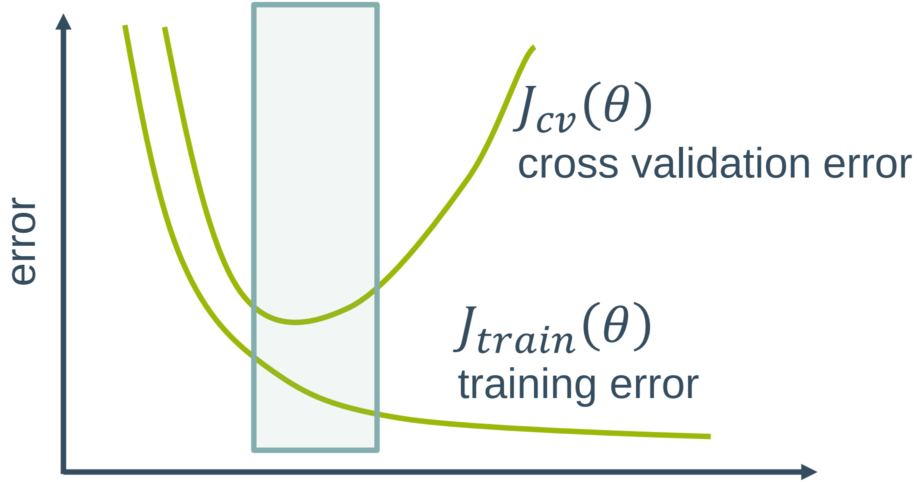
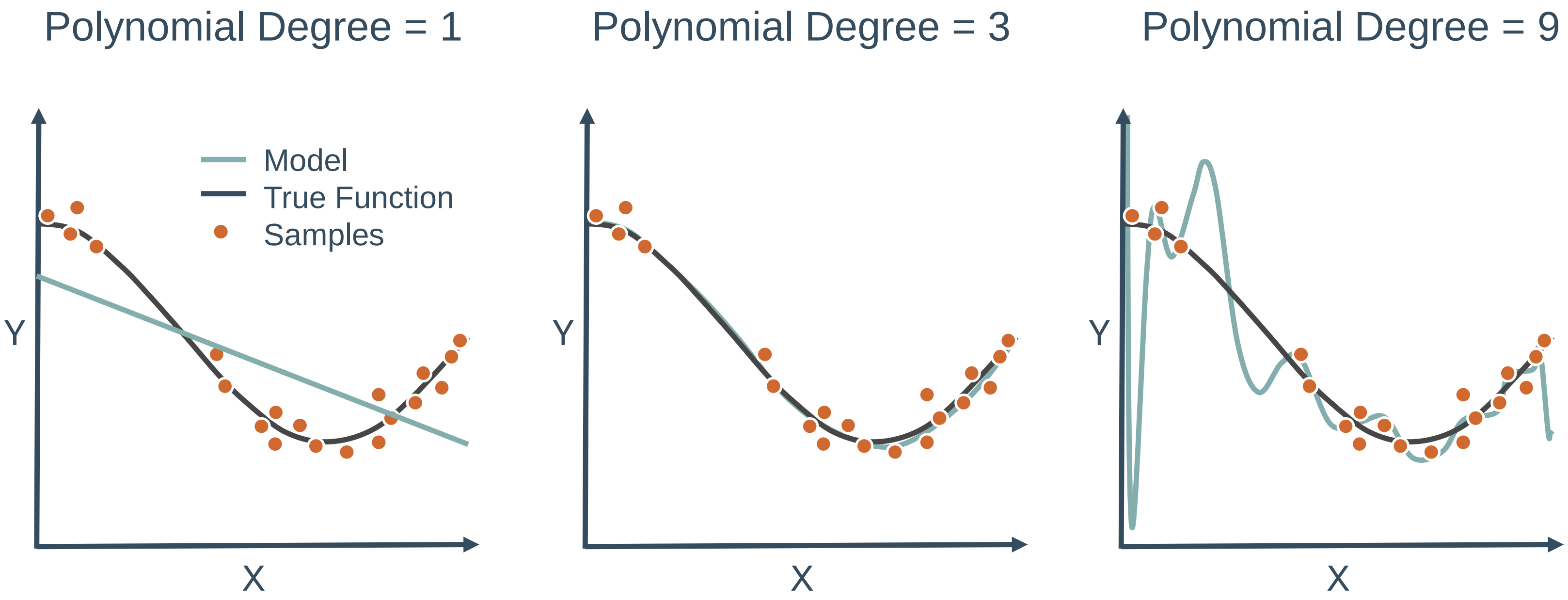
Intel Nervana™ AI Academy

REGULARIZATION AND FEATURE SELECTION

MODEL COMPLEXITY VS ERROR

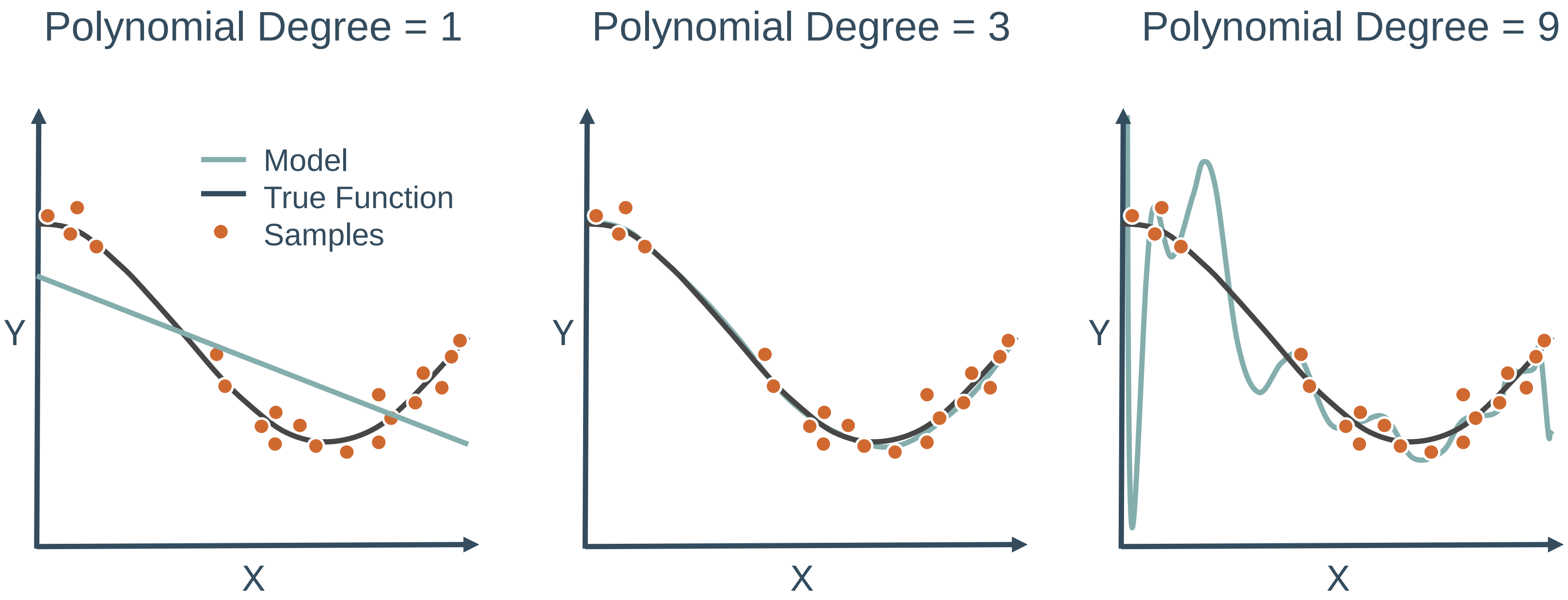


PREVENTING UNDER—AND OVERFITTING



How to use a degree 9 polynomial and prevent overfitting?

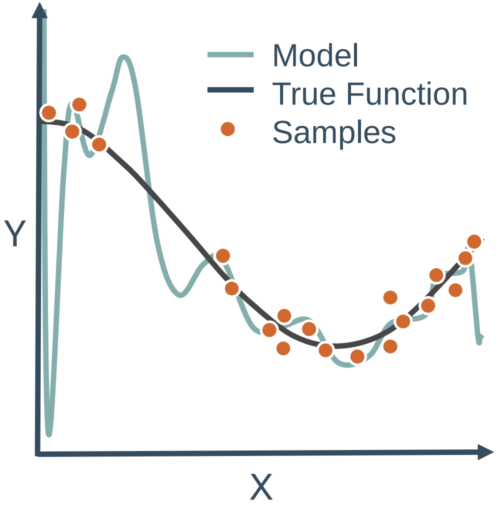
PREVENTING UNDER—AND OVERFITTING



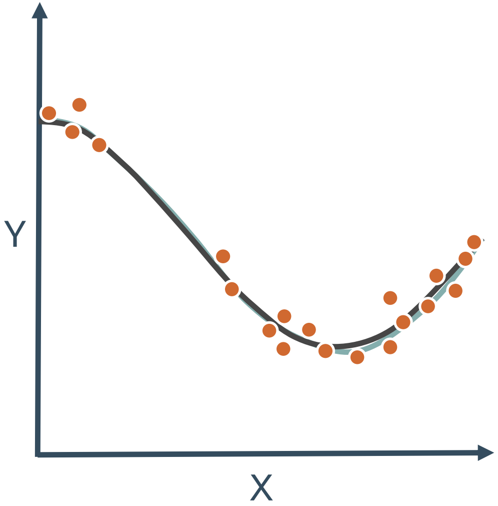
$$J(\beta_0, \beta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

REGULARIZATION

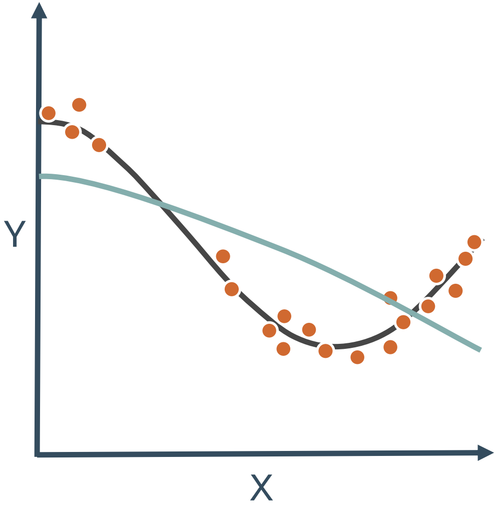
Poly Degree=9, λ=0.0



Poly Degree=9, λ=1e-5



Poly Degree=9, λ=0.1



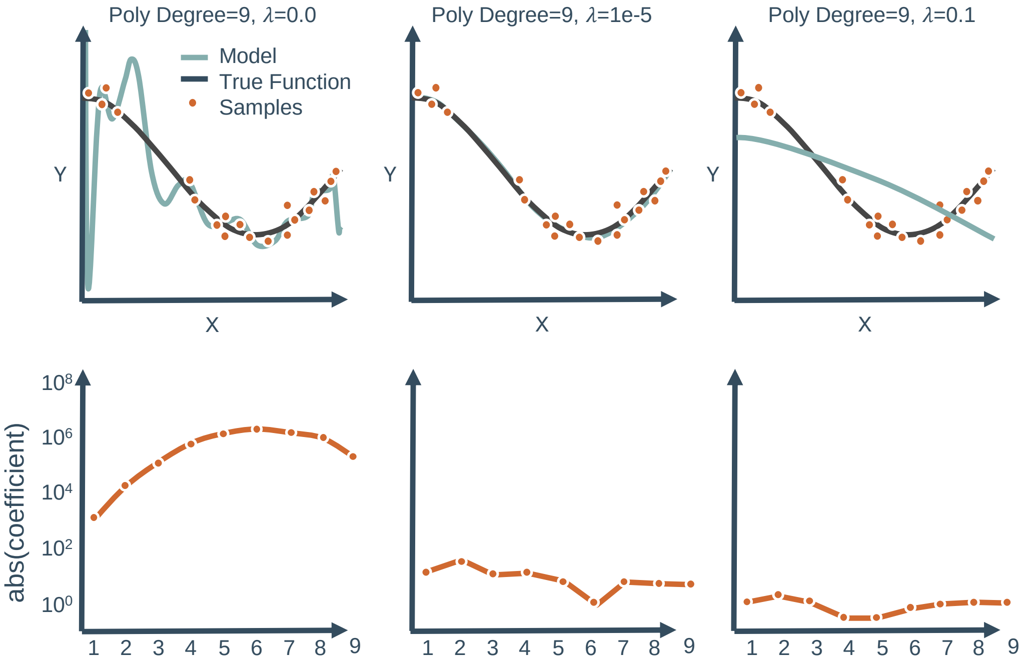
$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2 + \lambda \sum_{j=1}^{k} {\beta_j}^2$$

RIDGE REGRESSION (L2)

$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2 + \lambda \sum_{j=1}^{k} \beta_j{}^2$$

- Penalty shrinks magnitude of all coefficients
- Larger coefficients strongly penalized because of the squaring

EFFECT OF RIDGE REGRESSION ON PARAMETERS



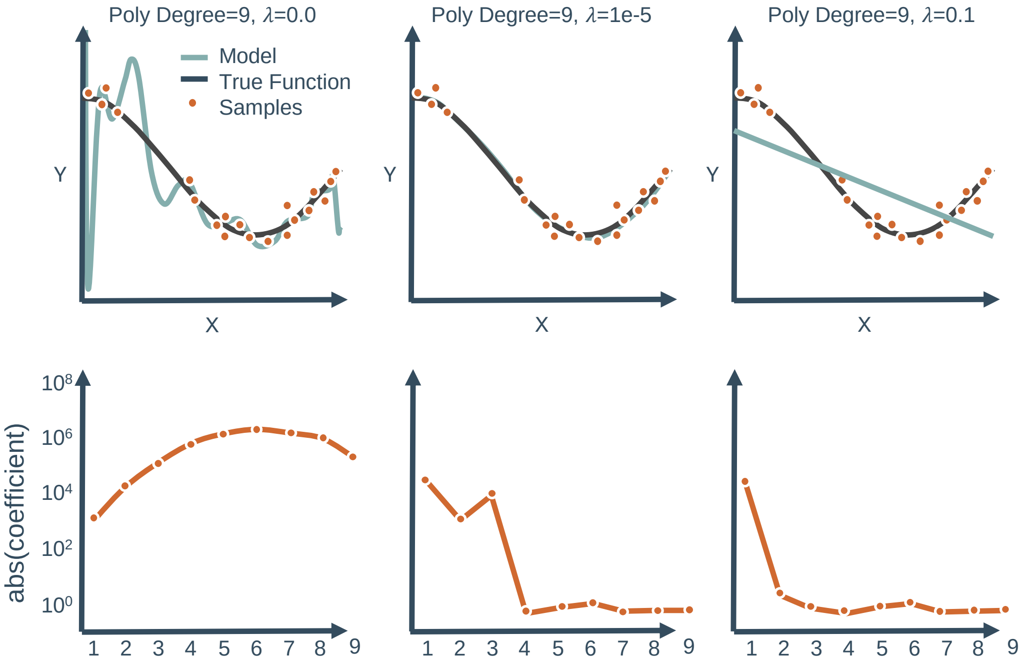
$$J(\beta_0, \beta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2 + \lambda \sum_{j=1}^{k} {\beta_j}^2$$

LASSO REGRESSION (L1)

$$J(\beta_0, \beta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2 + \lambda\sum_{j=1}^{k}|\beta_j|$$

- Penalty selectively shrinks some coefficients
- Can be used for feature selection
- Slower to converge than Ridge regression

EFFECT OF LASSO REGRESSION ON PARAMETERS



$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2 + \lambda \sum_{j=1}^{k} |\beta_j|$$

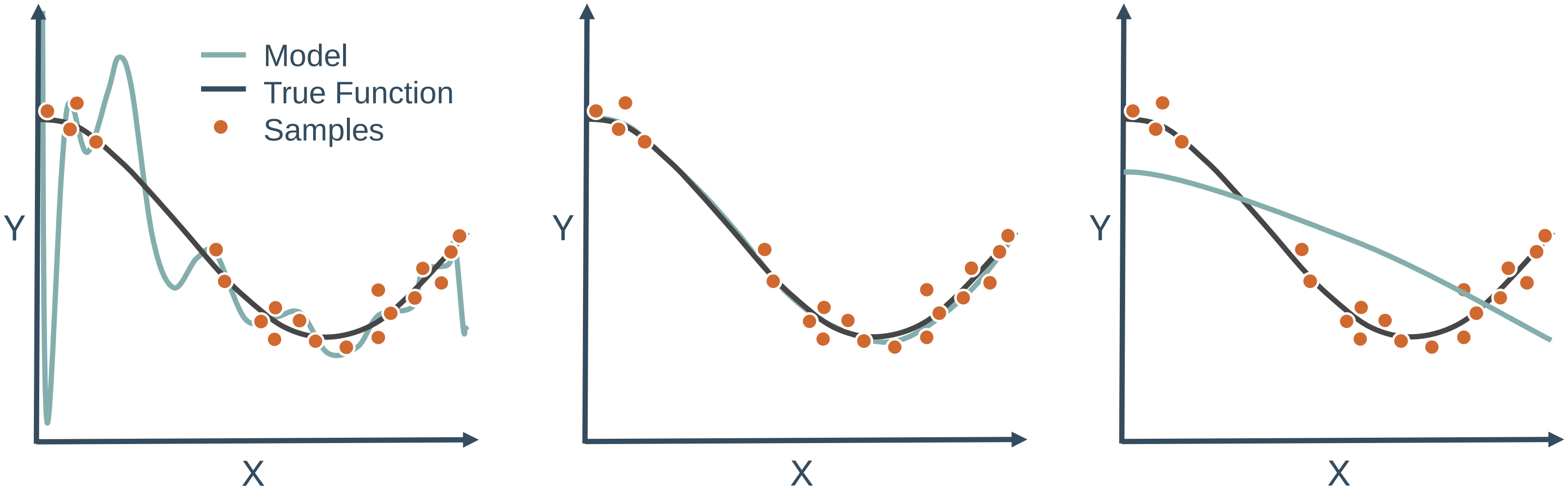
ELASTIC NET REGULARIZATION

$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2 + \lambda_1 \sum_{j=1}^{k} \left| \beta_j \right| + \lambda_2 \sum_{j=1}^{k} \beta_j^2$$

- Compromise of both Ridge and Lasso regression
- Requires tuning of additional parameter that distributes regularization penalty between L1 and L2

ELASTIC NET REGULARIZATION

Poly Degree=9, λ=0.0 | Poly Degree=9, λ=1e-5 | Poly Degree=9, λ=0.1



$$J(\beta_0, \beta_1) = \frac{1}{2m}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2 + \lambda_1 \sum_{j=1}^{k}\left|\beta_j\right| + \lambda_2 \sum_{j=1}^{k}\beta_j^2$$

HYPERPARAMETERS AND THEIR OPTIMIZATION

- Regularization coefficients (λ_1 and λ_2) are empirically determined

Use Test Data to Tune λ?

	Date	Title	Budget	DomesticTotalGross	Director	Rating	Runtime
0	2013-11-22	The Hunger Games: Catching Fire	130000000	424668047	Francis Lawrence	PG-13	146
1	2013-05-03	Iron Man 3	200000000	409013994	Shane Black	PG-13	129
2	2013-11-22	Frozen	150000000	400738009	Chris BuckJennifer Lee	PG	108
3	2013-07-03	Despicable Me 2	76000000	368061265	Pierre CoffinChris Renaud	PG	98
4	2013-06-14	Man of Steel	225000000	291045518	Zack Snyder	PG-13	143
5	2013-10-04	Gravity	[illegible]	[illegible]	Cuaron	PG-13	91
6	2013-06-21	Monsters University	[illegible]	[illegible]	anlon	G	107
7	2013-12-13	The Hobbit: The Deso	[illegible]	[illegible]	ckson	PG-13	161
8	2013-05-24	Fast & Furious 6	[illegible]	[illegible]	in	PG-13	130
9	2013-03-08	Oz The Great and Powerful	215000000	234911825	Sam Raimi	PG	127
10	2013-05-16	Star Trek Into Darkness	190000000	228778661	J.J. Abrams	PG-13	123
11	2013-11-08	Thor: The Dark World	170000000	206362140	Alan Taylor	PG-13	120
12	2013-06-21	World War Z	190000000	202359711	Marc Forster	PG-13	116
13	2013-03-22	The Croods	135000000	187168425	Kirk De MiccoChris Sanders	PG	98
14	2013-06-28	The Heat	[illegible]	[illegible]	g	R	117
15	2013-08-07	We're the Millers	[illegible]	[illegible]	Marshall Thurber	R	110
16	2013-12-13	American Hustle	[illegible]	[illegible]	. Russell	R	138
17	2013-05-10	The Great Gatsby	105000000	144840419	Baz Luhrmann	PG-13	143

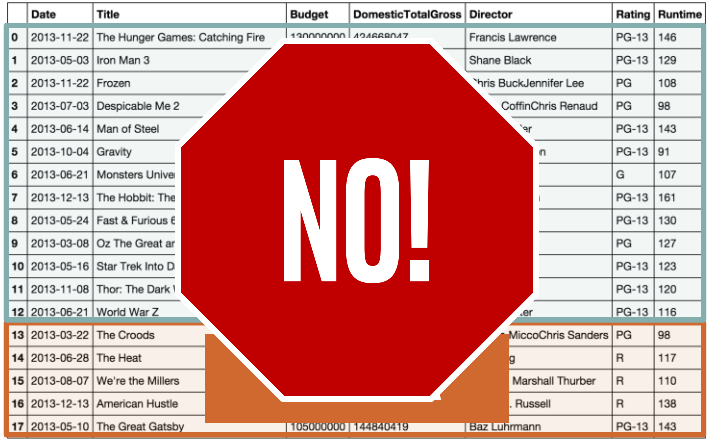
TRAINING DATA

TEST DATA

HYPERPARAMETERS AND THEIR OPTIMIZATION

- Regularization coefficients (λ_1 and λ_2) are empirically determined
- Want value that generalizes—do not use test data for tuning

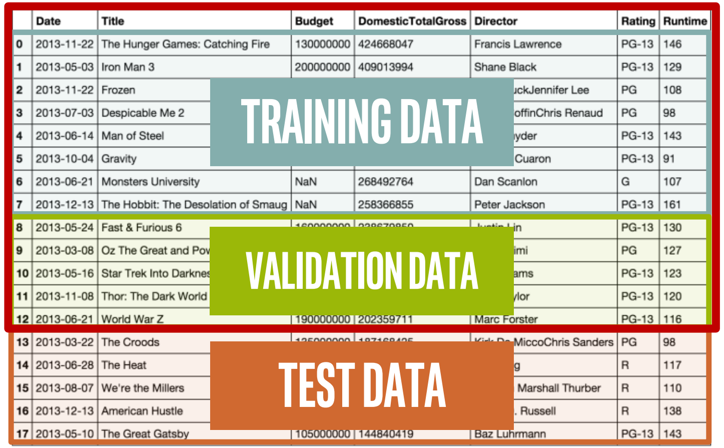
Use Test Data to Tune λ?



HYPERPARAMETERS AND THEIR OPTIMIZATION

- Regularization coefficients (λ_1 and λ_2) are empirically determined
- Want value that generalizes—do not use test data for tuning
- Create additional split of data to tune hyperparameters—validation set

Tune λ with Cross Validation



RIDGE REGRESSION: THE SYNTAX

Import the class containing the regression method

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from sklearn.linear_model import Ridge
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Create an instance of the class

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RR = Ridge(alpha=1.0)
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regularization parameter

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Import the class containing the regression method

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```

Create an instance of the class

```
RR = Ridge(alpha=1.0)
```

Fit the instance on the data and then predict the expected value

```
RR = RR.fit(X_train, y_train)

y_predict = RR.predict(X_test)
```

RIDGE REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import Ridge
```

Create an instance of the class

```
RR = Ridge(alpha=1.0)
```

Fit the instance on the data and then predict the expected value

```
RR = RR.fit(X_train, y_train)

y_predict = RR.predict(X_test)
```

The RidgeCV class will perform cross validation on a set of values for alpha.

LASSO REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import Lasso
```

Create an instance of the class

```
LR = Lasso(alpha=1.0)
```

Fit the instance on the data and then predict the expected value

```
LR = LR.fit(X_train, y_train)
y_predict = LR.predict(X_test)
```

The LassoCV class will perform cross validation on a set of values for alpha.

LASSO REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import Lasso
```

Create an instance of the class

```
LR = Lasso(alpha=1.0)
```

regularization parameter

Fit the instance on the data and then predict the expected value

```
LR = LR.fit(X_train, y_train)

y_predict = LR.predict(X_test)
```

The LassoCV class will perform cross validation on a set of values for alpha.

ELASTIC NET REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import ElasticNet
```

Create an instance of the class

```
EN = ElasticNet(alpha=1.0,l1_ratio=0.5)
```

Fit the instance on the data and then predict the expected value

```
EN = EN.fit(X_train, y_train)

y_predict = EN.predict(X_test)
```

The **ElasticNetCV** class will perform cross validation on a set of values for l1_ratio and alpha.

ELASTIC NET REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import ElasticNet
```

Create an instance of the class

```
EN = ElasticNet(alpha=1.0,l1_ratio=0.5)
```

alpha is the regularization parameter

Fit the instance on the data and then predict the expected value

```
EN = EN.fit(X_train, y_train)

y_predict = EN.predict(X_test)
```

The **ElasticNetCV** class will perform cross validation on a set of values for l1_ratio and alpha.

ELASTIC NET REGRESSION: THE SYNTAX

Import the class containing the regression method

```
from sklearn.linear_model import ElasticNet
```

Create an instance of the class

```
EN = ElasticNet(alpha=1.0,l1_ratio=0.5)
```

l1_ratio distributes alpha to L1/L2

Fit the instance on the data and then predict the expected value

```
EN = EN.fit(X_train, y_train)

y_predict = EN.predict(X_test)
```

The ElasticNetCV class will perform cross validation on a set of values for l1_ratio and alpha.

FEATURE SELECTION

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- **For L1-regularization, this is accomplished by driving some coefficients to zero**

FEATURE SELECTION

- Regularization performs feature selection by shrinking the contribution of features
- For L1-regularization, this is accomplished by driving some coefficients to zero
- Feature selection can also be performed by removing features

WHY IS FEATURE SELECTION IMPORTANT?

- Reducing the number of features is another way to prevent overfitting (similar to regularization)

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- Reducing the number of features is another way to prevent overfitting (similar to regularization)
- For some models, fewer features can improve fitting time and/or results
- Identifying most critical features can improve model interpretability

RECURSIVE FEATURE ELIMINATION: THE SYNTAX

Import the class containing the feature selection method

```
from sklearn.feature_selection import RFE
```

Create an instance of the class

```
rfeMod = RFE(est, n_features_to_select=5)
```

Fit the instance on the data and then predict the expected value

```
rfeMod = rfeMod.fit(X_train, y_train)

y_predict = rfeMod.predict(X_test)
```

The **RFECV** class will perform feature elimination using cross validation.

RECURSIVE FEATURE ELIMINATION: THE SYNTAX

Import the class containing the feature selection method

```
from sklearn.feature_selection import RFE
```

Create an instance of the class

```
rfeMod = RFE(est, n_features_to_select=5)
```

est is an instance of the model to use

Fit the instance on the data and then predict the expected value

```
rfeMod = rfeMod.fit(X_train, y_train)

y_predict = rfeMod.predict(X_test)
```

The **RFECV** class will perform feature elimination using cross validation.

RECURSIVE FEATURE ELIMINATION: THE SYNTAX

Import the class containing the feature selection method

```
from sklearn.feature_selection import RFE
```

Create an instance of the class

```
rfeMod = RFE(est, n_features_to_select=5)
```

final number of features

Fit the instance on the data and then predict the expected value

```
rfeMod = rfeMod.fit(X_train, y_train)

y_predict = rfeMod.predict(X_test)
```

The RFECV class will perform feature elimination using cross validation.

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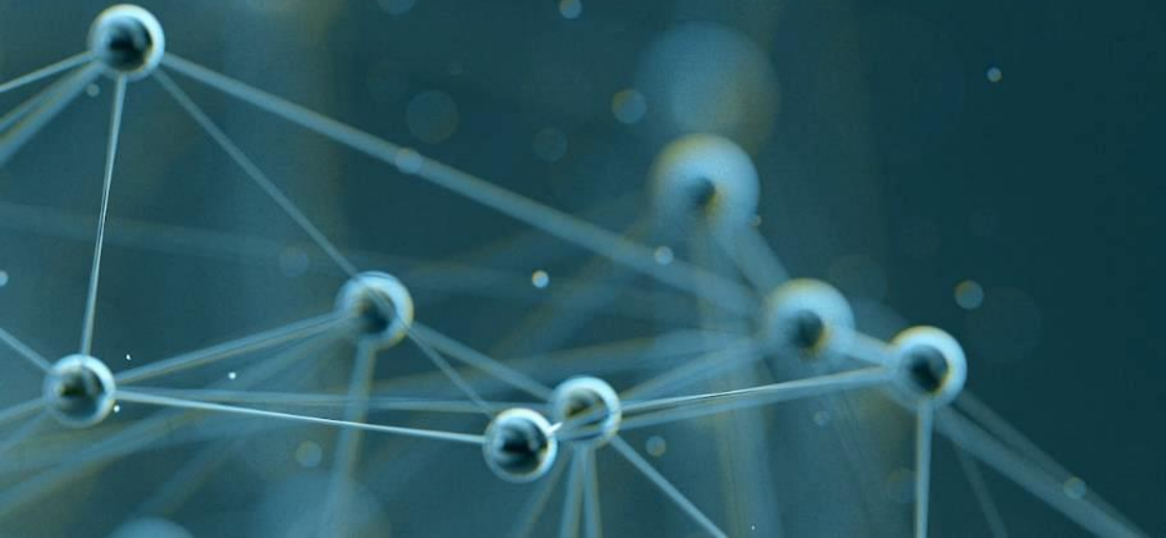
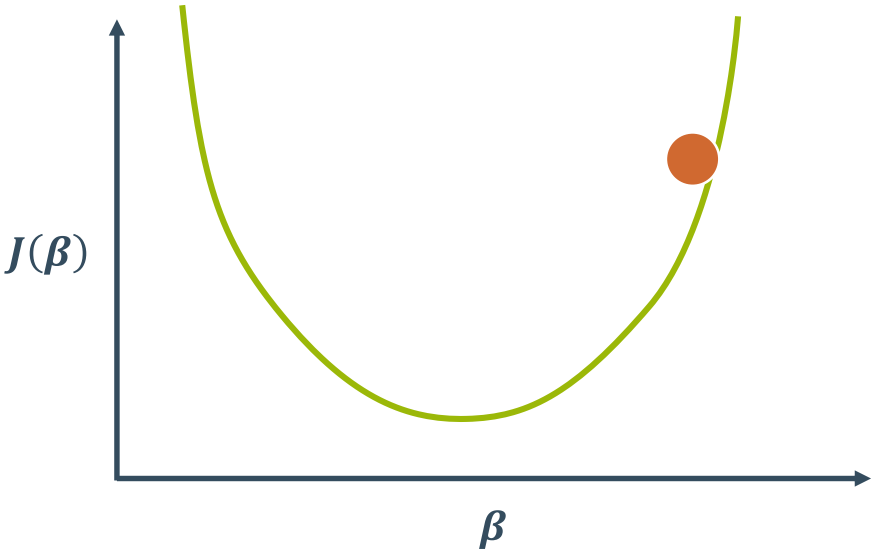
GRADIENT DESCENT



GRADIENT DESCENT

Start with a cost function J(β):



GRADIENT DESCENT

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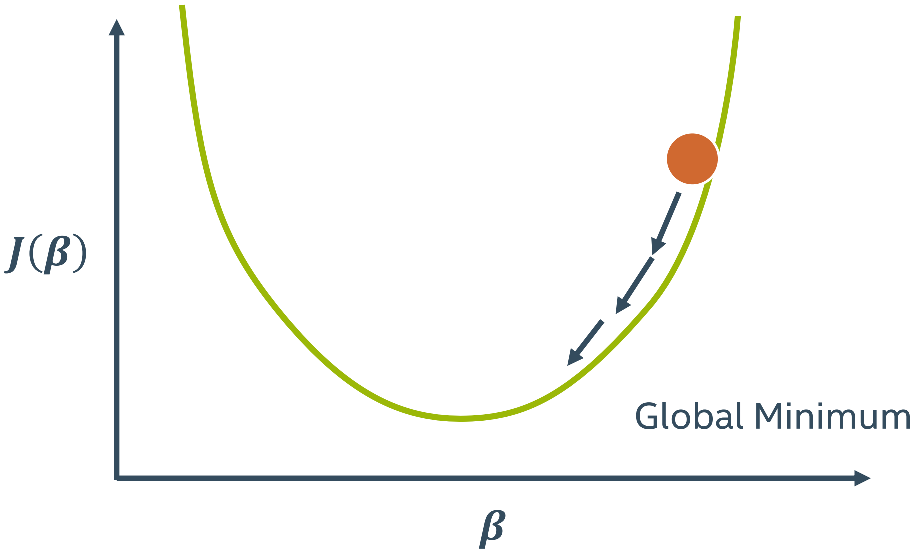


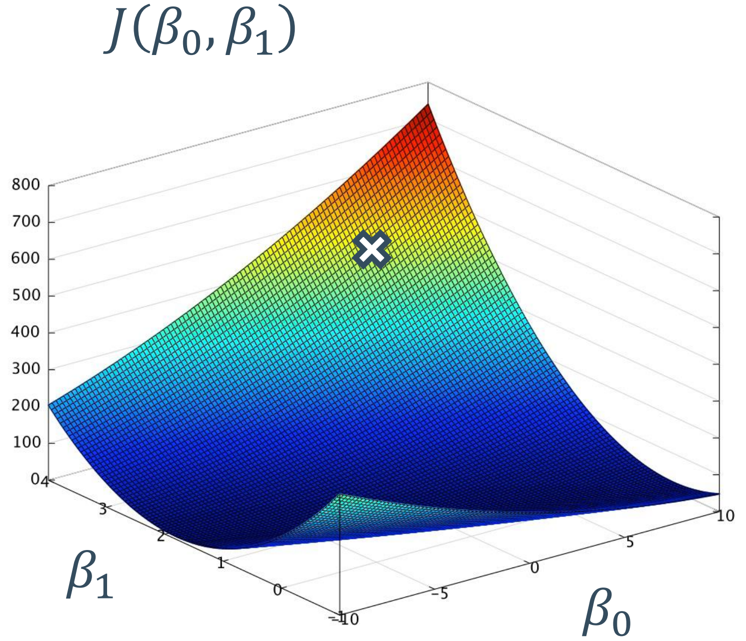
Then gradually move towards the minimum.

GRADIENT DESCENT WITH LINEAR REGRESSION

- Now imagine there are two parameters (β_0, β_1)

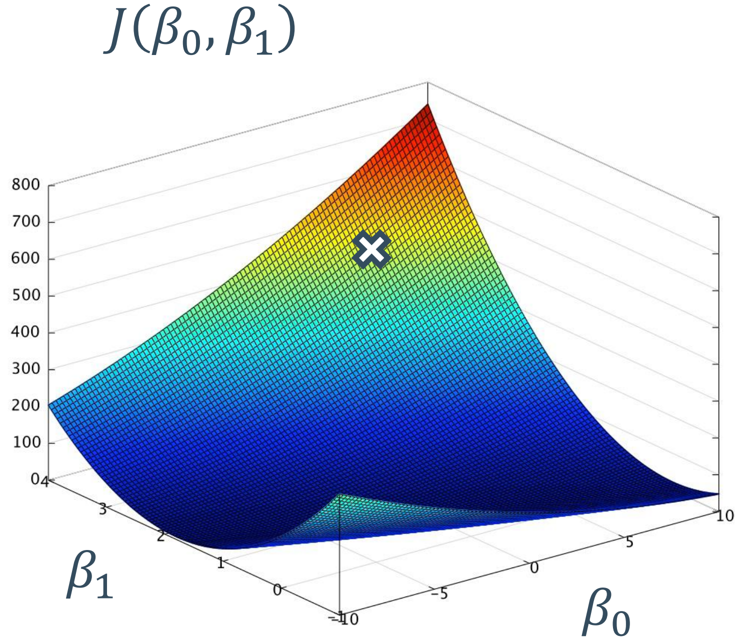
GRADIENT DESCENT WITH LINEAR REGRESSION

- Now imagine there are two parameters (β_0, β_1)
- This is a more complicated surface on which the minimum must be found



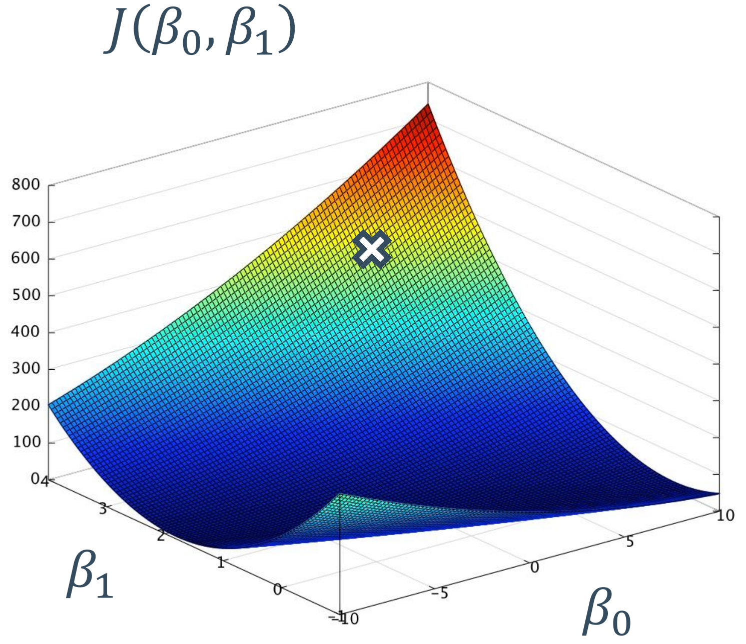
GRADIENT DESCENT WITH LINEAR REGRESSION

- Now imagine there are two parameters (β_0, β_1)
- This is a more complicated surface on which the minimum must be found
- How can we do this without knowing what $J(\beta_0, \beta_1)$ looks like?



GRADIENT DESCENT WITH LINEAR REGRESSION

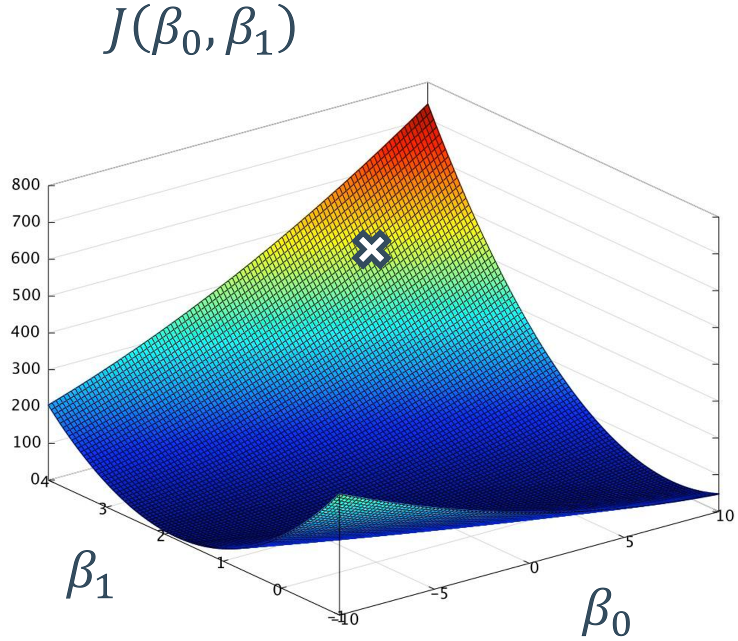
- Compute the gradient, $\nabla J(\beta_0, \beta_1)$, which points in the direction of the biggest increase!
- -$\nabla J(\beta_0, \beta_1)$(negative gradient) points to the biggest decrease at that point!



GRADIENT DESCENT WITH LINEAR REGRESSION

- The gradient is the a vector whose coordinates consist of the partial derivatives of the parameters

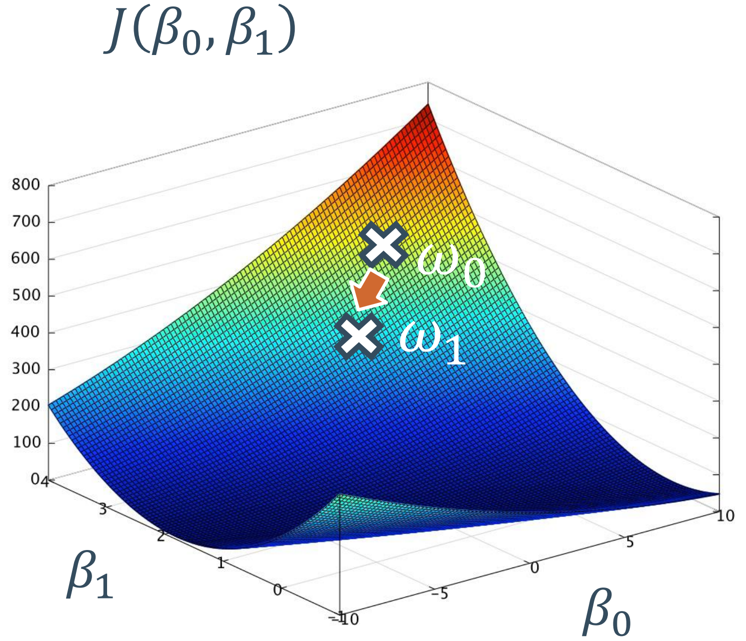
$$\nabla J(\beta_0, \dots, \beta_n) = < \frac{\partial J}{\partial \beta_0}, \dots, \frac{\partial J}{\partial \beta_n} >$$



GRADIENT DESCENT WITH LINEAR REGRESSION

- Then use the gradient (∇) and the cost function to calculate the next point (ω_1) from the current one (ω_0):

$$\omega_1 = \omega_0 - \alpha \nabla \frac{1}{2} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$

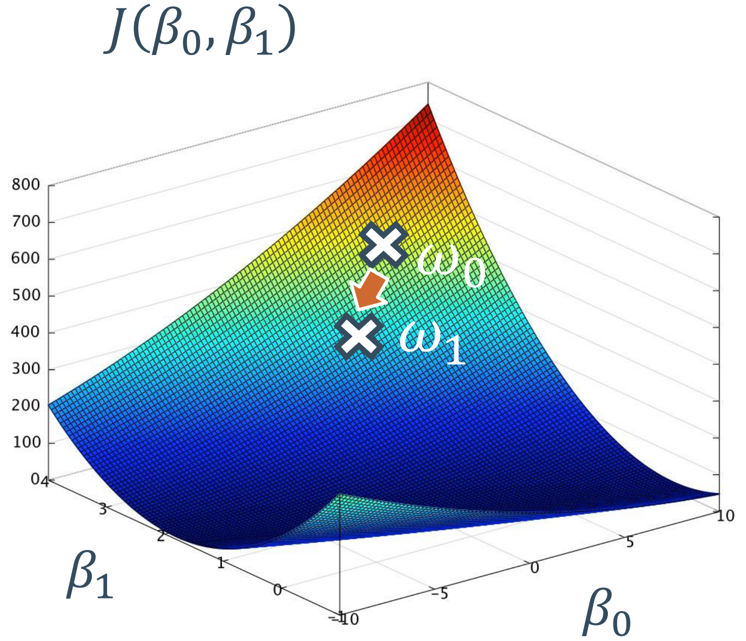


GRADIENT DESCENT WITH LINEAR REGRESSION

- Then use the gradient (∇) and the cost function to calculate the next point (ω_1) from the current one (ω_0):

$$\omega_1 = \omega_0 - \alpha\nabla\frac{1}{2}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

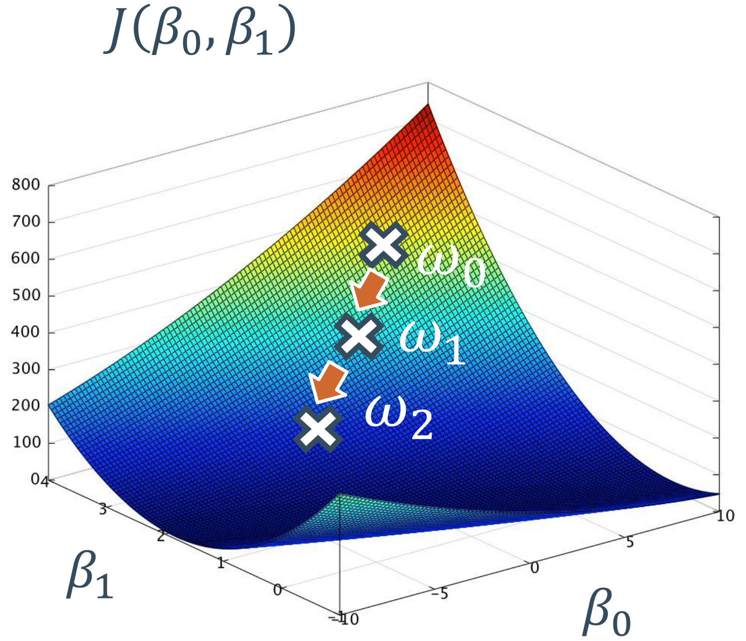
- The learning rate (α) is a tunable parameter that determines step size



GRADIENT DESCENT WITH LINEAR REGRESSION

- Each point can be iteratively calculated from the previous one

$$\omega_2 = \omega_1 - \alpha\nabla \frac{1}{2}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

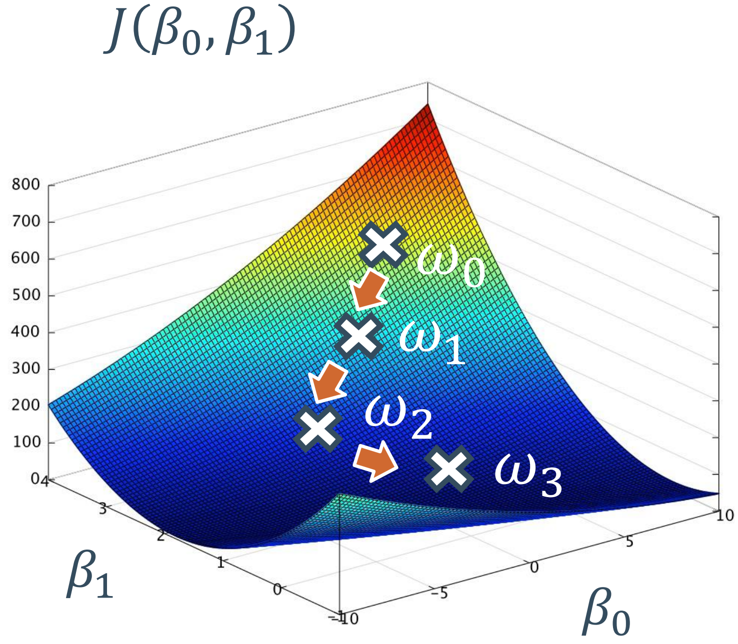


GRADIENT DESCENT WITH LINEAR REGRESSION

- Each point can be iteratively calculated from the previous one

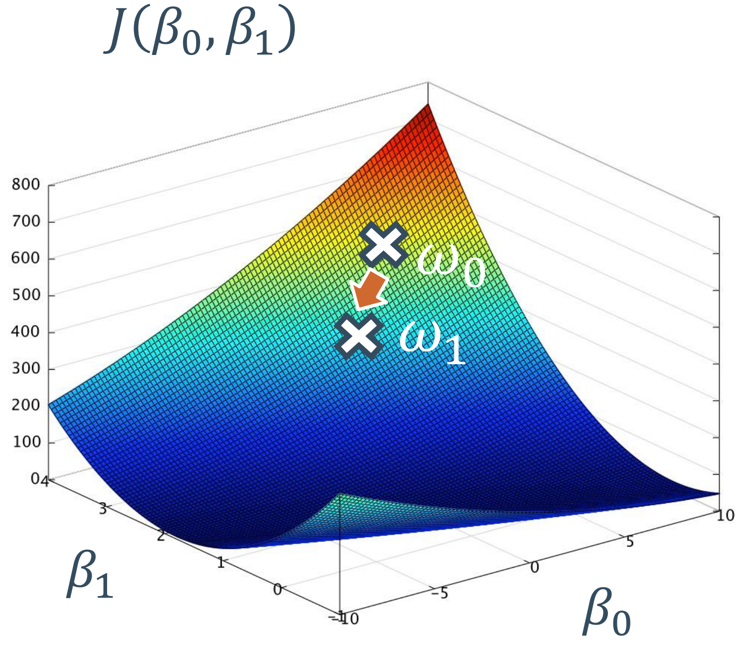
$$\omega_2 = \omega_1 - \alpha\nabla\frac{1}{2}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

$$\omega_3 = \omega_2 - \alpha\nabla\frac{1}{2}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$



STOCHASTIC GRADIENT DESCENT

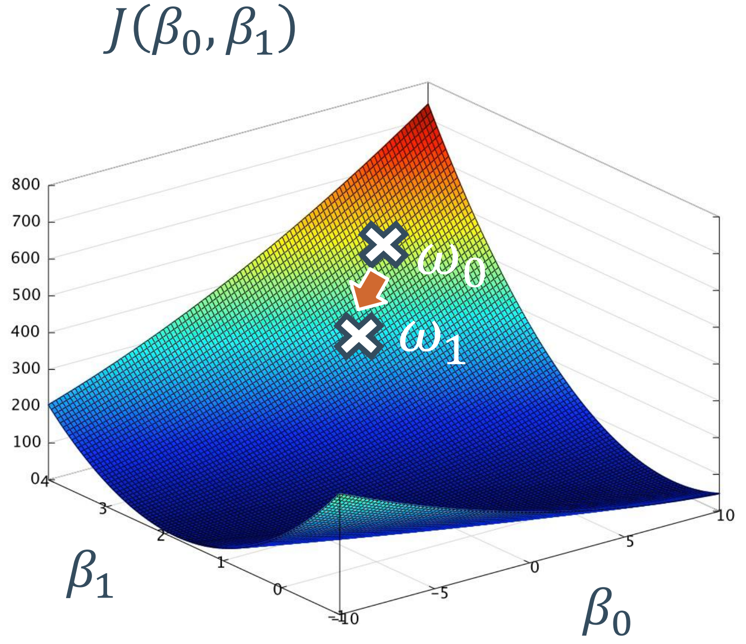
- Use a single data point to determine the gradient and cost function instead of all the data



STOCHASTIC GRADIENT DESCENT

- Use a single data point to determine the gradient and cost function instead of all the data

$$\omega_1 = \omega_0 - \alpha \nabla \frac{1}{2} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$



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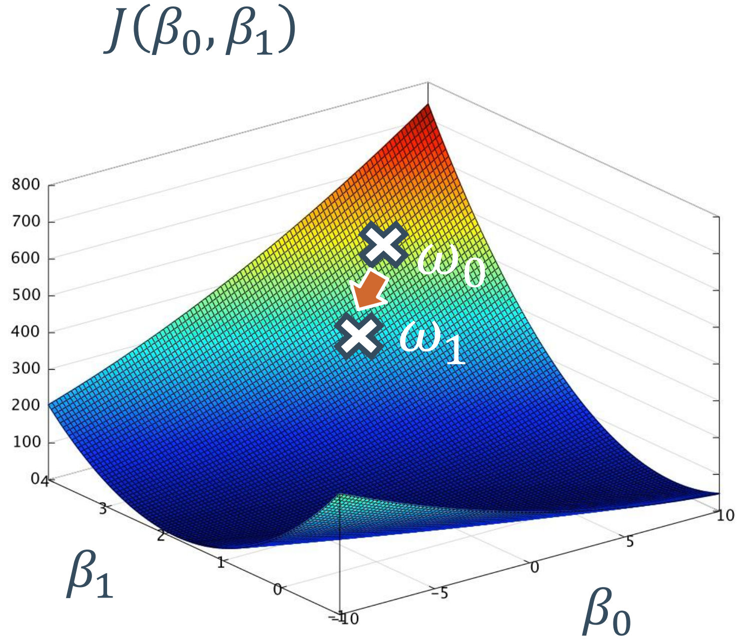
- Use a single data point to determine the gradient and cost function instead of all the data

$$\omega_1 = \omega_0 - \alpha\nabla \frac{1}{2}\cancel{\sum_{i=1}^{m}}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

$$\boxed{\omega_1 = \omega_0 - \alpha\nabla \frac{1}{2}\left(\left(\beta_0 + \beta_1 x_{obs}^{(0)}\right) - y_{obs}^{(0)}\right)^2}$$



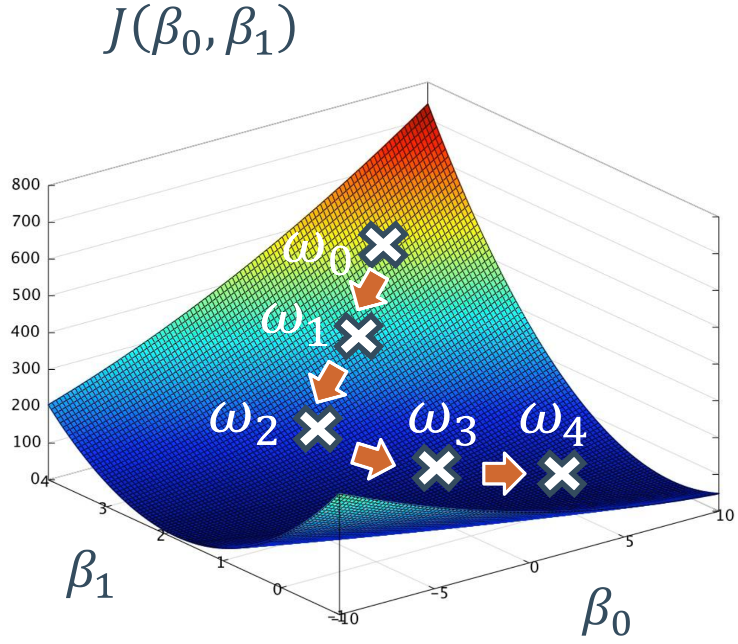
STOCHASTIC GRADIENT DESCENT

- Use a single data point to determine the gradient and cost function instead of all the data

$$\omega_1 = \omega_0 - \alpha\nabla\frac{1}{2}\left(\left(\beta_0 + \beta_1 x_{obs}^{(0)}\right) - y_{obs}^{(0)}\right)^2$$

$$\cdots$$

$$\omega_4 = \omega_3 - \alpha\nabla\frac{1}{2}\left(\left(\beta_0 + \beta_1 x_{obs}^{(3)}\right) - y_{obs}^{(3)}\right)^2$$



STOCHASTIC GRADIENT DESCENT

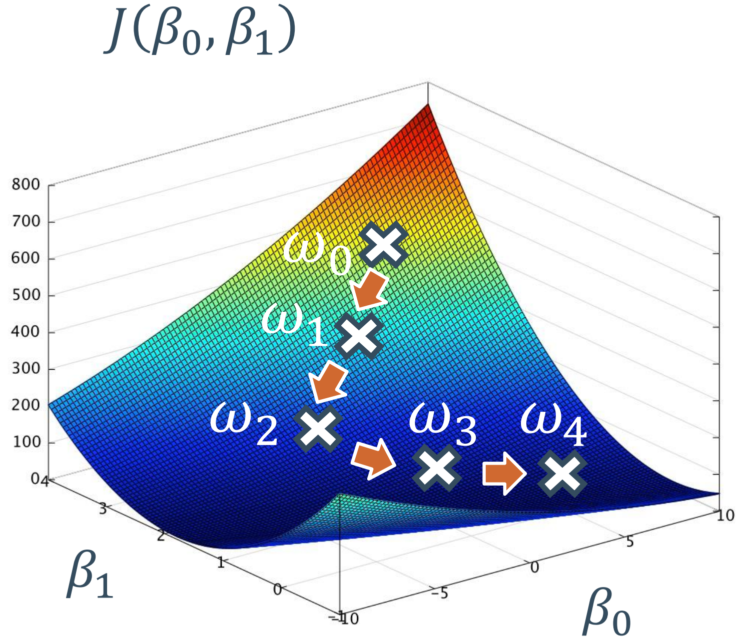
- Use a single data point to determine the gradient and cost function instead of all the data

$$\omega_1 = \omega_0 - \alpha\nabla\frac{1}{2}\left(\left(\beta_0 + \beta_1 x_{obs}^{(0)}\right) - y_{obs}^{(0)}\right)^2$$

$$\ldots$$

$$\omega_4 = \omega_3 - \alpha\nabla\frac{1}{2}\left(\left(\beta_0 + \beta_1 x_{obs}^{(3)}\right) - y_{obs}^{(3)}\right)^2$$

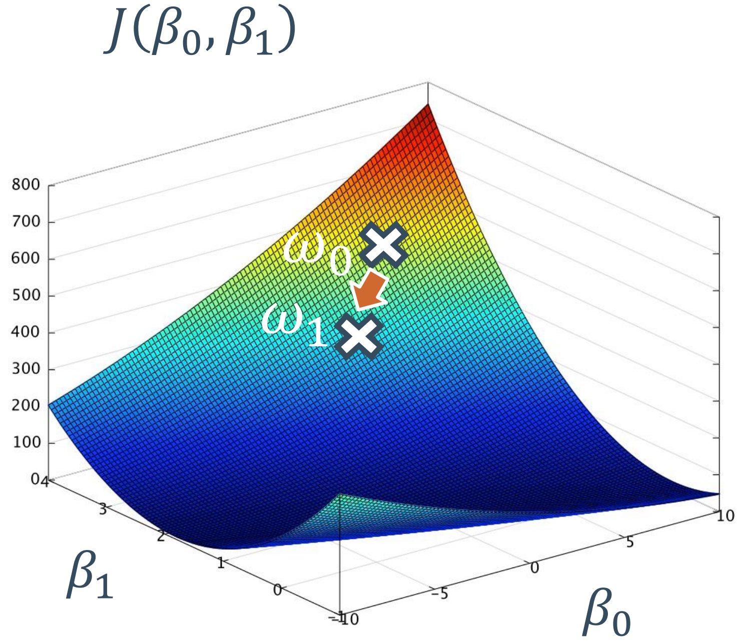
- Path is less direct due to noise in single data point—"stochastic"



MINI BATCH GRADIENT DESCENT

- Perform an update for every n training examples

$$\omega_1 = \omega_0 - \alpha\nabla\frac{1}{2}\sum_{i=1}^{n}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$



MINI BATCH GRADIENT DESCENT

- Perform an update for every n training examples

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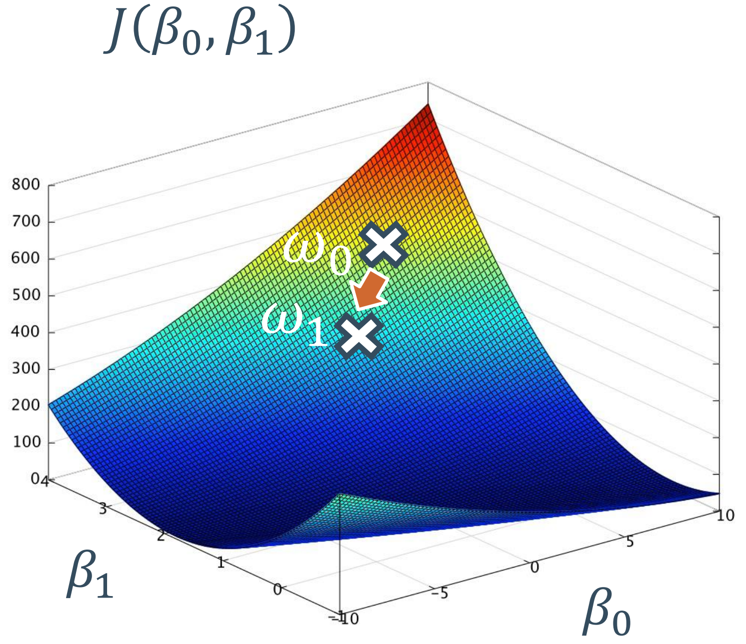

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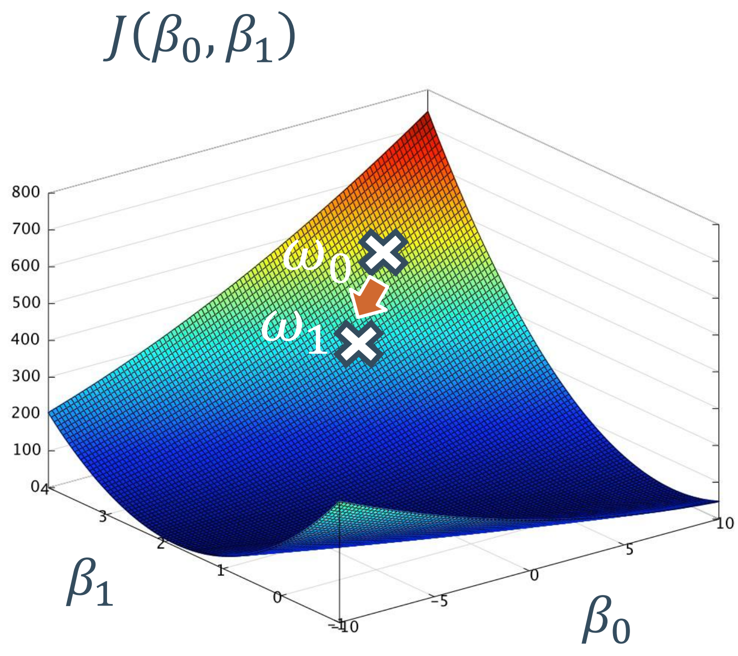

Best of both worlds:

- Reduced memory relative to "vanilla" gradient descent
- Less noisy than stochastic gradient descent

MINI BATCH GRADIENT DESCENT

- Mini batch implementation typically used for neural nets

MINI BATCH GRADIENT DESCENT

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- Batch sizes range from 50–256 points

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MINI BATCH GRADIENT DESCENT

- Mini batch implementation typically used for neural nets
- Batch sizes range from 50–256 points
- Trade off between batch size and learning rate (α)
- Tailor learning rate schedule: gradually reduce learning rate during a given epoch

STOCHASTIC GRADIENT DESCENT REGRESSION: SYNTAX

Import the class containing the regression model

```
from sklearn.linear_model import SGDRegressor
```

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squared_loss = linear regression

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regularization parameters

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Fit the instance on the data and then transform the data

```
SGDreg = SGDreg.fit(X_train, y_train)

y_pred = SGDreg.predict(X_test)
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Mini-batch version

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Other loss methods exist: epsilon_insensitive, huber, etc.

STOCHASTIC GRADIENT DESCENT CLASSIFICATION: THE SYNTAX

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log loss = logistic regression

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mini-batch version

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Other loss methods exist: hinge, squared_hinge, etc.

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See SVM lecture (week 7)

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