# Machine Learning - Regressions

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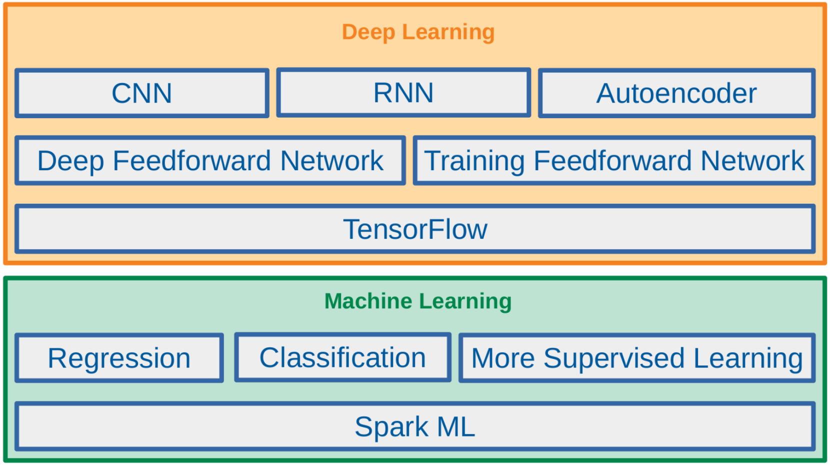
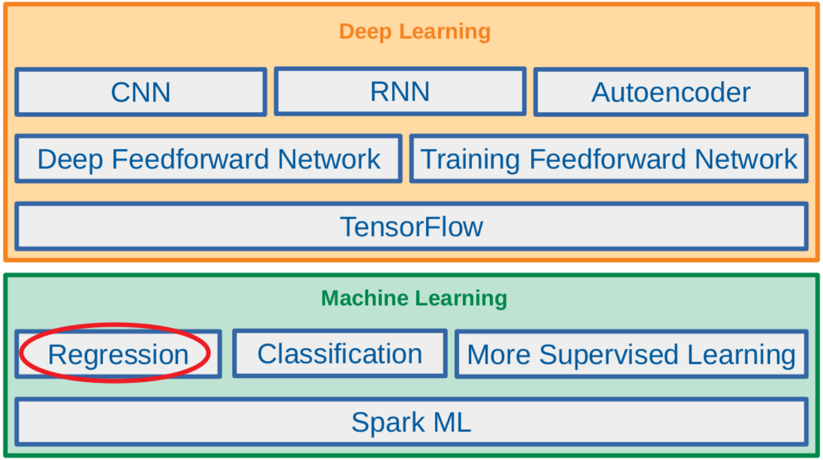
## The Course Web Page

https://id2223kth.github.io

## Where Are We?


Deep Learning
CNN
RNN
Autoencoder
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
Classification
More Supervised Learning
Spark ML

## Where Are We?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## Let's Start with an Example

## The Housing Price Example (1/3)

- Given the dataset of `m` houses.

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| ⋮ | ⋮ | ⋮ |

- Predict the prices of other houses, as a function of the size of living area and number of bedrooms?

## The Housing Price Example (2/3)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| $\vdots$ | $\vdots$ | $\vdots$ |

$$\mathbf{x}^{(1)} = \begin{bmatrix} 2104 \\ 3 \end{bmatrix} \quad y^{(1)} = 400 \qquad \mathbf{x}^{(2)} = \begin{bmatrix} 1600 \\ 3 \end{bmatrix} \quad y^{(2)} = 330 \qquad \mathbf{x}^{(3)} = \begin{bmatrix} 2400 \\ 3 \end{bmatrix} \quad y^{(3)} = 369$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)\intercal} \\ \mathbf{x}^{(2)\intercal} \\ \mathbf{x}^{(3)\intercal} \\ \vdots \end{bmatrix} = \begin{bmatrix} 2104 & 3 \\ 1600 & 3 \\ 2400 & 3 \\ \vdots & \vdots \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ \vdots \end{bmatrix}$$

- $\mathbf{x}^{(i)} \in \mathbb{R}^2$: $x_1^{(i)}$ is the living area, and $x_2^{(i)}$ is the number of bedrooms of the $i$th house in the training set.

## The Housing Price Example (3/3)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| $\vdots$ | $\vdots$ | $\vdots$ |

- Predict the prices of other houses $\hat{y}$ as a function of the size of their living areas $x_1$, and number of bedrooms $x_2$, i.e., $\hat{y} = f(x_1, x_2)$
- E.g., what is $\hat{y}$, if $x_1 = 4000$ and $x_2 = 4$?
- As an initial choice: $\hat{y} = f_w(\mathbf{x}) = w_1x_1 + w_2x_2$

## Linear Regression

## Linear Regression (1/2)

- Our goal: to build a system that takes input $\mathbf{x} \in \mathbb{R}^{\mathtt{n}}$ and predicts output $\hat{\mathtt{y}} \in \mathbb{R}$.
- In linear regression, the output $\hat{\mathtt{y}}$ is a linear function of the input $\mathbf{x}$.

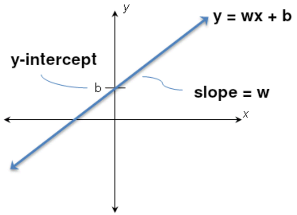
$$\hat{\mathtt{y}} = \mathtt{f}_{\mathtt{w}}(\mathbf{x}) = \mathtt{w}_1\mathtt{x}_1 + \mathtt{w}_2\mathtt{x}_2 + \cdots + \mathtt{w}_{\mathtt{n}}\mathtt{x}_{\mathtt{n}}$$
$$\hat{\mathtt{y}} = \mathbf{w}^{\mathsf{T}}\mathbf{x}$$

  - $\hat{\mathtt{y}}$: the predicted value
  - $\mathtt{n}$: the number of features
  - $\mathtt{x}_{\mathtt{i}}$: the $\mathtt{i}$th feature value
  - $\mathtt{w}_{\mathtt{j}}$: the $\mathtt{j}$th model parameter ($\mathbf{w} \in \mathbb{R}^{\mathtt{n}}$)

## Linear Regression (2/2)

- Linear regression often has one additional parameter, called intercept $\mathtt{b}$:

$$\hat{y} = \mathbf{w}^\intercal \mathbf{x} + \mathtt{b}$$



- Instead of adding the bias parameter $\mathtt{b}$, we can augment $\mathbf{x}$ with an extra entry that is always set to 1.

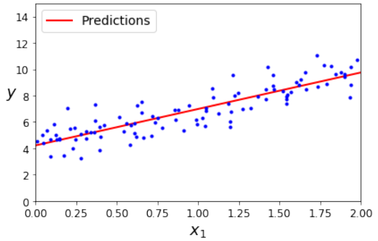
$$\hat{y} = f_w(\mathbf{x}) = w_0 x_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n, \text{ where } x_0 = 1$$

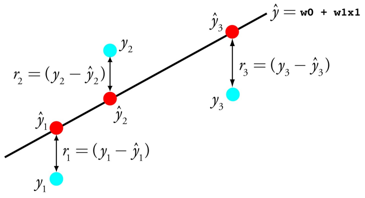
## Linear Regression - Model Parameters

- Parameters $\mathbf{w} \in \mathbb{R}^n$ are values that control the behavior of the model.
- $\mathbf{w}$ are a set of weights that determine how each feature affects the prediction.
  - $w_i > 0$: increasing the value of the feature $x_i$, increases the value of our prediction $\hat{y}$.
  - $w_i < 0$: increasing the value of the feature $x_i$, decreases the value of our prediction $\hat{y}$.
  - $w_i = 0$: the value of the feature $x_i$, has no effect on the prediction $\hat{y}$.

## How to Learn Model Parameters $\mathbf{w}$?

## Linear Regression - Cost Function (1/2)

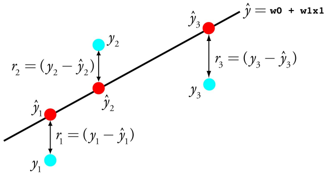



$\hat{y} = $ w0 + w1x1
$\hat{y}_3$
$y_2$
$r_2 = (y_2 - \hat{y}_2)$
$r_3 = (y_3 - \hat{y}_3)$
$y_3$
$\hat{y}_2$
$\hat{y}_1$
$r_1 = (y_1 - \hat{y}_1)$
$y_1$

- One reasonable model should make $\hat{y}$ close to $y$, at least for the training dataset.
- Residual: the difference between the dependent variable $y$ and the predicted value $\hat{y}$.

$$r^{(i)} = y^{(i)} - \hat{y}^{(i)}$$

## Linear Regression - Cost Function (2/2)



$\hat{y} =$ w0 + w1x1
$\hat{y}_3$
$y_2$
$r_2 = (y_2 - \hat{y}_2)$
$r_3 = (y_3 - \hat{y}_3)$
$y_3$
$\hat{y}_1$
$\hat{y}_2$
$r_1 = (y_1 - \hat{y}_1)$
$y_1$

- Cost function $\mathtt{J}(\mathbf{w})$
  - For each value of the $\mathbf{w}$, it measures how close the $\hat{\mathtt{y}}^{(\mathtt{i})}$ is to the corresponding $\mathtt{y}^{(\mathtt{i})}$.
  - We can define $\mathtt{J}(\mathbf{w})$ as the mean squared error (MSE):

$$\mathtt{J}(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) = \frac{1}{\mathtt{m}} \sum_{\mathtt{i}}^{\mathtt{m}} (\hat{\mathtt{y}}^{(\mathtt{i})} - \mathtt{y}^{(\mathtt{i})})^2$$

$$= \mathtt{E}[(\hat{\mathtt{y}} - \mathtt{y})^2] = \frac{1}{\mathtt{m}} ||\hat{\mathbf{y}} - \mathbf{y}||_2^2$$

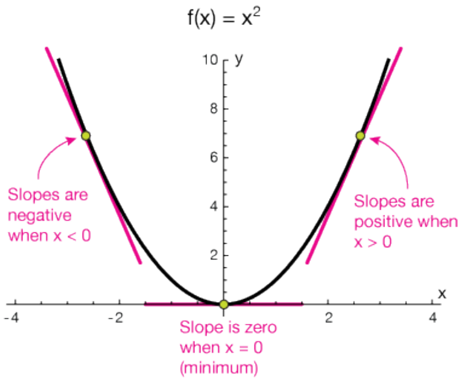
## How to Learn Model Parameters?

- We want to choose $\mathbf{w}$ so as to minimize $\mathtt{J}(\mathbf{w})$.
- Two approaches to find $\mathbf{w}$:
  - Normal equation
  - Gradient descent

## Normal Equation

## Derivatives and Gradient (1/3)

- The first derivative of $f(x)$, shown as $f'(x)$, shows the slope of the tangent line to the function at the poa $x$.
- $f(x) = x^2 \Rightarrow f'(x) = 2x$
- If $f(x)$ is increasing, then $f'(x) > 0$
- If $f(x)$ is decreasing, then $f'(x) < 0$
- If $f(x)$ is at local minimum/maximum, then $f'(x) = 0$



## Derivatives and Gradient (2/3)

- What if a function has multiple arguments, e.g., $f(x_1, x_2, \cdots, x_n)$
- Partial derivatives: the derivative with respect to a particular argument.
  - $\frac{\partial f}{\partial x_1}$, the derivative with respect to $x_1$
  - $\frac{\partial f}{\partial x_2}$, the derivative with respect to $x_2$
- $\frac{\partial f}{\partial x_i}$: shows how much the function $f$ will change, if we change $x_i$.
- Gradient: the vector of all partial derivatives for a function $f$.

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

## Derivatives and Gradient (3/3)

- What is the gradient of $f(x_1, x_2, x_3) = x_1 - x_1 x_2 + x_3^2$?

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1}(x_1 - x_1 x_2 + x_3^2) \\ \frac{\partial}{\partial x_2}(x_1 - x_1 x_2 + x_3^2) \\ \frac{\partial}{\partial x_3}(x_1 - x_1 x_2 + x_3^2) \end{bmatrix} = \begin{bmatrix} 1 - x_2 \\ -x_1 \\ 2x_3 \end{bmatrix}$$

## Normal Equation (1/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$\hat{y} = \mathbf{w}^\intercal \mathbf{x}$$

$$\mathbf{X} = \begin{bmatrix} [x_1^{(1)}, x_2^{(1)}, \cdots, x_n^{(1)}] \\ [x_1^{(2)}, x_2^{(2)}, \cdots, x_n^{(2)}] \\ \vdots \\ [x_1^{(m)}, x_2^{(m)}, \cdots, x_n^{(m)}] \end{bmatrix} = \begin{bmatrix} \mathbf{x}^{(1)\intercal} \\ \mathbf{x}^{(2)\intercal} \\ \vdots \\ \mathbf{x}^{(m)\intercal} \end{bmatrix} \qquad \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix}$$

$$\hat{\mathbf{y}} = \mathbf{w}^\intercal \mathbf{X}^\intercal \text{ or } \hat{\mathbf{y}} = \mathbf{X}\mathbf{w}$$

## Normal Equation (2/2)

- To minimize $J(\mathbf{w})$, we can simply solve for where its gradient is 0: $\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$

$$J(\mathbf{w}) = \frac{1}{m}||\hat{\mathbf{y}} - \mathbf{y}||_2^2, \nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m}||\hat{\mathbf{y}} - \mathbf{y}||_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} \frac{1}{m}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\intercal(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0$$

$$\Rightarrow \nabla_{\mathbf{w}} (\mathbf{w}^\intercal\mathbf{X}^\intercal\mathbf{X}\mathbf{w} - 2\mathbf{w}^\intercal\mathbf{X}^\intercal\mathbf{y} + \mathbf{y}^\intercal\mathbf{y}) = 0$$

$$\Rightarrow 2\mathbf{X}^\intercal\mathbf{X}\mathbf{w} - 2\mathbf{X}^\intercal\mathbf{y} = 0$$

$$\Rightarrow \mathbf{w} = (\mathbf{X}^\intercal\mathbf{X})^{-1}\mathbf{X}^\intercal\mathbf{y}$$

## Normal Equation - Example (1/7)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| 1416 | 2 | 232 |
| 3000 | 4 | 540 |

- Predict the value of $\hat{y}$, when $x_1 = 4000$ and $x_2 = 4$.
- We should find $w_0$, $w_1$, and $w_2$ in $\hat{y} = w_0 + w_1 x_1 + w_2 x_2$.
- $\mathbf{w} = (\mathbf{X}^\intercal \mathbf{X})^{-1} \mathbf{X}^\intercal \mathbf{y}$.

## Normal Equation - Example (2/7)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| 1416 | 2 | 232 |
| 3000 | 4 | 540 |

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

```
import breeze.linalg._

val X = new DenseMatrix(5, 3, Array(1.0, 1.0, 1.0, 1.0, 1.0,
                                    2104.0, 1600.0, 2400.0, 1416.0, 3000.0,
                                    3.0, 3.0, 3.0, 2.0, 4.0))
val y = new DenseVector(Array(400.0, 330.0, 369.0, 232.0, 540.0))
```

## Normal Equation - Example (3/7)

$$\mathbf{X}^\intercal\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 2104 & 1600 & 2400 & 1416 & 3000 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 10520 & 15 \\ 10520 & 23751872 & 33144 \\ 15 & 33144 & 47 \end{bmatrix}$$

```
val Xt = X.t
val XtX = Xt * X
```

## Normal Equation - Example (4/7)

$$(\mathbf{X}^\intercal\mathbf{X})^{-1} = \begin{bmatrix} 4.90366455e+00 & 7.48766737e-04 & -2.09302326e+00 \\ 7.48766737e-04 & 2.75281889e-06 & -2.18023256e-03 \\ -2.09302326e+00 & -2.18023256e-03 & 2.22674419e+00 \end{bmatrix}$$

```
val XtXInv = inv(XtX)
```

## Normal Equation - Example (5/7)

$$\mathbf{X}^\intercal \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 2104 & 1600 & 2400 & 1416 & 3000 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix} = \begin{bmatrix} 1871 \\ 4203712 \\ 5921 \end{bmatrix}$$

```
val Xty = Xt * y
```

## Normal Equation - Example (6/7)

$$\mathbf{w} = (\mathbf{X}^\intercal\mathbf{X})^{-1}\mathbf{X}^\intercal \mathrm{y} = \begin{bmatrix} 4.90366455\mathrm{e}+00 & 7.48766737\mathrm{e}-04 & -2.09302326\mathrm{e}+00 \\ 7.48766737\mathrm{e}-04 & 2.75281889\mathrm{e}-06 & -2.18023256\mathrm{e}-03 \\ -2.09302326\mathrm{e}+00 & -2.18023256\mathrm{e}-03 & 2.22674419\mathrm{e}+00 \end{bmatrix} \begin{bmatrix} 1871 \\ 4203712 \\ 5921 \end{bmatrix}$$

$$= \begin{bmatrix} -7.04346018e+01 \\ 6.38433756e-02 \\ 1.03436047e+02 \end{bmatrix}$$

```
val w = XtXInv * Xty
```

## Normal Equation - Example (7/7)

- Predict the value of $y$, when $x_1 = 4000$ and $x_2 = 4$.

$$\hat{y} = -7.04346018e+01 + 6.38433756e-02 \times 4000 + 1.03436047e+02 \times 4 \approx 599$$

```
val test =  new DenseVector(Array(1.0, 4000.0, 4.0))

val yHat = w * test
```

## Normal Equation in Spark

```scala
case class house(x1: Long, x2: Long, y: Long)

val trainData = Seq(house(2104, 3, 400), house(1600, 3, 330), house(2400, 3, 369),
                    house(1416, 2, 232), house(3000, 4, 540)).toDF

val testData = Seq(house(4000, 4, 0)).toDF
```

```scala
import org.apache.spark.ml.feature.VectorAssembler

val va = new VectorAssembler().setInputCols(Array("x1", "x2")).setOutputCol("features")

val train = va.transform(trainData)
val test = va.transform(testData)
```

```scala
import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setFeaturesCol("features").setLabelCol("y").setSolver("normal")
val lrModel = lr.fit(train)
lrModel.transform(test).show
```

## Normal Equation - Computational Complexity

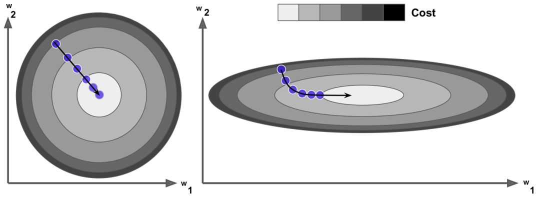
- The computational complexity of inverting $\mathbf{X}^\intercal\mathbf{X}$ is $\mathtt{O}(\mathtt{n}^3)$.
    - For an $\mathtt{m} \times \mathtt{n}$ matrix (where $\mathtt{n}$ is the number of features).
- But, this equation is linear with regards to the number of instances in the training set (it is $\mathtt{O}(\mathtt{m})$).
    - It handles large training sets efficiently, provided they can fit in memory.

## Gradient Descent

## Gradient Descent (1/2)

- Gradient descent is a generic optimization algorithm capable of finding optimal solutions to a wide range of problems.

- The idea: to tweak parameters iteratively in order to minimize a cost function.

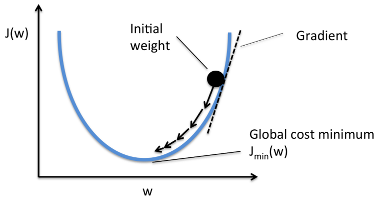


## Gradient Descent (2/2)

- Suppose you are lost in the mountains in a dense fog.
- You can only feel the slope of the ground below your feet.
- A strategy to get to the bottom of the valley is to go downhill in the direction of the steepest slope.

## Gradient Descent - Iterative Optimization Algorithm

- Choose a starting point, e.g., filling **w** with random values.
- If the stopping criterion is true return the current solution, otherwise continue.
- Find a descent direction, a direction in which the function value decreases near the current point.
- Determine the step size, the length of a step in the given direction.



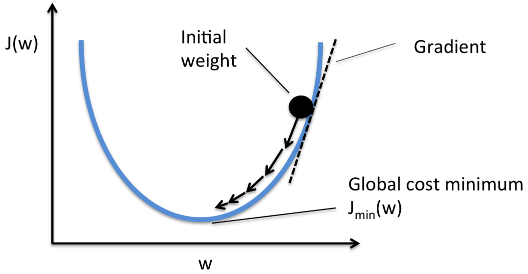
## Gradient Descent - Key Points

- Stopping criterion
- Descent direction
- Step size (learning rate)

## Gradient Descent - Stopping Criterion

- The cost function minimum property: the gradient has to be zero.

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = 0$$

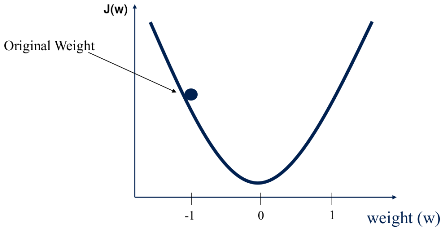


## Gradient Descent - Descent Direction (1/2)

- Direction in which the function value decreases near the current point.
- Find the direction of descent (slope).
- Example:

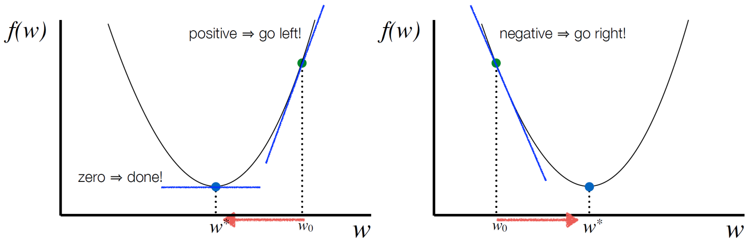
$$J(w) = w^2$$

$$\frac{\partial J(w)}{\partial w} = 2w = -2 \text{ at } w = -1$$



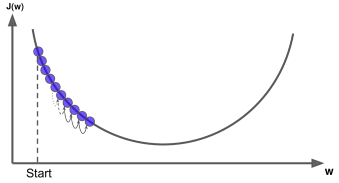
# Gradient Descent - Descent Direction (2/2)

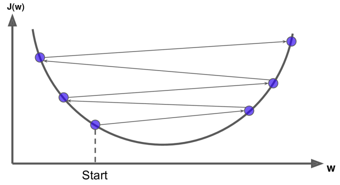
- Follow the opposite direction of the slope.



## Gradient Descent - Learning Rate

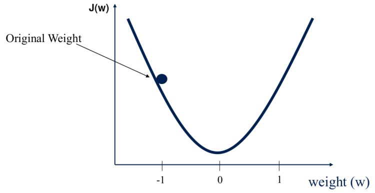
- Learning rate: the length of steps.
- If it is too small: many iterations to converge.
- If it is too high: the algorithm might diverge.





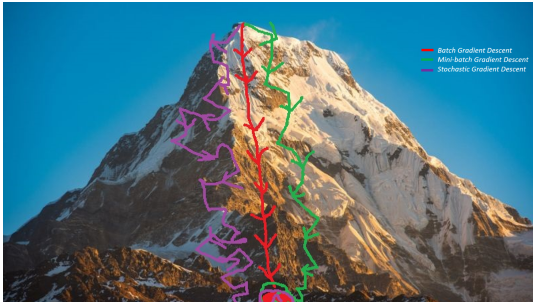
## Gradient Descent - How to Learn Model Parameters $\mathbf{w}$?

- Goal: find $\mathbf{w}$ that minimizes $J(\mathbf{w}) = \sum_{i=1}^{m}(\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)})^2$.
- Start at a random point, and repeat the following steps, until the stopping criterion is satisfied:
  1. Determine a descent direction $\frac{\partial J(\mathbf{w})}{\partial w}$
  2. Choose a step size $\eta$
  3. Update the parameters: $w^{(next)} = w - \eta \frac{\partial J(\mathbf{w})}{\partial w}$ (should be done for all parameters simultanously)



## Gradient Descent - Different Algorithms

- Batch gradient descent
- Stochastic gradient descent
- Mini-batch gradient descent



[https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3]

## Batch Gradient Descent

## Batch Gradient Descent (1/2)

- Repeat the following steps, until the stopping criterion is satisfied:

  1. Determine a descent direction $\frac{\partial J(\mathbf{w})}{\partial w}$ for all parameters $\mathbf{w}$.

$$J(\mathbf{w}) = \sum_{i=1}^{m} (\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)})^2$$

$$\frac{\partial J(\mathbf{w})}{\partial w_j} = \frac{2}{m} \sum_{i=1}^{m} (\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)}) x_j^{(i)} \qquad \nabla_{\mathbf{w}} J(\mathbf{w}) = \begin{bmatrix} \frac{\partial J(\mathbf{w})}{\partial w_0} \\ \frac{\partial J(\mathbf{w})}{\partial w_1} \\ \vdots \\ \frac{\partial J(\mathbf{w})}{\partial w_n} \end{bmatrix} = \frac{2}{m} \mathbf{X}^\intercal (\mathbf{X}\mathbf{w} - \mathbf{y})$$

  2. Choose a step size $\eta$
  3. Update the parameters: $\mathbf{w}^{(\text{next})} = \mathbf{w} - \eta \nabla_{\mathbf{w}} J(\mathbf{w})$

## Batch Gradient Descent (2/2)

- The algorithm is called Batch Gradient Descent, because at each step, calculations are over the full training set $\mathbf{X}$.
- As a result it is slow on very large training sets, i.e., large `m`.
- But, it scales well with the number of features `n`.

## Batch Gradient Descent - Example (1/5)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| 1416 | 2 | 232 |
| 3000 | 4 | 540 |

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

## Batch Gradient Descent - Example (2/5)

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

$$\begin{aligned}\frac{\partial J(\mathbf{w})}{\partial w_0} &= \frac{2}{m}\sum_{i=1}^{m}(\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)})x_0^{(i)} \\ &= \frac{2}{5}[(w_0 + 2104w_1 + 3w_2 - 400) + (w_0 + 1600w_1 + 3w_2 - 330) + \\ &(w_0 + 2400w_1 + 3w_2 - 369) + (w_0 + 1416w_1 + 2w_2 - 232) + (w_0 + 3000w_1 + 4w_2 - 540)]\end{aligned}$$

## Batch Gradient Descent - Example (3/5)

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

$$\frac{\partial J(\mathbf{w})}{\partial w_1} = \frac{2}{m}\sum_{i=1}^{m}(\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)})x_1^{(i)}$$
$$= \frac{2}{5}[2104(w_0 + 2104w_1 + 3w_2 - 400) + 1600(w_0 + 1600w_1 + 3w_2 - 330)+$$
$$2400(w_0 + 2400w_1 + 3w_2 - 369) + 1416(w_0 + 1416w_1 + 2w_2 - 232) + 3000(w_0 + 3000w_1 + 4w_2 - 540)]$$

## Batch Gradient Descent - Example (4/5)

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

$$\frac{\partial J(\mathbf{w})}{\partial w_2} = \frac{2}{m}\sum_{i=1}^{m}(\mathbf{w}^\intercal \mathbf{x}^{(i)} - y^{(i)})x_2^{(i)}$$

$$= \frac{2}{5}[3(w_0 + 2104w_1 + 3w_2 - 400) + 3(w_0 + 1600w_1 + 3w_2 - 330) +$$

$$3(w_0 + 2400w_1 + 3w_2 - 369) + 2(w_0 + 1416w_1 + 2w_2 - 232) + 4(w_0 + 3000w_1 + 4w_2 - 540)]$$

## Batch Gradient Descent - Example (5/5)

$$\mathtt{w}_0^{(\mathtt{next})} = \mathtt{w}_0 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_0}$$

$$\mathtt{w}_1^{(\mathtt{next})} = \mathtt{w}_1 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_1}$$

$$\mathtt{w}_2^{(\mathtt{next})} = \mathtt{w}_2 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_2}$$

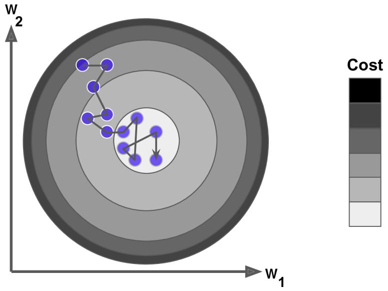
## Stochastic Gradient Descent

## Stochastic Gradient Descent (1/3)

- Batch gradient descent problem: it's slow, because it uses the whole training set to compute the gradients at every step.
- Stochastic gradient descent computes the gradients based on only a single instance.
  - It picks a random instance in the training set at every step.

## Stochastic Gradient Descent (2/3)

- The algorithm is much faster, but less regular than batch gradient descent.
  - Instead of decreasing until it reaches the minimum, the cost function will bounce up and down.
  - It never settles down.



## Stochastic Gradient Descent (3/3)

- With randomness the algorithm can never settle at the minimum.
- One solution is simulated annealing: start with large learning rate, then make it smaller and smaller.
- Learning schedule: the function that determines the learning rate at each step.

## Stochastic Gradient Descent - Example (1/3)

| Living area | No. of bedrooms | Price |
|---|---|---|
| 2104 | 3 | 400 |
| 1600 | 3 | 330 |
| 2400 | 3 | 369 |
| 1416 | 2 | 232 |
| 3000 | 4 | 540 |

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

## Stochastic Gradient Descent - Example (2/3)

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 2104 & 3 \\ 1 & 1600 & 3 \\ 1 & 2400 & 3 \\ 1 & 1416 & 2 \\ 1 & 3000 & 4 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 400 \\ 330 \\ 369 \\ 232 \\ 540 \end{bmatrix}$$

$$\frac{\partial J(\mathbf{w})}{\partial w_0} = \frac{2}{m}(\mathbf{w}^\mathsf{T}\mathbf{x}^{(i)} - y^{(i)})x_0^{(i)} = \frac{2}{5}[(w_0 + 1600w_1 + 3w_2 - 330)]$$

$$\frac{\partial J(\mathbf{w})}{\partial w_1} = \frac{2}{m}(\mathbf{w}^\mathsf{T}\mathbf{x}^{(i)} - y^{(i)})x_1^{(i)} = \frac{2}{5}[1416(w_0 + 1416w_1 + 2w_2 - 232)]$$

$$\frac{\partial J(\mathbf{w})}{\partial w_2} = \frac{2}{m}(\mathbf{w}^\mathsf{T}\mathbf{x}^{(i)} - y^{(i)})x_2^{(i)} = \frac{2}{5}[3(w_0 + 2104w_1 + 3w_2 - 400)]$$

## Stochastic Gradient Descent - Example (3/3)

$$\mathtt{w}_0^{(\mathtt{next})} = \mathtt{w}_0 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_0}$$

$$\mathtt{w}_1^{(\mathtt{next})} = \mathtt{w}_1 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_1}$$

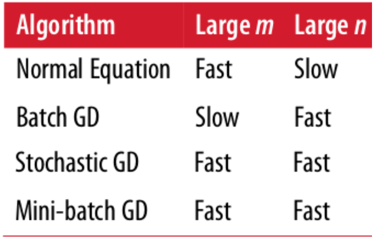
$$\mathtt{w}_2^{(\mathtt{next})} = \mathtt{w}_2 - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_2}$$

## Mini-Batch Gradient Descent

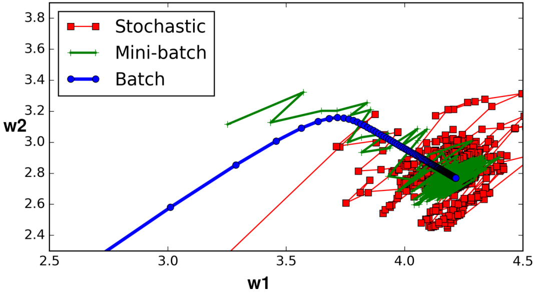
## Mini-Batch Gradient Descent

- Batch gradient descent: at each step, it computes the gradients based on the full training set.
- Stochastic gradient descent: at each step, it computes the gradients based on just one instance.
- Mini-batch gradient descent: at each step, it computes the gradients based on small random sets of instances called mini-batches.

## Comparison of Algorithms for Linear Regression



| Algorithm | Large *m* | Large *n* |
|---|---|---|
| Normal Equation | Fast | Slow |
| Batch GD | Slow | Fast |
| Stochastic GD | Fast | Fast |
| Mini-batch GD | Fast | Fast |



## Gradient Descent in Spark

```
val data = spark.read.format("libsvm").load("data.txt")
```

```
import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setMaxIter(10)

val lrModel = lr.fit(data)
```

```
println(s"Coefficients: ${lrModel.coefficients} Intercept: ${lrModel.intercept}")

val trainingSummary = lrModel.summary
println(s"RMSE: ${trainingSummary.rootMeanSquaredError}")
```

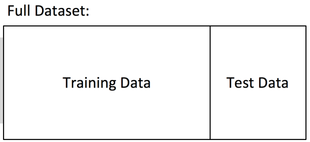
## Generalization

## Training Data and Test Data

- Split data into a training set and a test set.
- Use training set when training a machine learning model.
  - Compute training error on the training set.
  - Try to reduce this training error.
- Use test set to measure the accuracy of the model.
  - Test error is the error when you run the trained model on test data (new data).

```
val data = spark.read.format("libsvm").load("data.txt")

val Array(trainDF, testDF) = data.randomSplit(Array(0.8, 0.2))
```



## Generalization

- **Generalization**: make a model that performs well on test data.
  - Have a small test error.

- Challenges
  1. Make the training error small.
  2. Make the gap between training and test error small.

## More About The Test Error

- The test error is defined as the expected value of the error on test set.

$$\mathtt{MSE} = \frac{1}{k}\sum_{i}^{k}(\hat{y}^{(i)} - y^{(i)})^2, \text{ k: the num. of instances in the test set}$$
$$= E[(\hat{y} - y)^2]$$

- A model's test error can be expressed as the sum of bias and variance.

$$E[(\hat{y} - y)^2] = \mathtt{Bias}[\hat{y}, y]^2 + \mathtt{Var}[\hat{y}] + \varepsilon^2$$

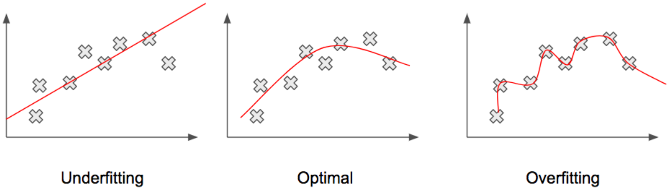
## Bias and Underfitting

- Bias: the expected deviation from the true value of the function.

$$\mathtt{Bias}[\hat{y}, y] = \mathtt{E}[\hat{y}] - y$$

- A high-bias model is most likely to underfit the training data.
  - High error value on the training set.

- Underfitting happens when the model is too simple to learn the underlying structure of the data.

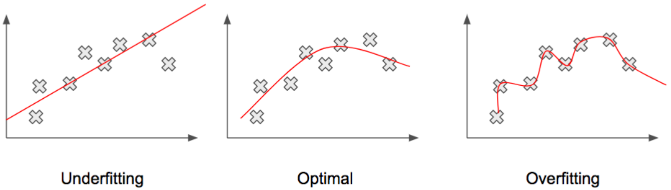


## Variance and Overfitting

- Variance: how much a model changes if you train it on a different training set.

$$\mathtt{Var}[\hat{y}] = \mathtt{E}[(\hat{y} - \mathtt{E}[\hat{y}])^2]$$

- A high-variance model is most likely to overfit the training data.
  - The gap between the training error and test error is too large.
- Overfitting happens when the model is too complex relative to the amount and noisiness of the training data.

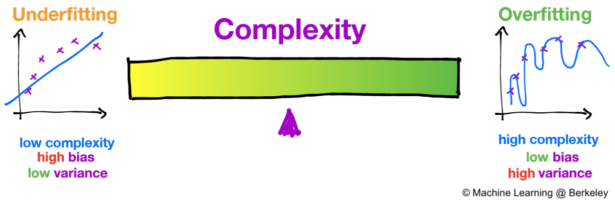


## The Bias/Variance Tradeoff (1/2)

- Assume a model with two parameters $\mathtt{w}_0$ (intercept) and $\mathtt{w}_1$ (slope): $\hat{\mathtt{y}} = \mathtt{w}_0 + \mathtt{w}_1\mathtt{x}$
- They give the learning algorithm two degrees of freedom.
- We tweak both the $\mathtt{w}_0$ and $\mathtt{w}_1$ to adapt the model to the training data.
- If we forced $\mathtt{w}_0 = 0$, the algorithm would have only one degree of freedom and would have a much harder time fitting the data properly.

## The Bias/Variance Tradeoff (2/2)

- Increasing degrees of freedom will typically increase its variance and reduce its bias.
- Decreasing degrees of freedom increases its bias and reduces its variance.
- This is why it is called a tradeoff.



[https://ml.berkeley.edu/blog/2017/07/13/tutorial-4]

## Regularization (1/2)

- One way to reduce the risk of overfitting is to have fewer degrees of freedom.
- Regularization is a technique to reduce the risk of overfitting.
- For a linear model, regularization is achieved by constraining the weights of the model.

$$\mathtt{J}(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) + \lambda \mathtt{R}(\mathbf{w})$$

## Regularization (2/2)

- Lasso regression ($l1$): $\mathtt{R}(\mathbf{w}) = \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} |\mathtt{w}_\mathtt{i}|$ is added to the cost function:

$$\mathtt{J}(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) + \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} |\mathtt{w}_\mathtt{i}|$$

- Ridge regression ($l2$): $\mathtt{R}(\mathbf{w}) = \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} \mathtt{w}_\mathtt{i}^2$ is added to the cost function.

$$\mathtt{J}(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) + \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} \mathtt{w}_\mathtt{i}^2$$

- ElasticNet: a middle ground between $l1$ and $l2$ regularization.

$$\mathtt{J}(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) + \alpha\lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} |\mathtt{w}_\mathtt{i}| + (1-\alpha)\lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} \mathtt{w}_\mathtt{i}^2$$

## Regularization in Spark

$$J(w) = MSE(w) + \alpha\lambda \sum_{i=1}^{n} |w_i| + (1-\alpha)\lambda \sum_{i=1}^{n} w_i^2$$

- If $\alpha = 0$: *l*2 regularization
- If $\alpha = 1$: *l*1 regularization
- For $\alpha$ in $(0, 1)$: a combination of *l*1 and *l*2 regularizations

```
import org.apache.spark.ml.regression.LinearRegression

val lr = new LinearRegression().setElasticNetParam(0.8)

val lrModel = lr.fit(data)
```

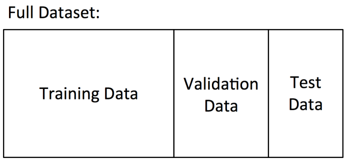
## Hyperparameters

## Hyperparameters and Validation Sets (1/2)

- Hyperparameters are settings that we can use to control the behavior of a learning algorithm.
- The values of hyperparameters are not adapted by the learning algorithm itself.
  - E.g., the $\alpha$ and $\lambda$ values for regularization.
- We do not learn the hyperparameter.
  - It is not appropriate to learn that hyperparameter on the training set.
  - If learned on the training set, such hyperparameters would always result in overfitting.

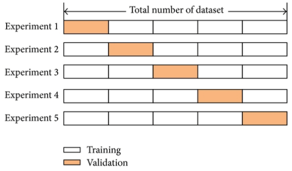
## Hyperparameters and Validation Sets (2/2)

- To find hyperparameters, we need a validation set of examples that the training algorithm does not observe.
- We construct the validation set from the training data (not the test data).
- We split the training data into two disjoint subsets:
  1. One is used to learn the parameters.
  2. The other one (the validation set) is used to estimate the test error during or after training, allowing for the hyperparameters to be updated accordingly.



## Cross-Validation

- Cross-validation: a technique to avoid wasting too much training data in validation sets.
- The training set is split into complementary subsets.
- Each model is trained against a different combination of these subsets and validated against the remaining parts.
- Once the model type and hyperparameters have been selected, a final model is trained using these hyperparameters on the full training set, and the test error is measured on the test set.



## Hyperparameters and Cross-Validation in Spark (1/2)

- `CrossValidator` to optimize hyperparameters in algorithms and model selection.
- It requires the following items:
  - `Estimator`: algorithm or Pipeline to tune.
  - Set of `ParamMaps`: parameters to choose from (also called a parameter grid).
  - `Evaluator`: metric to measure how well a fitted Model does on held-out test data.

## Hyperparameters and Cross-Validation in Spark (2/2)

```
// construct a grid of parameters to search over.
// this grid has 2 x 2 = 4 parameter settings for CrossValidator to choose from.
val paramGrid = new ParamGridBuilder()
  .addGrid(lr.regParam, Array(0.1, 0.01))
  .addGrid(lr.elasticNetParam, Array(0.0, 1.0))
  .build()
```

```
val lr = new LinearRegression()

// num folds = 3 => (2 x 2) x 3 = 12 different models being trained
val cv = new CrossValidator()
  .setEstimator(lr)
  .setEvaluator(new RegressionEvaluator())
  .setEstimatorParamMaps(paramGrid)
  .setNumFolds(3)

val cvModel = cv.fit(trainDF)
```

## Summary

## Summary

- Linear regression model $\hat{y} = \mathbf{w}^\top \mathbf{x}$
  - Learning parameters $\mathbf{w}$
  - Cost function $J(\mathbf{w})$
  - Learn parameters: normal equation, gradient descent (batch, stochastic, mini-batch)
- Generalization
  - Overfitting vs. underfitting
  - Bias vs. variance
  - Regularization: Lasso regression, Ridge regression, ElasticNet
- Hyperparameters and cross-validation

## Reference

- Ian Goodfellow et al., Deep Learning (Ch. 4, 5)
- Aurélien Géron, Hands-On Machine Learning (Ch. 2, 4)
- Matei Zaharia et al., Spark - The Definitive Guide (Ch. 27)

Questions?