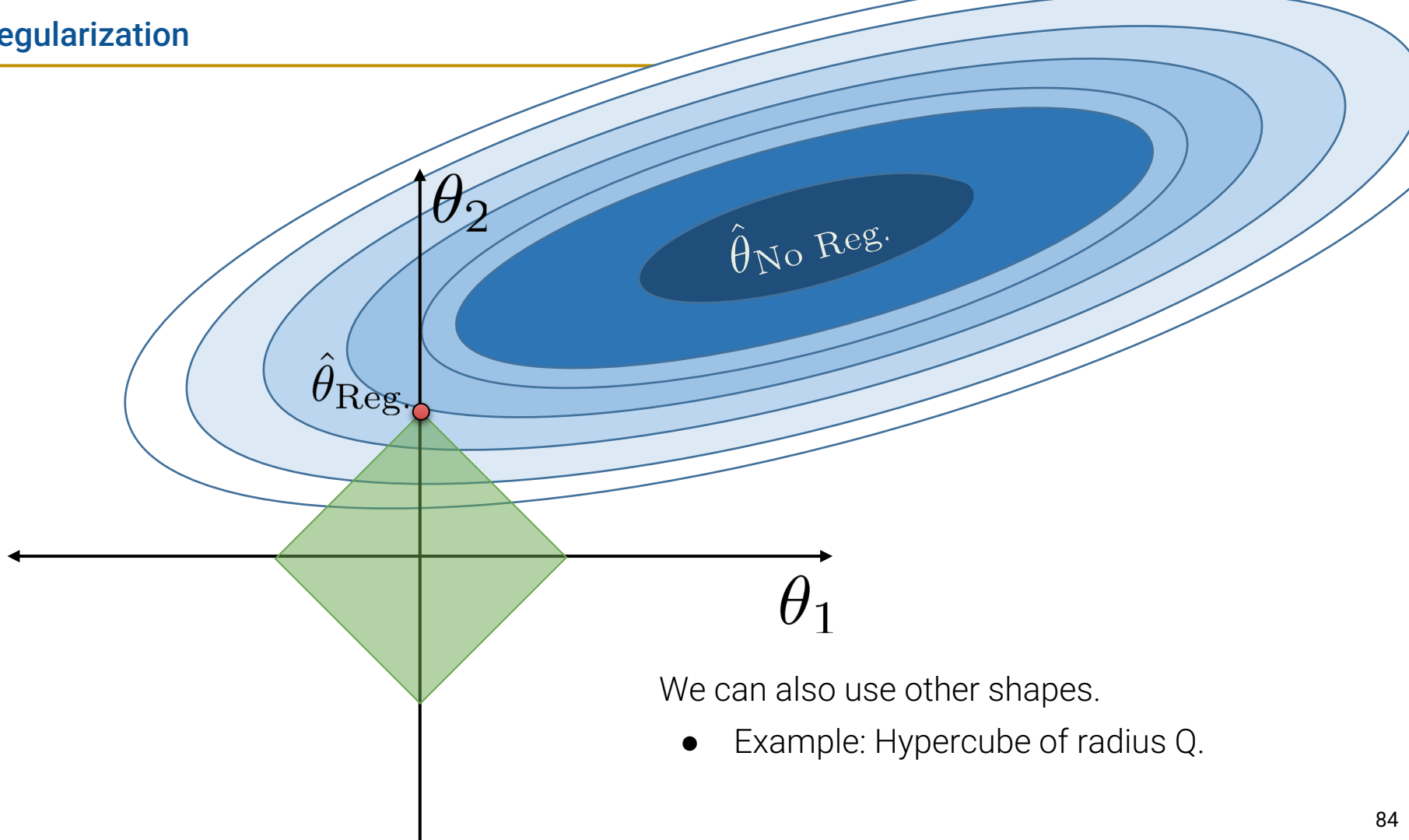
Cross Validation

- The Holdout Method
- K-Fold Cross Validation
- Test Sets

Regularization

- L2 Regularization (Ridge)
- Scaling Data for Regularization
- **L1 Regularization (LASSO)**

L1 Regularization



We can also use other shapes.

- Example: Hypercube of radius Q.

L1 Regularization in Equation Form

Using a hypercube is known as **L1 regularization**. Expressed mathematically in the two equivalent forms below:

Problem 1: Find thetas that minimize:

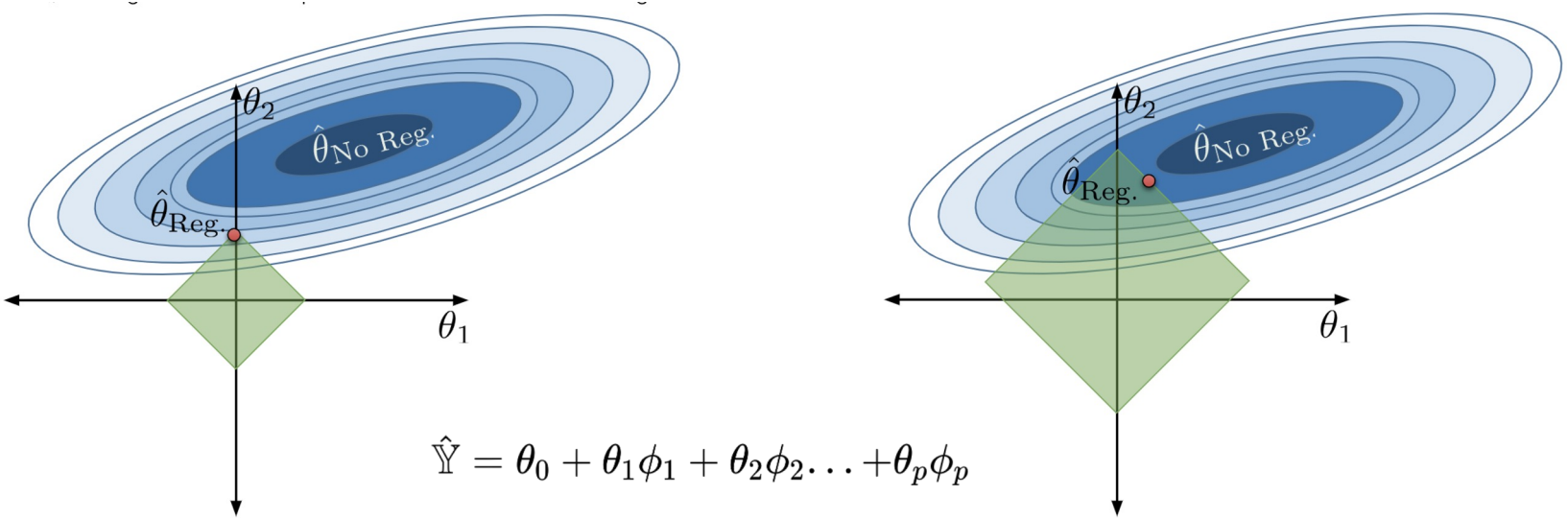
$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_1 + ... + \theta_d\phi_d))^2 \qquad \textbf{such that} \sum_{j=1}^{d}|\theta_j| \leq Q$$

Problem 2: Find thetas that minimize:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1\phi_1 + ... + \theta_d\phi_d))^2 + \alpha\sum_{j=1}^{d}|\theta_j|$$

Size of Q

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



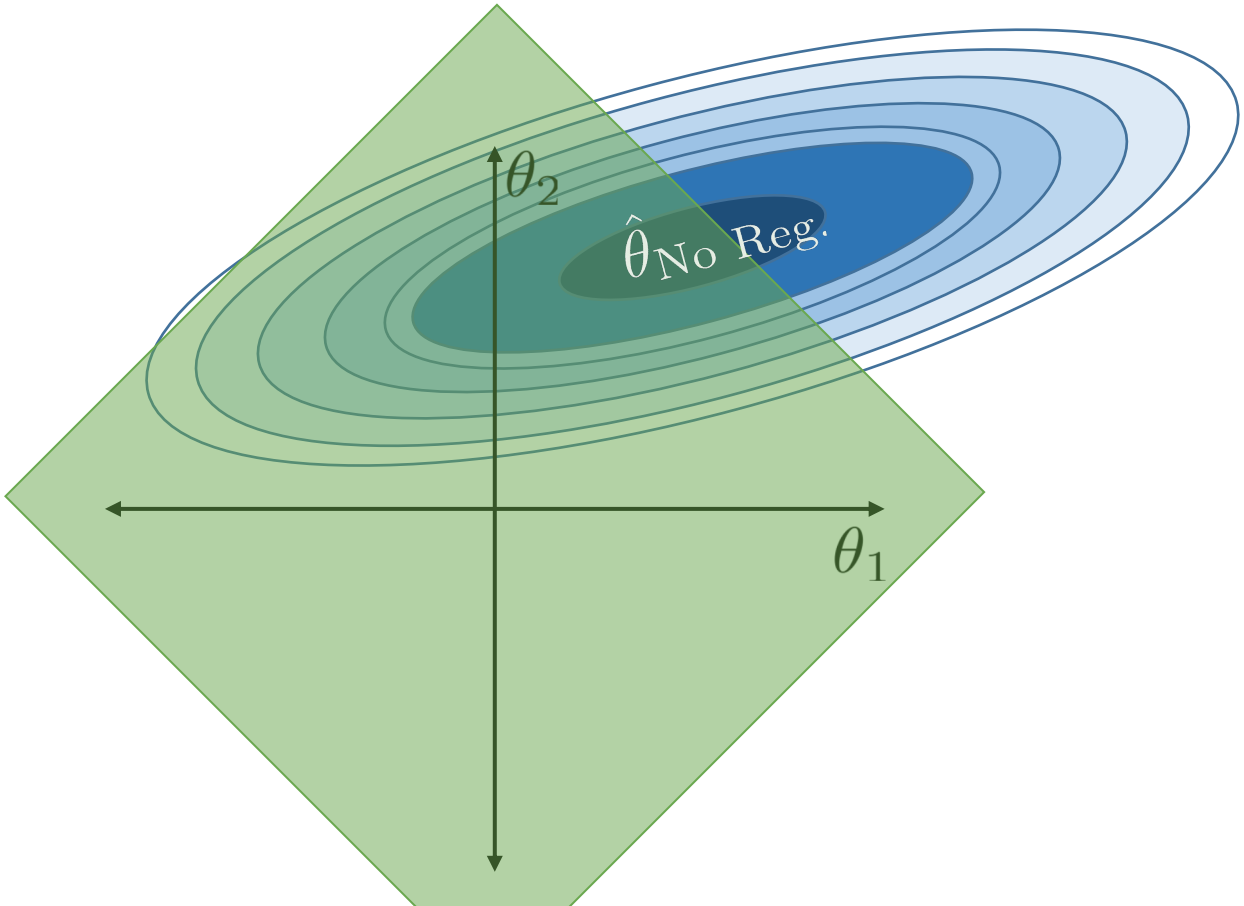
$$\hat{\mathbb{Y}} = \theta_0 + \theta_1\phi_1 + \theta_2\phi_2 \ldots + \theta_p\phi_p$$

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.

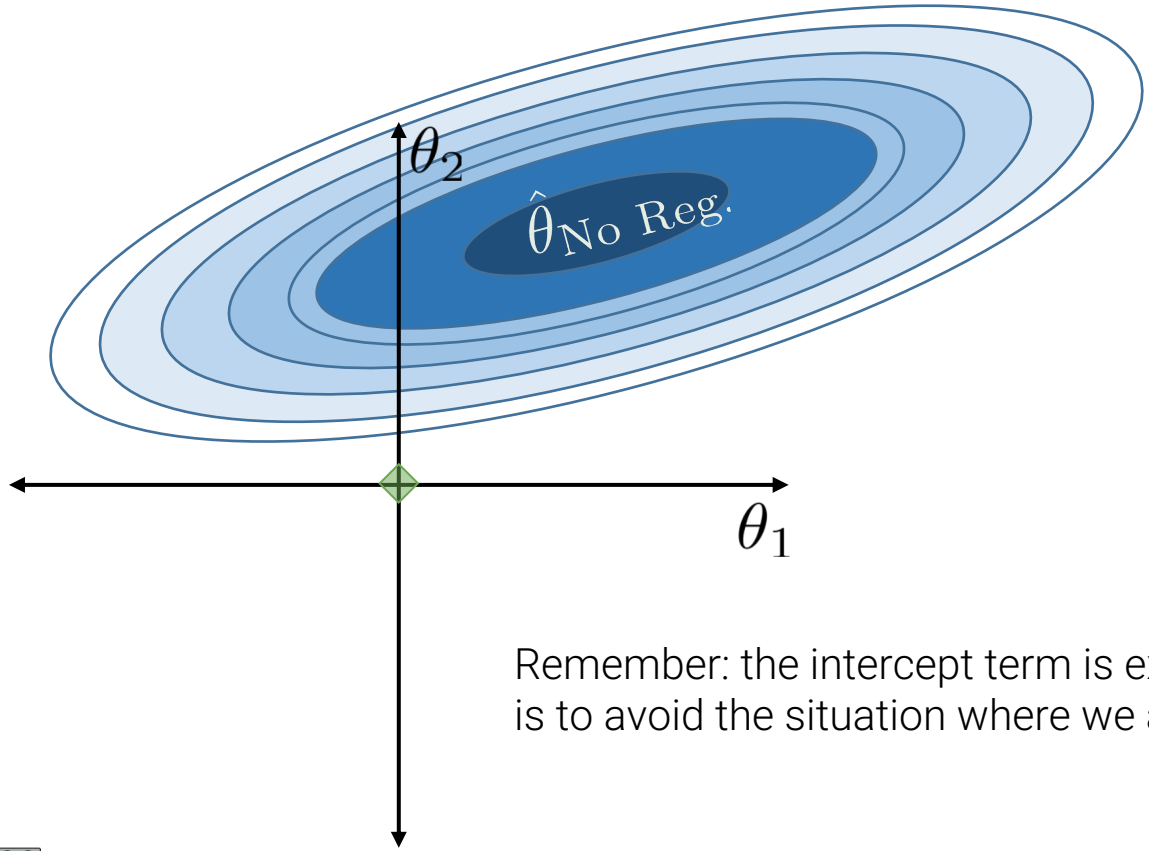
Size of Q

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:

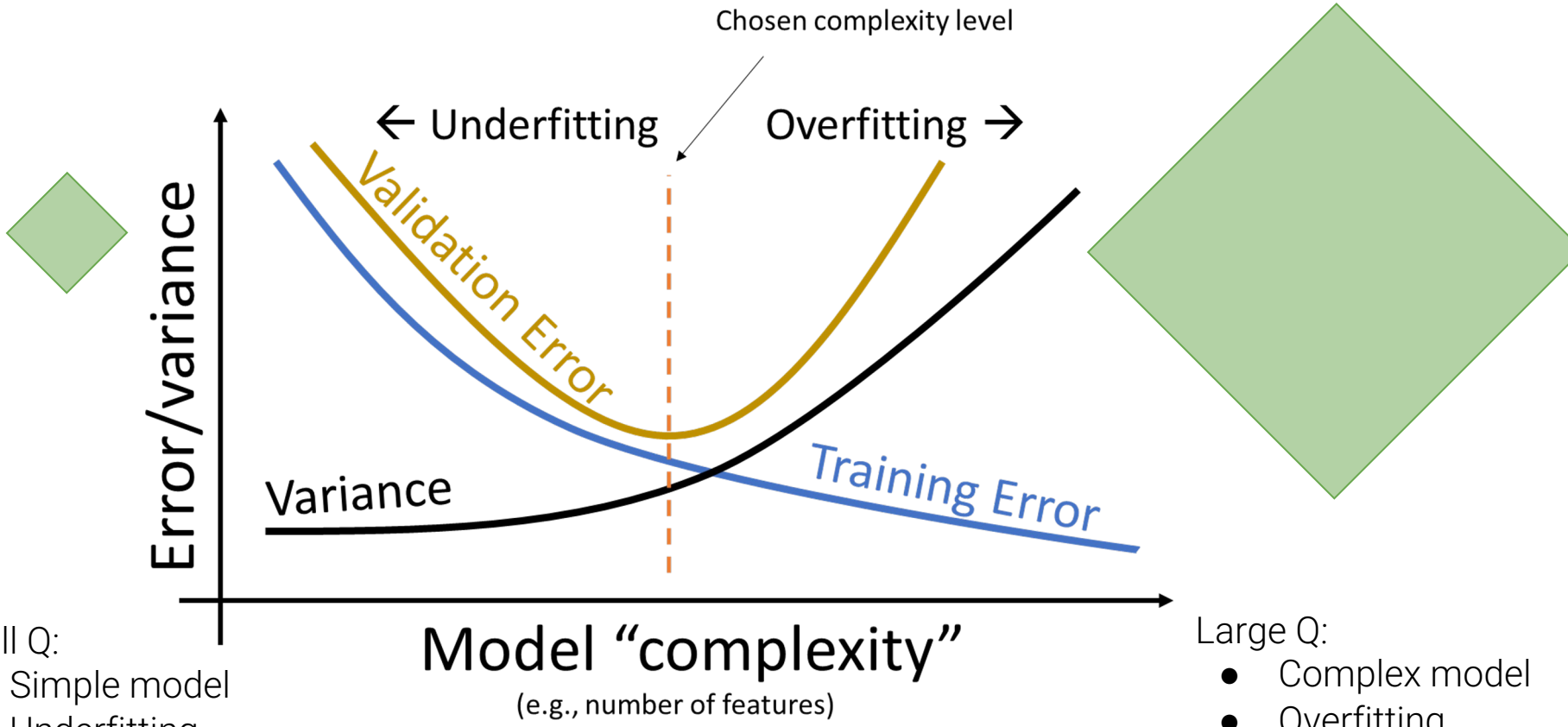
$$\hat{\mathbb{Y}} = (0)\phi_1 + (0)\phi_2 + \ldots = 0$$

If the model has an intercept term:

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

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 Regularized OLS in sklearn

In sklearn, we use the Lasso module.

- Note: Performing OLS with L1 regularization is also called **LASSO regression**.

```
from sklearn.linear_model import Lasso
lasso_model = Lasso(alpha = 10**1)
lasso_model.fit(vehicle_data_with_squared_features, vehicle_data["mpg"])
lasso_model.coef_
```

```
array([-0.00000000e+00, -1.88104942e-02, -0.00000000e+00, -1.19625308e-03,
        8.84657720e-06,  8.77253835e-04,  3.16759194e-06, -3.21738391e-05,
       -1.29386937e-05])
```

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.

Summary of Regression Methods

Our regression models are summarized below.

- The “Objective” column gives the function that our gradient descent optimizer minimizes.
- Note that this table uses lambda instead of alpha for regularization strength. Both are common.

Name	Model	Loss	Reg.	Objective	Solution
OLS	$\hat{\mathbb{Y}} = \mathbb{X}\theta$	Squared loss	None	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2$	$\hat{\theta}_{\text{OLS}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$
Ridge Regression	$\hat{\mathbb{Y}} = \mathbb{X}\theta$	Squared loss	L2	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2 + \lambda\sum_{j=1}^{d}\theta_i^2$	$\hat{\theta}_{\text{ridge}} = (\mathbb{X}^T\mathbb{X} + n\lambda I)^{-1}\mathbb{X}^T\mathbb{Y}$
LASSO	$\hat{\mathbb{Y}} = \mathbb{X}\theta$	Squared loss	L1	$\frac{1}{n}\|\|\mathbb{Y} - \mathbb{X}\theta\|\|_2^2 + \lambda\sum_{j=1}^{d}\|\theta_i\|$	**No closed form**