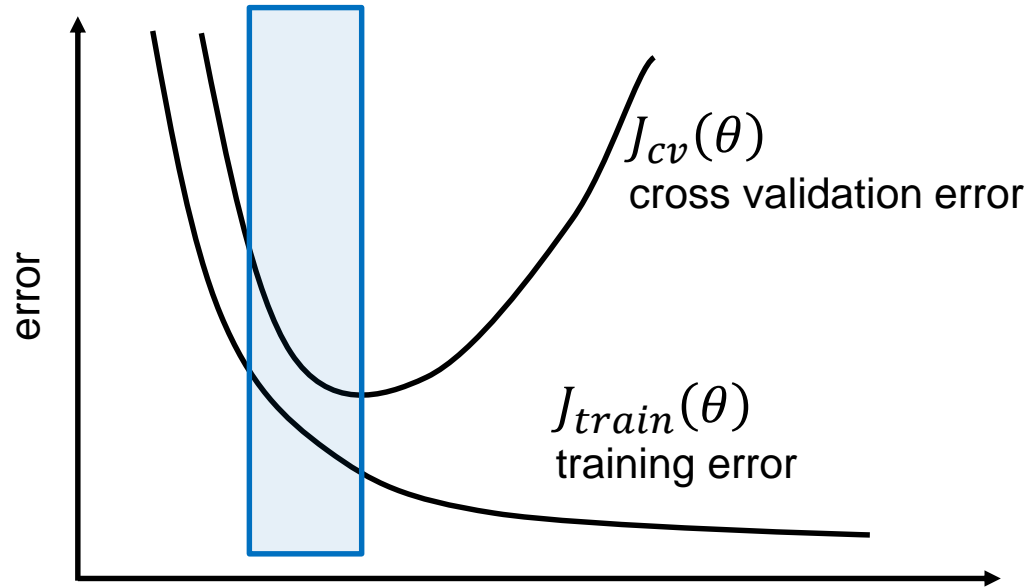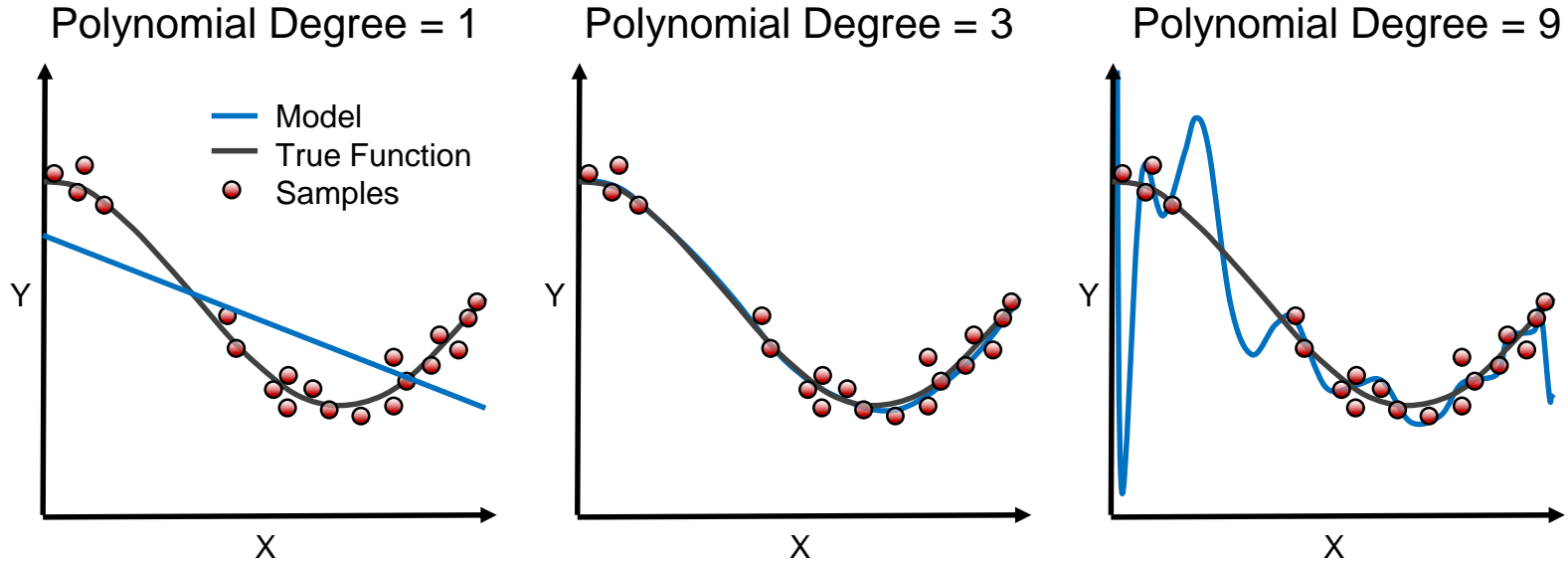# Chapter 4

Regularization Gradient Descent

Regularization
Feature Selection

Model Complexity vs Error
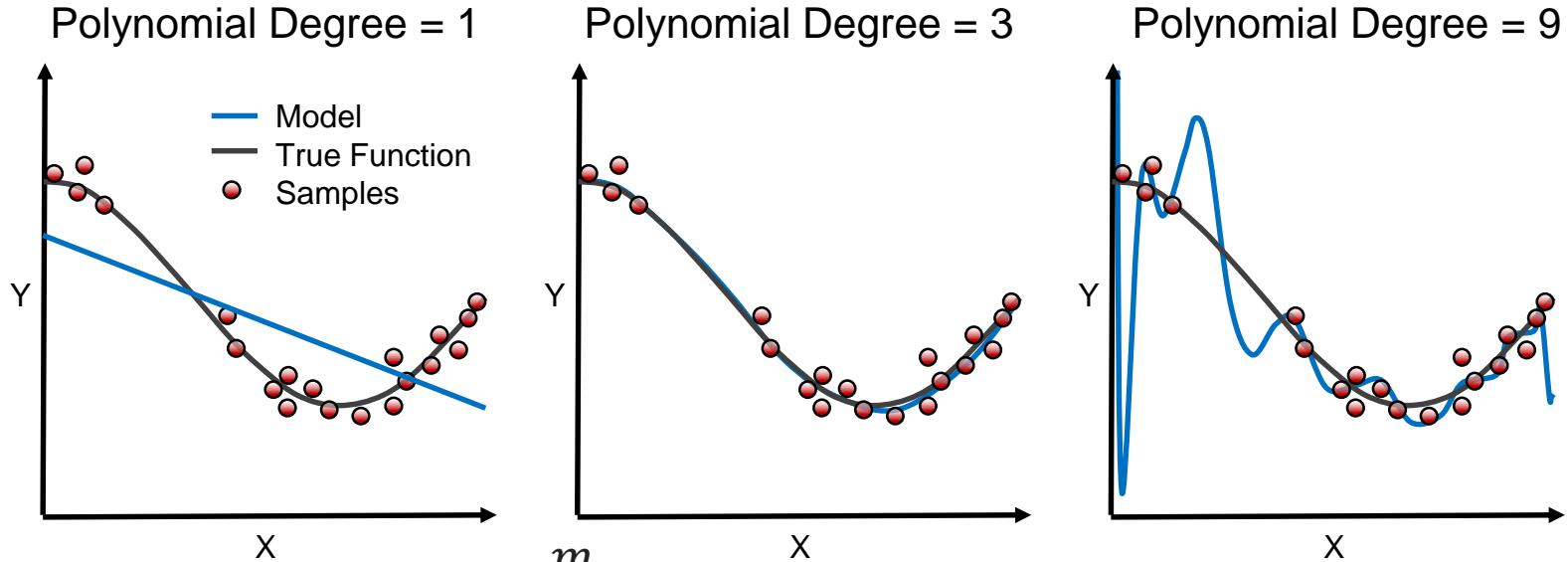
Preventing Under- and Overfitting
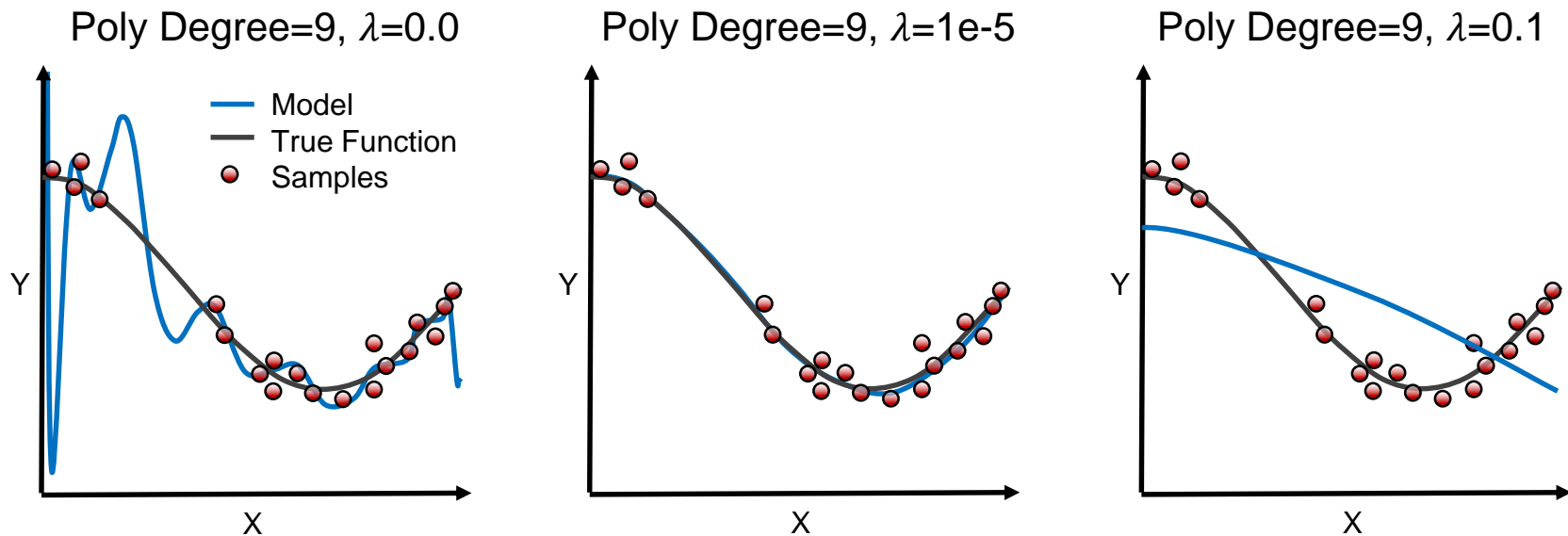
Polynomial Degree = 1

Polynomial Degree = 3

Polynomial Degree = 9

- How to use a degree 9 polynomial and prevent overfitting?

Preventing Under- and Overfitting

Polynomial Degree = 1

Y

X

Polynomial Degree = 3

Y

X

Polynomial Degree = 9

Y

X

— Model
— True Function
● Samples

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

(intel)
Software

Regularization

Poly Degree=9, λ=0.0

Poly Degree=9, λ=1e-5

Poly Degree=9, λ=0.1

- Model
- True Function
- Samples

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

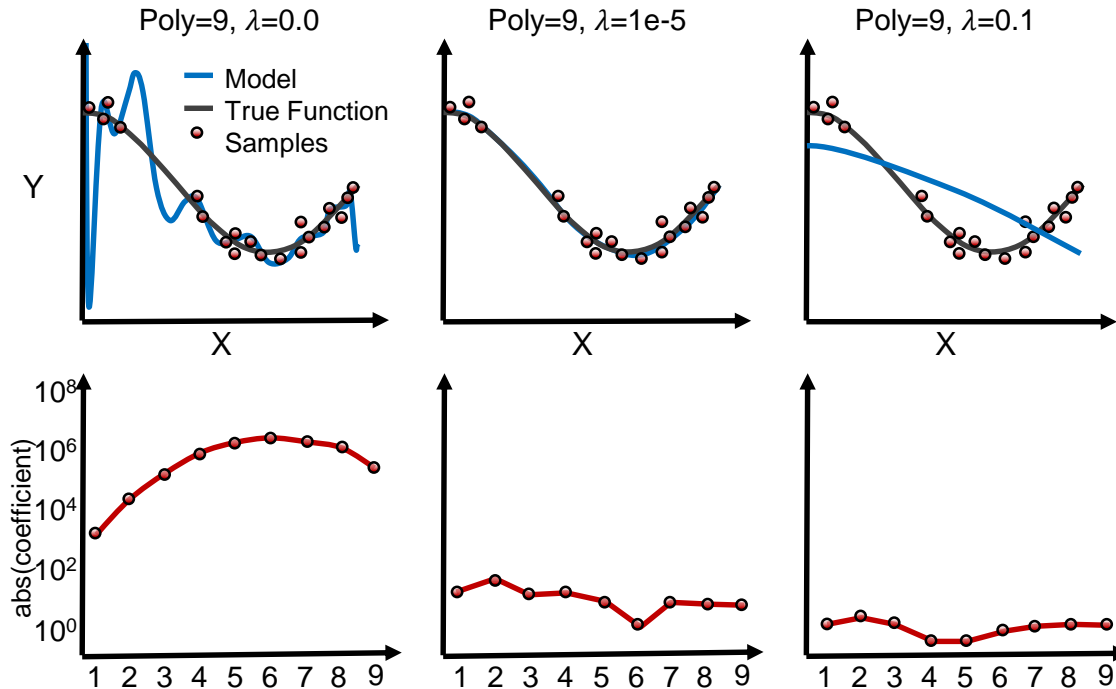# Ridge Regression (L2)

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

- Penalty shrinks magnitude of all coefficients

- Larger coefficients strongly penalized because of the squaring
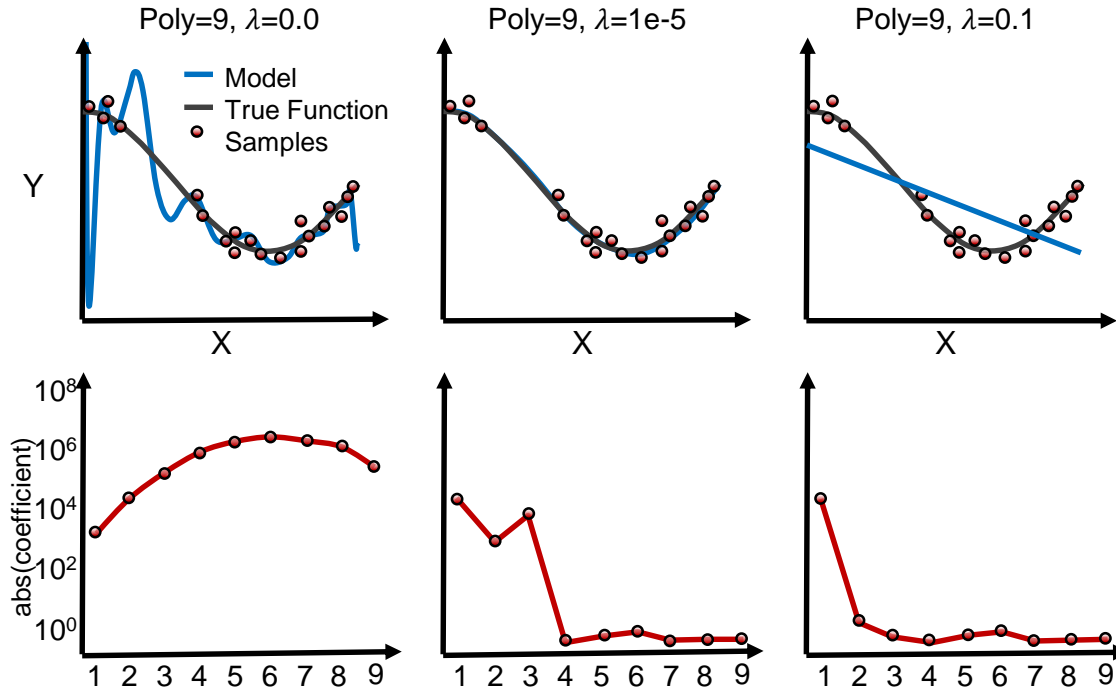
Effect of Ridge Regression on Parameters

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

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
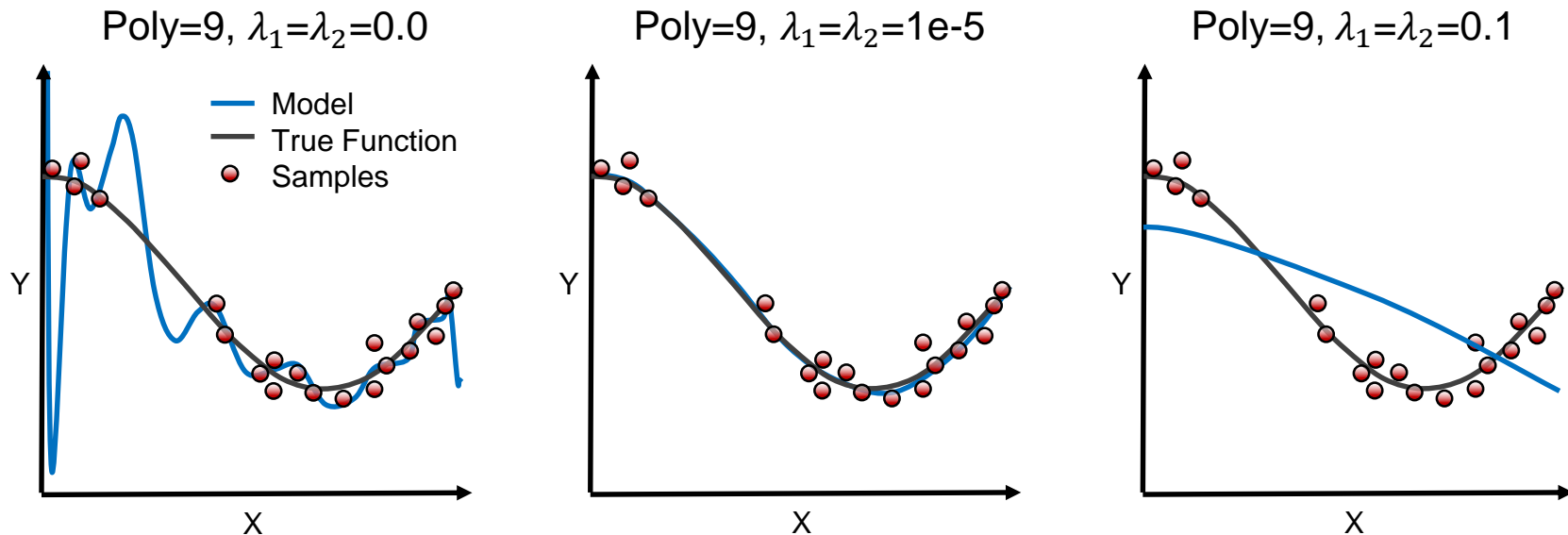
Effect of Lasso Regression on Parameters

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

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

Elastic Net Regularization

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

- Compromise of both Ridge and Lasso regression

- Requires tuning of additional parameter that distributes regularization penalty between L1 and L2

Elastic Net Regularization

Poly=9, $\lambda_1=\lambda_2=0.0$

Poly=9, $\lambda_1=\lambda_2=$1e-5

Poly=9, $\lambda_1=\lambda_2=0.1$

- Model
- True Function
- Samples

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

Hyperparameters and Their Optimization

- Regularization coefficients (λ_1 and λ_2) are empirically determined

Use Test Data to Tune λ?

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			uaron	PG-13	91
6	2013-06-21	Monsters University			on	G	107
7	2013-12-13	The Hobbit: The De			kson	PG-13	161
8	2013-05-24	Fast & Furious 6	160000000	238679850	Justin Lin	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				R	117
15	2013-08-07	We're the Millers			Marshall Thurber	R	110
16	2013-12-13	American Hustle			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

from sklearn.linear_model import **Ridge**

alpha.

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)

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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)

regularization
parameter

alpha.

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)
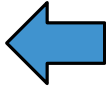
alpha.

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

- Regularization performs feature selection by shrinking the contribution of features

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

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- 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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- For some models, fewer features can improve fitting time and/or results

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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)

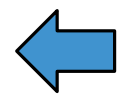**The RFECV class will perform feature elimination using cross validation.**

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

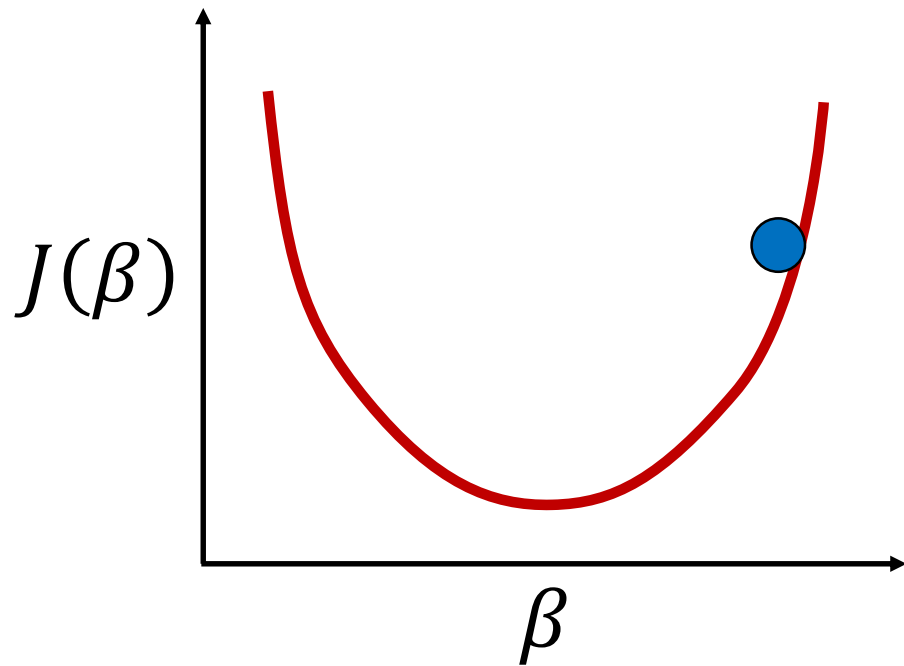**Fit the instance on the data and then predict the expected value**

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

    y_predict = **rfeMod**.**predict**(X_test)

The RFECV class will perform feature elimination using cross validation.
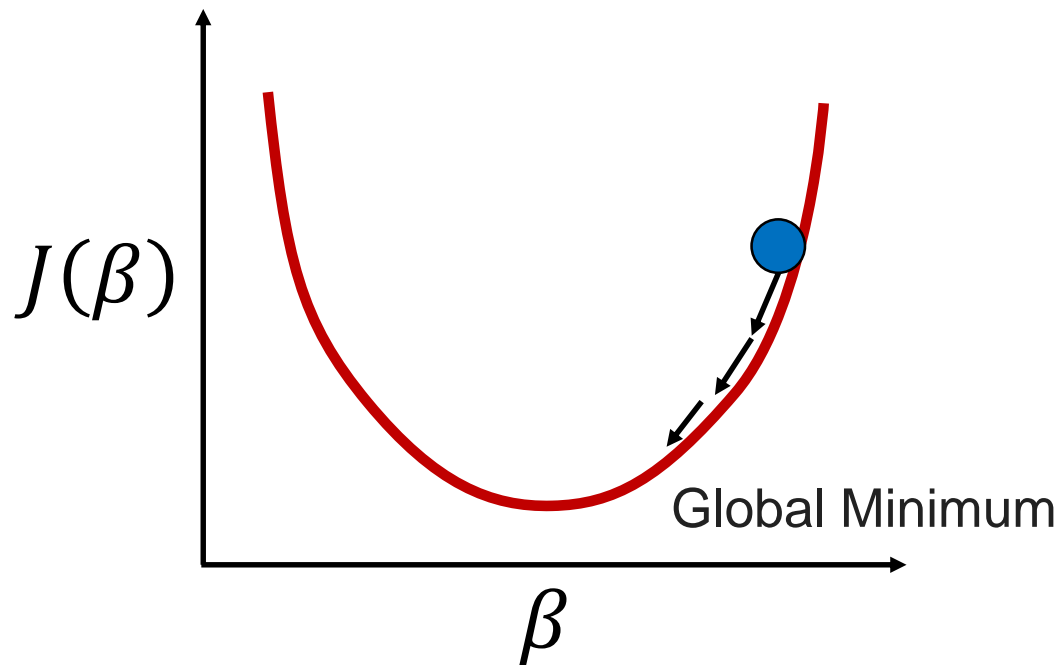
Gradient Descent

Gradient Descent

Start with a cost function J(β):

$J(\beta)$

β

Gradient Descent

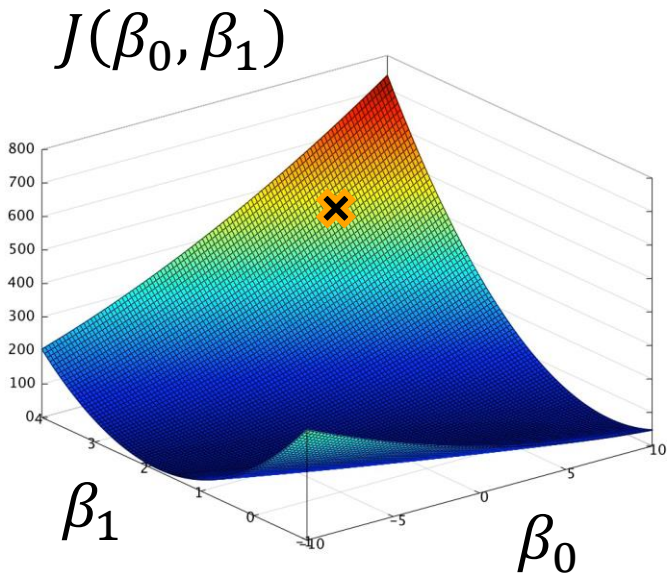Start with a cost function J(β):

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

$$J(\beta_0, \beta_1)$$

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

- How can we do this without knowing what $J(\beta_0, \beta_1)$ looks like?

$$J(\beta_0, \beta_1)$$

β_1

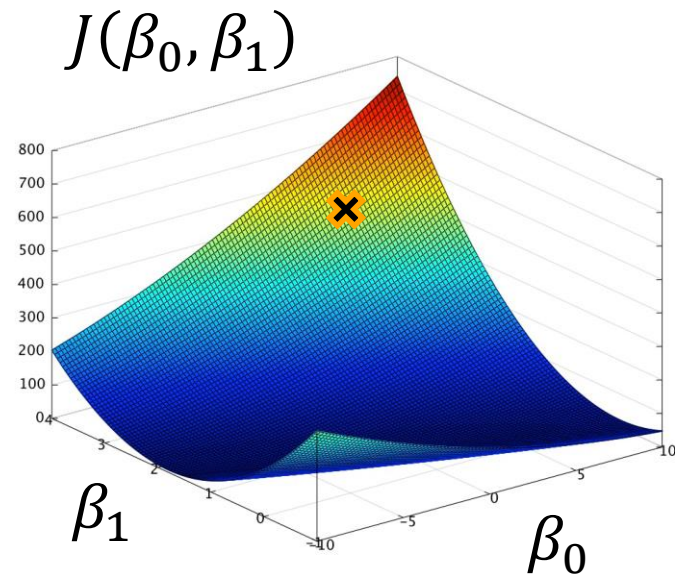β_0
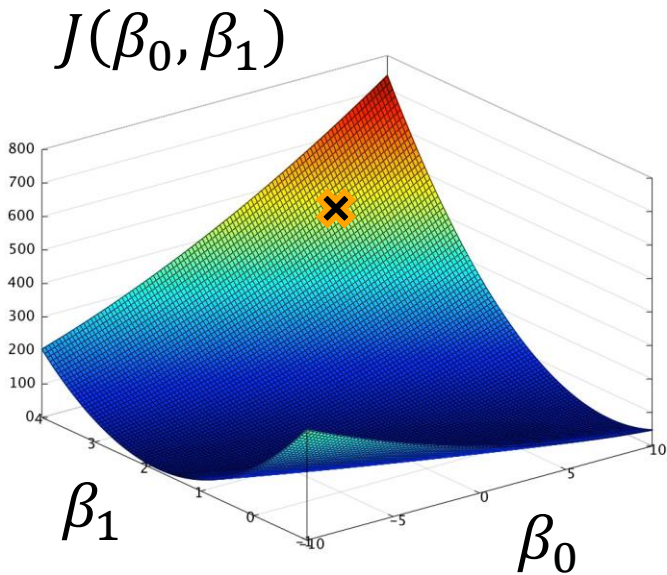
Gradient Descent with Linear Regression

- 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!

$J(\beta_0, \beta_1)$

β_1

β_0
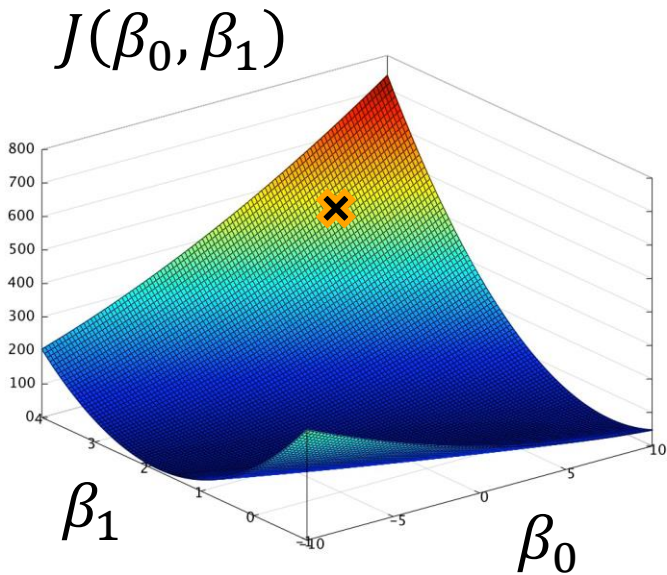
Gradient Descent with Linear Regression

- The gradient is the a vector whose coordinates consist of the partial derivatives of the parameters
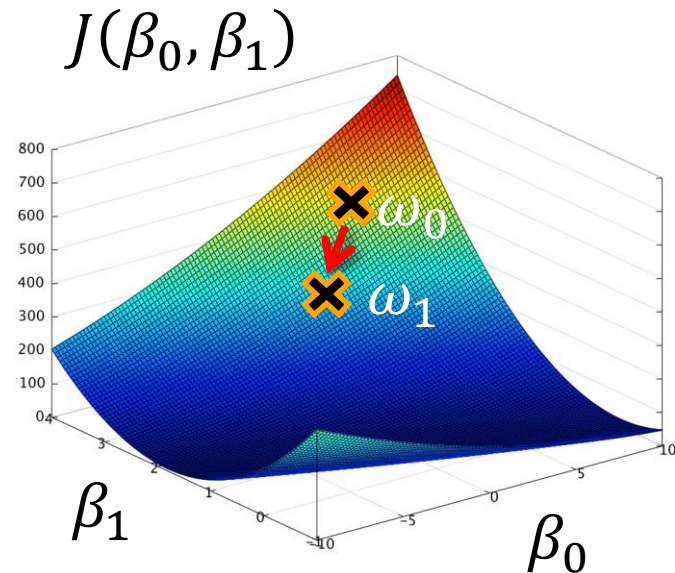
$$\nabla J(\beta_0, \ldots, \beta_n) = \left\langle \frac{\partial J}{\partial \beta_0}, \ldots, \frac{\partial J}{\partial \beta_n} \right\rangle$$

$J(\beta_0, \beta_1)$

β_1

β_0

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):

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

$J(\beta_0, \beta_1)$

ω_0
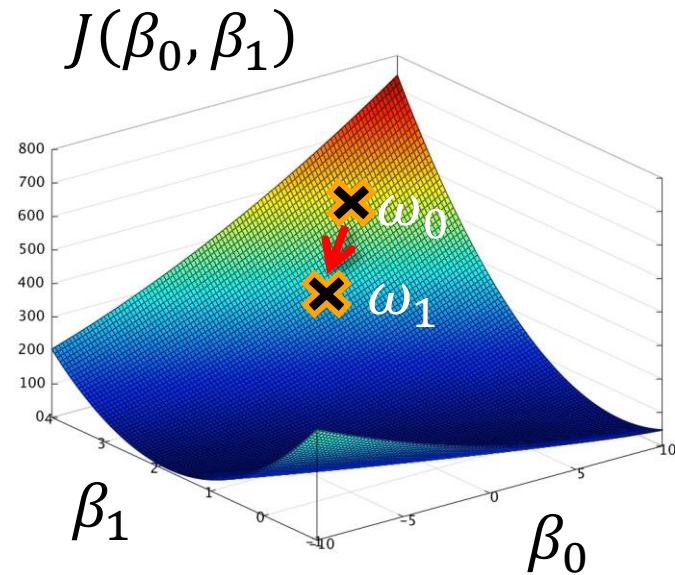
ω_1

β_1

β_0

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):

$$\omega_1 = \omega_0 - \alpha \nabla \frac{1}{2} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$
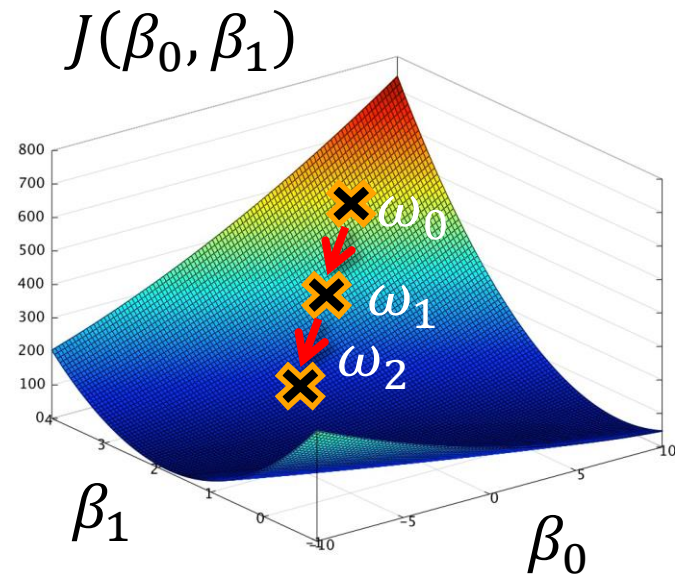
- The learning rate (α) is a tunable parameter that determines step size

Gradient Descent with Linear Regression

- Each point can be iteratively calculated from the previous one

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

$J(\beta_0, \beta_1)$

ω_0

ω_1
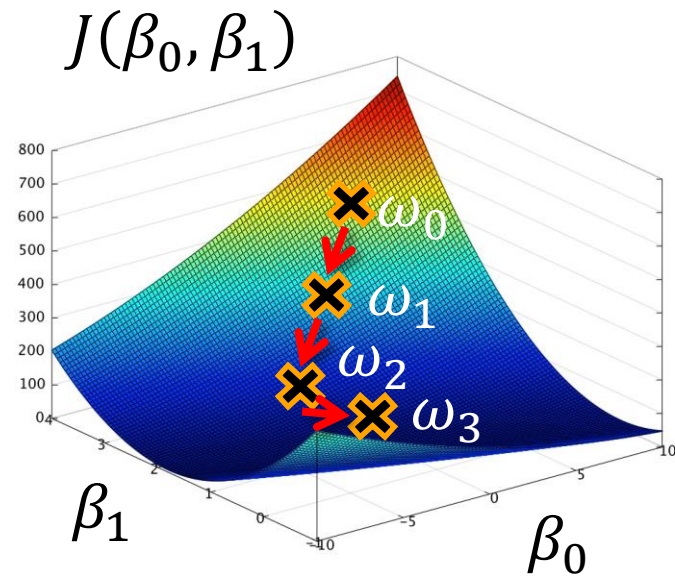
ω_2

β_1

β_0

Gradient Descent with Linear Regression

- Each point can be iteratively calculated from the previous one

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

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

$J(\beta_0, \beta_1)$

Stochastic Gradient Descent

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

Stochastic Gradient Descent

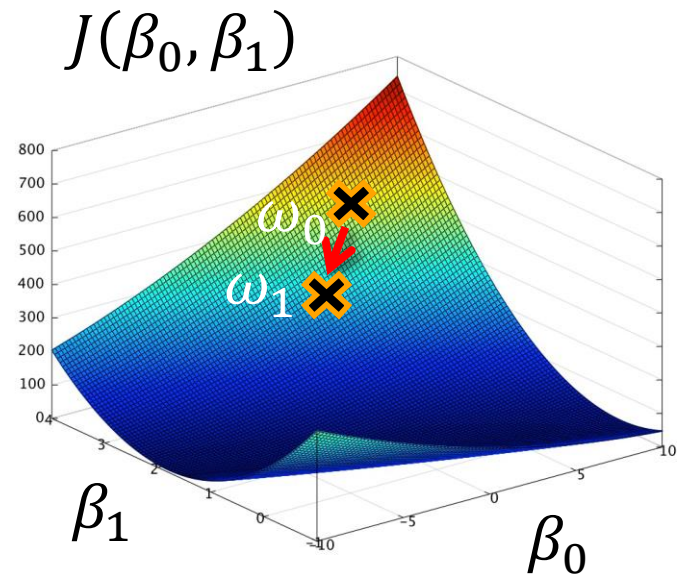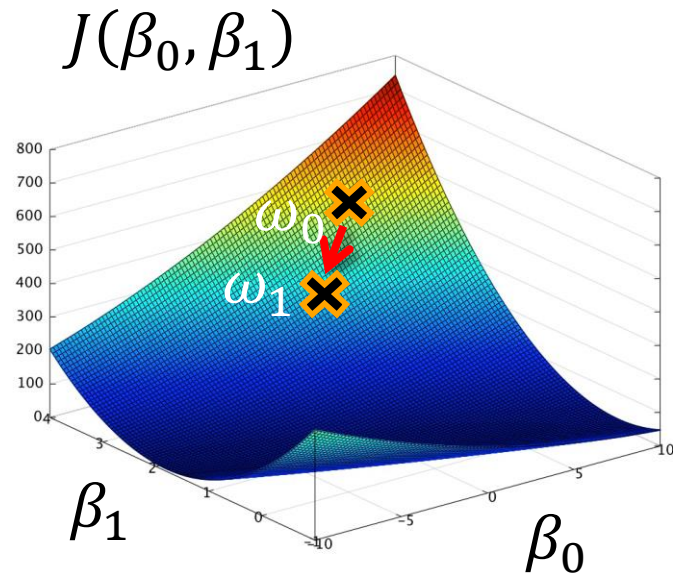- Use a single data point to determine the gradient and cost function instead of all the data

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

Stochastic Gradient Descent

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

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

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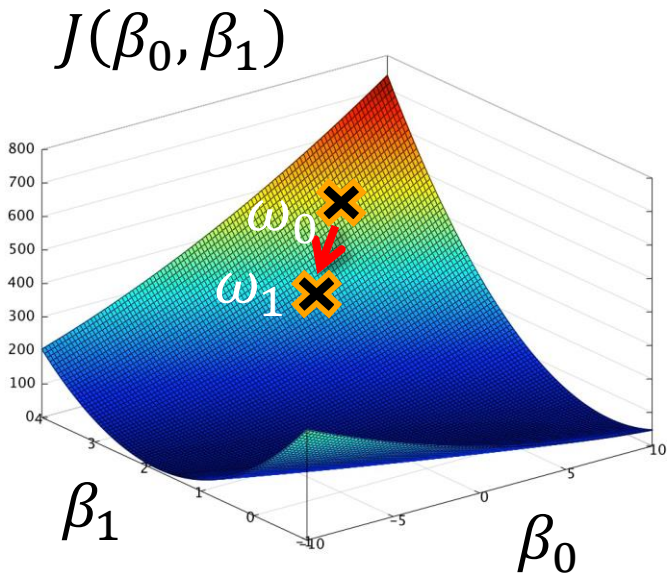

$J(\beta_0, \beta_1)$

Stochastic Gradient Descent

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

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

$$\dots$$

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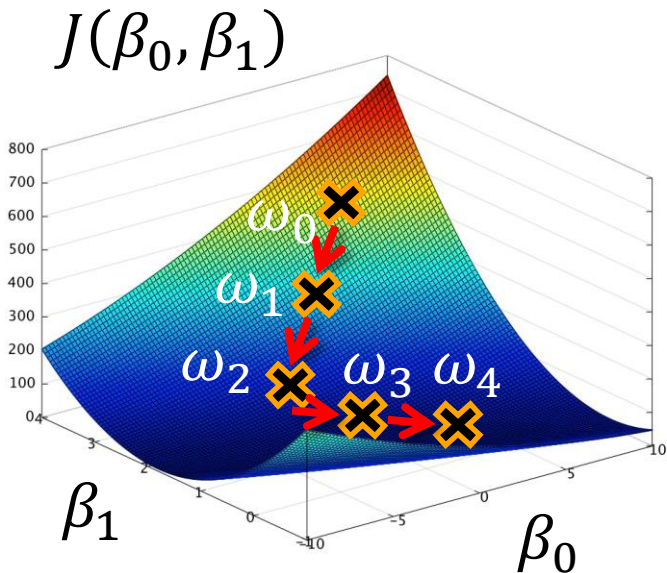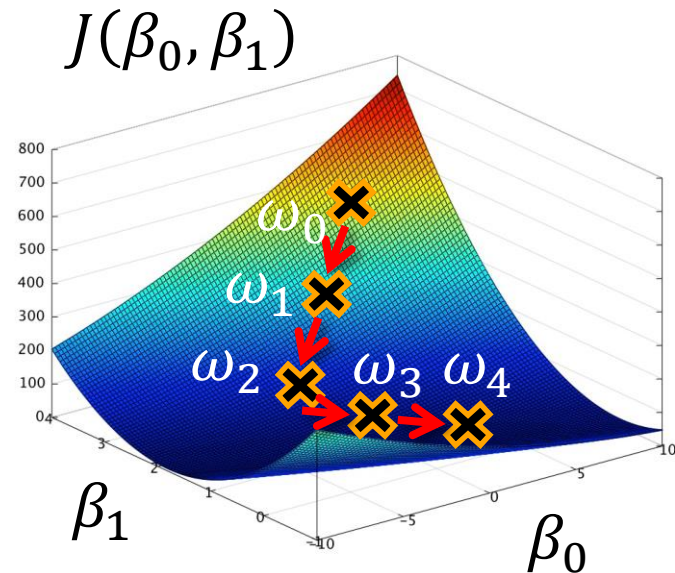
Stochastic Gradient Descent

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

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

$$\dots$$

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

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

$J(\beta_0, \beta_1)$

ω_0 ω_1 ω_2 ω_3 ω_4

β_1 β_0

Mini Batch Gradient Descent

- Perform an update for every n training examples

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

$J(\beta_0, \beta_1)$

Mini Batch Gradient Descent

- Perform an update for every n training examples

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

$$J(\beta_0, \beta_1)$$
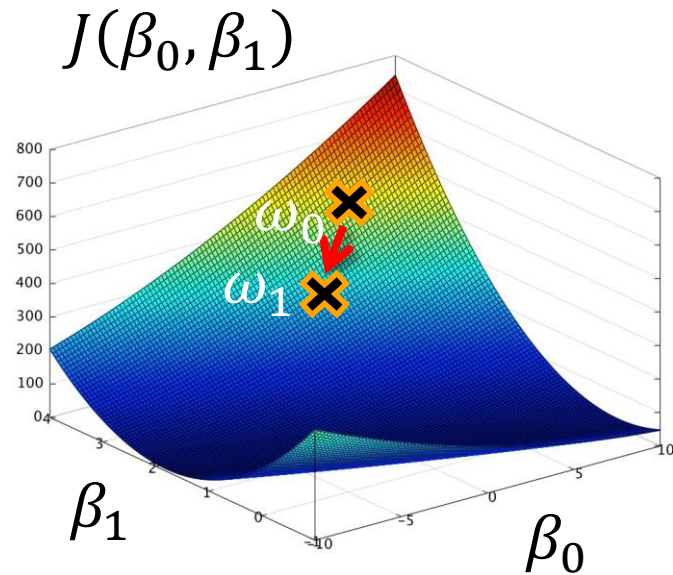
Mini Batch Gradient Descent

- Perform an update for every n training examples

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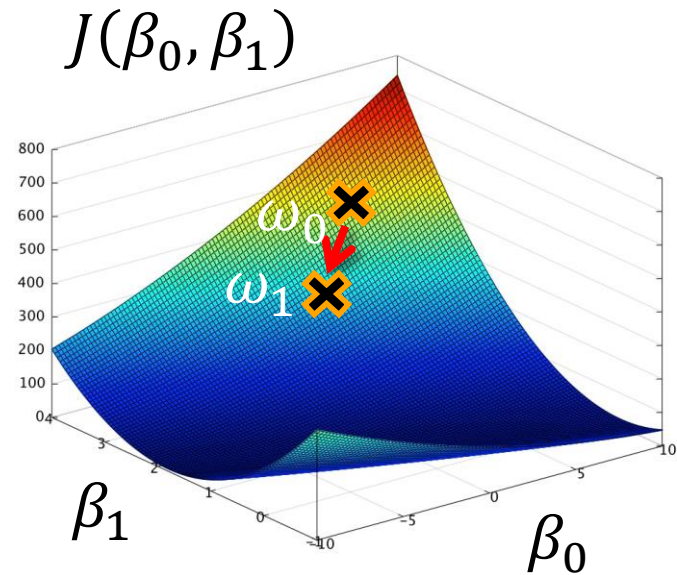
Best of both worlds:

- Reduced memory relative to "vanilla" gradient descent

- Less noisy than stochastic gradient descent

$J(\beta_0, \beta_1)$

ω_0

ω_1

β_1

β_0
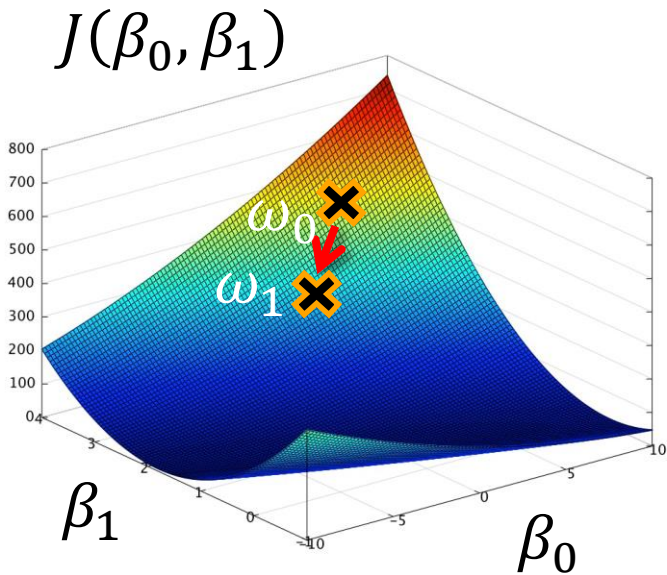
Mini Batch Gradient Descent

- Mini batch implementation typically used for neural nets

Mini Batch Gradient Descent

- Mini batch implementation typically used for neural nets

- Batch sizes range from 50-256 points

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)

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
```

Stochastic Gradient Descent Regression: Syntax

Import the class containing the regression model

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

Create an instance of the class

```
SGDreg = SGDRregressor(loss='squared_loss',
                       alpha=0.1, penalty='l2')
```

Stochastic Gradient Descent Regression: Syntax

Import the class containing the regression model

from sklearn.linear_model import **SGDRegressor**

Create an instance of the class

SGDreg = **SGDRregressor**(**loss='squared_loss',**

alpha=0.1, penalty='l2')

⬅ squared_loss = linear regression

Stochastic Gradient Descent Regression: Syntax

Import the class containing the regression model

from sklearn.linear_model import **SGDRegressor**

Create an instance of the class

SGDreg = **SGDRregressor**(**loss='squared_loss',**

alpha=0.1, penalty='l2')
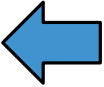
regularization parameters

Stochastic Gradient Descent Regression: Syntax

Import the class containing the regression model

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

Create an instance of the class

```
SGDreg = SGDRregressor(loss='squared_loss',
                        alpha=0.1, penalty='l2')
```

Fit the instance on the data and then transform the data

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

y_pred = SGDreg.predict(X_test)
```

Stochastic Gradient Descent Regression: Syntax

Import the class containing the regression model

from sklearn.linear_model import **SGDRegressor**

Create an instance of the class

SGDreg = **SGDRregressor**(**loss='squared_loss',**

alpha=0.1, penalty='l2')

Fit the instance on the data and then transform the data

SGDreg = **SGDreg**.**partial_fit**(X_train, y_train)

y_pred = **SGDreg**.**predict**(X_test)

← mini-batch version

Stochastic Gradient Descent Regression: The Syntax

Import the class containing the regression model

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

Create an instance of the class

```
SGDreg = SGDRregressor(loss='squared_loss',
                       alpha=0.1, penalty='l2')
```

Fit the instance on the data and then transform the data

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

y_pred = SGDreg.predict(X_test)
```

Other loss methods exist: epsilon_insensitive, huber, etc.

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

```
from sklearn.linear_model import SGDClassifier
```

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

```
from sklearn.linear_model import SGDClassifier
```

Create an instance of the class

```
SGDclass = SGDClassifier(loss='log',
                         alpha=0.1, penalty='l2')
```
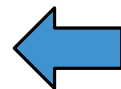
Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

from sklearn.linear_model import **SGDClassifier**

Create an instance of the class

SGDclass = **SGDClassifier(loss='log',**

alpha=0.1, penalty='l2')

log loss =
logistic regression

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

```
from sklearn.linear_model import SGDClassifier
```

Create an instance of the class

```
SGDclass = SGDClassifier(loss='log',
                alpha=0.1, penalty='l2')
```

Fit the instance on the data and then transform the data

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

y_pred = SGDclass.predict(X_test)
```

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

from sklearn.linear_model import **SGDClassifier**

Create an instance of the class

SGDclass = SGDClassifier(loss='log',

alpha=0.1, penalty='l2')

Fit the instance on the data and then transform the data

SGDclass = SGDclass.partial_fit(X_train, y_train)

y_pred = SGDclass.predict(X_test)

mini-batch version

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model

```
from sklearn.linear_model import SGDClassifier
```

Create an instance of the class

```
SGDclass = SGDClassifier(loss='log',
                alpha=0.1, penalty='l2')
```

Fit the instance on the data and then transform the data

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

y_pred = SGDclass.predict(X_test)
```

Other loss methods exist: hinge, squared_hinge, etc.

Stochastic Gradient Descent Classification: The Syntax

Import the class containing the classification model
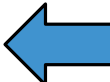
```
from sklearn.linear_model import SGDClassifier
```

Create an instance of the class

```
SGDclass = SGDClassifier(loss='log',
                         alpha=0.1, penalty='l2')
```

Fit the instance on the data and then transform the data

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

y_pred = SGDclass.predict(X_test)
```

Other loss methods exist: hinge, squared_hinge, etc.

See SVM lecture (week 7)

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