# SDM274: Al and Machine Learning

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Lecture: Regression and Linear Regression

- Regression Problems
- Linear Regression

#### o What should I watch this Friday?



#### o What should I watch this Friday?



o Goal: Predict movie rating automatically!



o Goal: How many followers will I get?



. Goal: Predict the price of the house



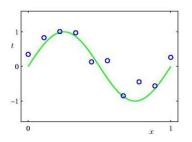
# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these t

(e.g., a rating: a real number between 0-10, # of followers, house price)

- Predicting continuous outputs is called regression
- What do I need in order to predict these outputs?
  - Features (inputs), we'll call these *x* (or **x** if vectors)
  - Training examples, many x(i) for which t(i) is known (e.g., many movies for which we know the rating)
  - A model, a function that represents the relationship between x and t
  - A loss or a cost or an objective function, which tells us how well our model approximates the training examples
  - Optimization, a way of finding the parameters of our model that minimizes the loss function

### Simple 1-D regression



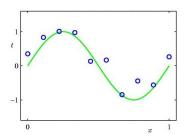
- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in x, but may be displaced in

$$t(x) = f(x) + \epsilon$$

with  $\epsilon$  some noise

- In green is the "true" curve that we don't know
- Goal: We want to fit a curve to these points

### Simple 1-D regression

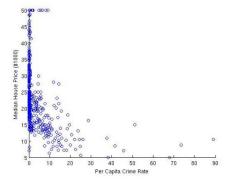


#### Key Questions:

- ► How do we parametrize the model?
- What loss (objective) function should we use to judge the fit?
- ► How do we optimize fit to unseen test data (generalization)?

### Example: Boston Housing data

- Estimate median house price in a neighborhood based on neighborhood statistics
- Look at first possible attribute (feature): per capita crime rate



- Use this to predict house prices in other neighborhoods
- Is this a good input (attribute) to predict house prices?

### Represent the Data

- Data is described as pairs  $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$ 
  - $x \in \mathbb{R}$  is the input feature (per capita crime rate)
  - ▶  $t \in \mathbb{R}$  is the target output (median house price)
  - ightharpoonup (i) simply indicates the training examples (we have N in this case)
- Here t is continuous, so this is a regression problem
- Model outputs y, an estimate of t

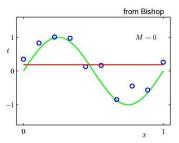
$$y(x) = w_0 + w_1 x$$

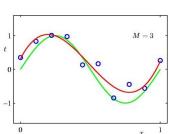
- What type of model did we choose?
- Divide the dataset into training and testing examples
  - ► Use the training examples to construct hypothesis, or function approximator, that maps *x* to predicted *y*
  - Evaluate hypothesis on test set

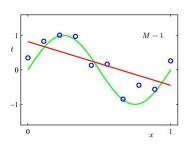
### Noise

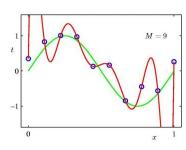
- A simple model typically does not exactly fit the data
  - lack of fit can be considered noise
- Sources of noise:
  - Imprecision in data attributes (input noise, e.g., noise in per-capita crime)
  - ► Errors in data targets (mis-labeling, e.g., noise in house prices)
  - Additional attributes not taken into account by data attributes, affect target values (latent variables). In the example, what else could affect house prices?
  - Model may be too simple to account for data targets

# Which fit is best?









### Summary of Regression

### Regression: to predict continuous outputs *t*

- Consider proper features (inputs): X (or x if vectors)
- Training examples, many x(i) for which t(i) is known (labeled)
- A model, a function that represents the relationship between x and t

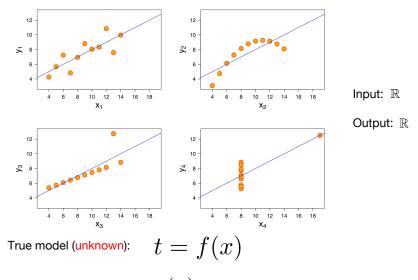
$$y = f(x, w)$$

- A loss or a cost or an objective function, which tells us how well our model approximates the training examples
- Optimization, a way of finding the parameters w of our model that minimizes the loss function

# Linear Regression

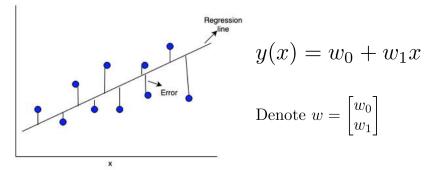
- Linear regression
  - continuous outputs
  - ► simple model (linear)
- Introduce key concepts:
  - loss functions
  - generalization
  - optimization
  - model complexity
  - regularization

# Linear regression model



lacksquare Linear regression model:  $y(x)=w_0+w_1x$ 

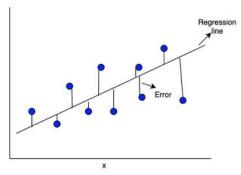
# Loss function: Mean Squared Error (MSE)



■ Standard loss/cost/objective function measures the mean squared error between *y* and the true value *t* 

$$l(w) = \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - y^{(n)} \right]^{2}$$
$$= \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - (w_0 + w_1 x^{(n)}) \right]^{2}$$

# Loss function: Mean Squared Error (MSE)



The loss is the mean of the sequared vertical errors

 Standard loss/cost/objective function measures the mean squared error between y and the true value t

$$l(w) = \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - y^{(n)} \right]^{2}$$
$$= \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - (w_0 + w_1 x^{(n)}) \right]^{2}$$

# Loss function: Mean Squared Error (MSE)

MSE loss:

$$l(w) = \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - y^{(n)} \right]^{2}$$

```
def mean_squared_error(true, pred):
    squared_error = np.square(true - pred)
    sum_squared_error = np.sum(squared_error)
    mse_loss = sum_squared_error / true.size
    return mse_loss
```

### Other loss function: Root Mean Squared Error (RMSE)

RMSE= 
$$\sqrt{\frac{1}{N}} \sum_{n=1}^{N} [t^{(n)} - y^{(n)}]^2$$

```
def root_mean_squared_error(true, pred):
    squared_error = np.square(true - pred)
    sum_squared_error = np.sum(squared_error)
    rmse_loss = np.sqrt(sum_squared_error / true.size)
    return rmse_loss
```

### Other loss function: Relative Squared Error (RSE)

RSE= 
$$\frac{\sum_{n=1}^{N} [t^{(n)} - y^{(n)}]^2}{\sum_{n=1}^{N} [t^{(n)} - \bar{t}]^2}, \quad \bar{t} = \frac{1}{N} \sum_{n=1}^{N} t^{(n)}$$

Merit: Insensitive to the mean and scale of samples

```
def relative_squared_error(true, pred):
    true_mean = np.mean(true)
    squared_error_num = np.sum(np.square(true - pred))
    squared_error_den = np.sum(np.square(true - true_mean))
    rse_loss = squared_error_num / squared_error_den
    return rse_loss
```

# Other loss function: Mean Absolute Error (MAE)

MAE= 
$$\frac{1}{N} \sum_{n=1}^{N} |t^{(n)} - y^{(n)}|$$

```
def mean_absolute_error(true, pred):
    abs_error = np.abs(true - pred)
    sum_abs_error = np.sum(abs_error)
    mae_loss = sum_abs_error / true.size
    return mae_loss
```

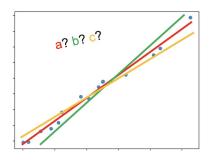
### Other loss function: Relative Absolute Error (RAE)

RAE= 
$$\frac{\sum_{n=1}^{N} |t^{(n)} - y^{(n)}|}{\sum_{n=1}^{N} |t^{(n)} - \bar{t}|}, \quad \bar{t} = \frac{1}{N} \sum_{n=1}^{N} t^{(n)}$$

```
def relative_absolute_error(true, pred):
    true_mean = np.mean(true)
    squared_error_num = np.sum(np.abs(true - pred))
    squared_error_den = np.sum(np.abs(true - true_mean))
    rae_loss = squared_error_num / squared_error_den
    return rae_loss
```

# Optimization in training

- lacktriangle Linear regression model:  $y(x)=w_0+w_1x$
- MSE loss:  $l(w) = \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} y^{(n)} \right]^2$
- How do we obtain weights w? Find w that minimizes loss l(w)

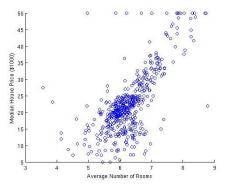


# Multi-dimensional Inputs

• One method of extending the model is to consider other input dimensions

$$y(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2$$

• In the Boston housing example, we can look at the number of rooms



# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations
- Each house is a data point n, with observations indexed by j:

$$\mathbf{x}^{(n)} = \left(x_1^{(n)}, \cdots, x_j^{(n)}, \cdots, x_d^{(n)}\right)$$

• We can incorporate the bias  $w_0$  into  $\mathbf{w}$ , by using  $x_0 = 1$ , then

$$y(\mathbf{x}) = w_0 + \sum_{j=1}^d w_j x_j = \mathbf{w}^T \mathbf{x}$$

• We can then solve for  $\mathbf{w} = (w_0, w_1, \dots, w_d)$ . How?

# Optimization in training

■ Linear regression model:

ssion model: 
$$y(x) = w^T \mathbf{x}, \quad \mathbf{x} = \begin{bmatrix} 1 \\ x \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}, \quad w = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

MSE loss:

$$l(w) = \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - y(x^{(n)}) \right]^{2}$$
$$= \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - w^{T} \mathbf{x}^{(n)} \right]^{2}$$

■ How do we obtain weights w? Find w that minimizes loss l(w)

### Detour: Gradients

- We can concatenate partial derivatives of a multivariate function with respect to all its variables to obtain the gradient vector of the function.
- $\begin{array}{c} \blacksquare \text{ Let } f: \mathbb{R}^n \to \mathbb{R} & \text{ . Then the gradient of the function is} \\ \nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_n}\right]^\top, \end{array}$

where  $\nabla_{\mathbf{x}} f(\mathbf{x})$  is often replaced by  $\nabla f(\mathbf{x})$  when there is no ambiguity.

#### **Detour: Convex function**

**Definition 1.** A function  $f: \mathbb{R}^n \to \mathbb{R}$  is convex if its domain is a convex set and for all x, y in its domain, and all  $\lambda \in [0, 1]$ , we have

$$f(\lambda x + (1 - \lambda)y) \le \lambda f(x) + (1 - \lambda)f(y).$$

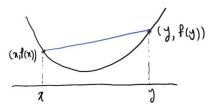
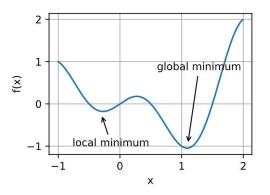


Figure 1: An illustration of the definition of a convex function

### **Detour: Local minima**

$$f(x) = x \cdot \cos(\pi x) \text{ for } -1.0 \le x \le 2.0$$



The cost function usually has many local optima.

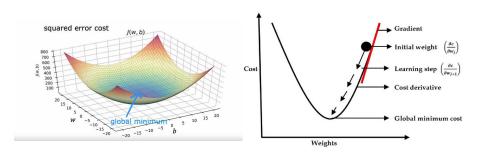
$$\nabla f(\bar{x}) = 0$$

### **Detour: Global optimal**

Corollary 1. Consider an unconstrained optimization problem

$$\min f(x)$$
s.t.  $x \in \mathbb{R}^n$ ,

where f is convex and differentiable. Then, any point  $\bar{x}$  that satisfies  $\nabla f(\bar{x}) = 0$  is a global minimum.



### Back to our problem

Linear regression model:

ssion model: 
$$y(x) = w^T \mathbf{x}, \quad \mathbf{x} = \begin{bmatrix} 1 \\ x \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}, \quad w = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

■ MSE loss:

$$l(w) = \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - y(x^{(n)}) \right]^{2}$$
$$= \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - w^{T} \mathbf{x}^{(n)} \right]^{2}$$

Find w that minimizes loss l(w)

□ Let x be an n-dimensional vector, the following rules are often used.

- For all  $\mathbf{A} \in \mathbb{R}^{m \times n}$ ,  $\nabla_{\mathbf{X}} \mathbf{A} \mathbf{X} = \mathbf{A}^{\top}$ ,
- For all  $\mathbf{A} \in \mathbb{R}^{n \times m}$ ,  $\nabla_{\mathbf{X}} \mathbf{X}^{\top} \mathbf{A} = \mathbf{A}$ ,
- For all  $\mathbf{A} \in \mathbb{R}^{n \times n}$ ,  $\nabla_{\mathbf{X}} \mathbf{X}^{\top} \mathbf{A} \mathbf{X} = (\mathbf{A} + \mathbf{A}^{\top}) \mathbf{X}$ ,
- $\nabla_{\mathbf{x}} \|\mathbf{x}\|^2 = \nabla_{\mathbf{x}} \mathbf{x}^{\top} \mathbf{x} = 2\mathbf{x}$ .

### Least square solution

The cost function l(w) is convex

$$l(w) = \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - y(x^{(n)}) \right]^{2}$$
$$= \frac{1}{2N} \sum_{n=1}^{N} \left[ t^{(n)} - w^{T} \mathbf{x}^{(n)} \right]^{2}$$

We take the gradient and let it equal to 0. Then find the solution.

$$\nabla l(w) = -\frac{1}{N} \sum_{n=1}^{N} \left( t^{(n)} - w^T \mathbf{x}^{(n)} \right) \mathbf{x}^{(n)} = 0$$

# Least square solution

In the matirx form, we have

$$\nabla l(w) = -\frac{1}{N} \mathbf{X}^T (t - \mathbf{X} w) = 0$$

$$\mathbf{X} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ \vdots \\ (\mathbf{x}^{(N)})^T \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}_1^{(1)} & \cdots & \mathbf{x}_d^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \mathbf{x}_1^{(N)} & \cdots & \mathbf{x}_d^{(N)} \end{bmatrix}, \quad t = \begin{bmatrix} t^{(1)} \\ \vdots \\ (t^{(N)} \end{bmatrix}$$

# Least square solution

Take N=2 for an example:

$$\nabla l(w) = -\frac{1}{N} \left\{ \begin{bmatrix} t^{(1)} - w^T \mathbf{x}^{(1)} \end{bmatrix} \mathbf{x}^{(1)} + \begin{bmatrix} t^{(2)} - w^T \mathbf{x}^{(2)} \end{bmatrix} \mathbf{x}^{(2)} \right\}$$

$$= -\frac{1}{N} \left\{ \begin{bmatrix} \mathbf{x}^{(1)} & \mathbf{x}^{(2)} \end{bmatrix} \begin{bmatrix} t^{(1)} - w^T \mathbf{x}^{(1)} \\ t^{(2)} - w^T \mathbf{x}^{(2)} \end{bmatrix} \right\} t^{-1}$$

$$= -\frac{1}{N} \mathbf{X}^T (t - \mathbf{X} w) = 0$$

$$w = \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{X}^T t$$

## Linear regression with least square solution

```
import numpy as np
import matplotlib.pyplot as plt
class OLSLinearRegression:

✓ Explain | Doc | Test | X
    def _ols(self, X, y):
        # Least square estimation
        return np.linalq.inv(X.T @ X) @ X.T @ y
    M Explain | Doc | Test | X
    def _preprocess_data_X(self, X):
        # Extend X by addiing a constant 1 as the first element
        m. n = X.shape # m represent the sample number, and n represent the feature number
        X_ = np.empty([m, n+1])
        X [:, 0] = 1
        X_{[:, 1:]} = X
        return X_
```

# Linear regression with least square solution

```
def train(self, X train, y train):
    # Train the model
    X_train = self._preprocess_data_X(X_train)
    self.W = self._ols(X_train, y_train)

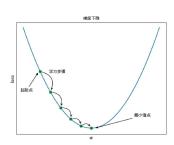
# Explain|Doc|Test|X
def predict(self, X):
    # Predict the output for a given input
    X = self._preprocess_data_X(X)
    return X @ self.W
```

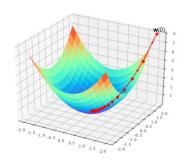
#### Gradient descent idea

- One straightforward method: gradient descent
- initialize w (e.g., randomly)
- > repeatedly update w based on the gradient

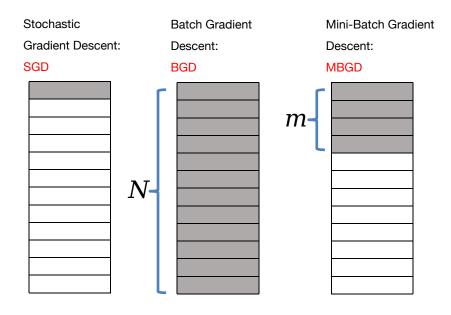
$$w \leftarrow w - \lambda \nabla l(w)$$

 $\triangleright$   $\lambda$  is the learning rate





## Three ways of gradient descent



#### Stochastic Gradient Descent (SGD)

#### Algorithm 1. Stochastic gradient descent (SGD)

- 1. Initialize w (e.g., randomly)
- **2. for** i = 1 to n\_epoch **do**
- 3. Randomly shuffle and pick one sample  $(x^{(n)}, t^{(n)})$  in the training set
- 4. Update:

$$w \leftarrow w + \lambda \left[ t^{(n)} - y(x^{(n)}) \right] \mathbf{x}^{(n)}$$

error

- 5. end for
- SGD: update the parameters for each sample in turn, according to its own gradient
- As error approaches zero, so does the update (w stops changing)

## Batch Gradient Descent (BGD)

#### Algorithm 2. Batch gradient descent (BGD)

- 1. Initialize w (e.g., randomly)
- **2. for** i = 1 to n\_epoch **do**
- 3. Update:

$$w \leftarrow w + \lambda \frac{1}{N} \sum_{n=1}^{N} \left[ t^{(n)} - y(x^{(n)}) \right] \mathbf{x}^{(n)}$$

4. end for

- BGD: avarage updates across every sample in training set, then change the parameters according to the gradient
- As error approaches zero, so does the update (*w* stops changing)

## Batch Gradient Descent (BGD)

Algorithm 2. Batch gradient descent (BGD)

■ Update in the matrix form:

$$w \leftarrow w + \lambda \frac{1}{N} \mathbf{X}^T (t - \mathbf{X}w)$$

### Mini-Batch Gradient Descent (MBGD)

#### Algorithm 3. Mini-Batch gradient descent (MBGD)

- 1. Initialize w (e.g., randomly)
- **2. for** i = 1 to n\_epoch **do**
- 3. shuffle the training set and partition into a number of mini-batches
- 4. **for** j = 1 to floor $(\frac{N}{m})$ , **do**
- 5. Update:

$$w \leftarrow w + \lambda \frac{1}{m} \sum_{n \in \mathcal{B}_j} \left[ t^{(n)} - y(x^{(n)}) \right] \mathbf{x}^{(n)}$$

- 6. end for
- 7. end for

### Mini-Batch Gradient Descent (MBGD)

Algorithm 3. Mini-Batch gradient descent (MBGD)

■ Update in the matrix form:

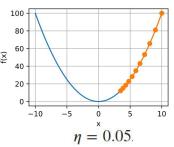
$$w \leftarrow w + \lambda \frac{1}{m} \mathbf{X}_{\mathcal{B}_i}^T (t_{\mathcal{B}_i} - \mathbf{X}_{\mathcal{B}_i} w)$$

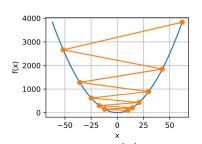
# Why gradient descent works?

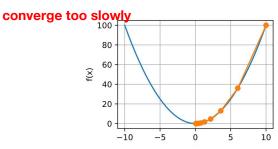
Gradient descent in one dimension is an excellent example to explain why the gradient descent algorithm may reduce the value of the objective function.

$$f(x+\epsilon) = f(x) + \epsilon f'(x) + \mathcal{O}(\epsilon^2).$$
 Taylor expansion choose  $\epsilon = -\eta f'(x)$ . 
$$f(x-\eta f'(x)) = f(x) - \eta f'^2(x) + \mathcal{O}(\eta^2 f'^2(x)).$$
 
$$f(x-\eta f'(x)) \lessapprox f(x).$$
 
$$x \leftarrow x - \eta f'(x)$$
 then f(x) decreases

# Learning rate is a hyper-parameter



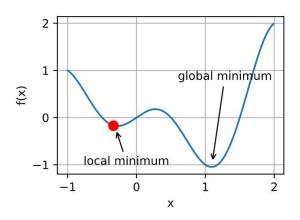




 $\eta = 0.2$ 

diverge

# Trap into local minima



```
class GDLinearRegression:
        Explain | Doc | Test | X
        def __init__(self, n_feature = 1, n_iter = 200, lr = 1e-3, tol = None):
           self.n_iter = n_iter # Maximum interation steps
           self.lr = lr # Learning rate
           self.W = np.random.random(n_feature + 1) * 0.05 # Molel parameters
           self.loss = [] # The loss value
        M Explain | Doc | Test | X
        def _loss(self, y, y_pred):
            return np.sum((v pred - v) ** 2) / v.size
        // Explain | Doc | Test | X
        def _gradient(self, X, y, y_pred):
            return (y pred-y) @ X / y.size
45
```

```
def _preprocess_data(self, X):
    m, n = X.shape
    X_{-} = np.empty([m, n+1])
    X_{[:, 0]} = 1
    X_{[:,1:]} = X
    return X
M Explain | Doc | Test | X
def _predict(self, X):
    return X @ self.W

✓ Explain | Doc | Test | X
def predict(self, X):
    X = self._preprocess_data(X)
    return X @ self.W
```

```
def batch_update(self, X, y):
    if self.tol is not None:
        loss_old = np.inf
    for iter in range(self.n_iter):
        y pred = self. predict(X)
        loss = self._loss(y, y_pred)
        # print(loss)
        self.loss.append(loss)
        if self.tol is not None:
            if np.abs(loss_old - loss) < self.tol:</pre>
                break
            loss old = loss
        grad = self._gradient(X, y, y_pred)
        self.W = self.W - self.lr * grad
```

```
def train(self, X_train, y_train):
             X_train = self._preprocess_data(X_train)
             self.batch_update(X_train, y_train)
         M Explain | Doc | Test | X
         def plot loss(self):
             plt.plot(self.loss)
             plt.grid()
             plt.show()
88
     if __name__ == '__main__':
         X \text{ train} = \text{np.arange}(100).reshape}(100,1)
         a. b = 1.10
         y train = a * X train + b
         v train = v train.flatten()
         _, n_feature = X_train.shape
         print(n feature)
         qd lreg 1 = GDLinearRegression(n feature=n feature, n iter=3000, lr=0.001, tol=0.00001)
         qd lreq 1.train(X train, y train)
         ad lrea 1.plot loss()
         print(f'Learned weights are {qd lreq 1.W}')
```