01_Linear_Regression

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[1]:
```
import torch
from matplotlib import pyplot as plt
%matplotlib inline
```

1 Linear Regression

- In a regression task, we have access to a dataset composed of pairs of inputs and outputs. The goal is to find a model (possibly defined by parameters) that allows predicting the output associated to a new input.
- Predicting the price of rent, the length of a hospital stay, and the demand for a product are examples of regression tasks.
- *Linear regression* is one of the simplest regression models. It assumes that the observation $\mathbf{x}$ and the target y are related linearly, so that y can be computed as a weighted sum of the elements in $\mathbf{x}$.

2 A Simple Example

- Consider the task of estimating the price of a house (in pounds) based on its area (in square feet) and age (in years).
- Linear regression would suppose that the target (price) can be expressed as a weighted sum of the features (elements of the observation, which are area and age) plus a constant:

$$\text{price} = w_{\text{area}} \cdot \text{area} + w_{\text{age}} \cdot \text{age} + b.$$

- In this context, w_{area} and w_{age} are called *weights*, and b is called a *bias*.
  - The weights determine how each feature influences the prediction.
  - The bias is the prediction for when all features are zero.
- In order to find the weights and bias required to predict the price of a new house, we can use a *training* dataset composed of pairs of inputs and outputs. Each input would be a vector composed of the area and the age of a house, and each output would be the known sale price for that house.
- The goal is not to accurately predict known sales prices, but to generalize (make good predictions for new houses)

- In what follows, we let $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(n)}, y^{(n)})$ denote a dataset with n examples, where each observation $\mathbf{x}^{(i)}$ corresponds to the target $y^{(i)}$.

3 Linear Model

- If the observations are composed of d features, the prediction $\hat{y}$ computed by a linear model defined by the weights $\mathbf{w} = [w_1, w_2, \ldots, w_d]^T$ and the bias b for an observation $\mathbf{x} = [x_1, x_2, \ldots, x_d]^T$ would be

$$\hat{y} = w_1 x_1 + \cdots + w_d x_d + b.$$

- Using the dot product, we can rewrite the previous equation as

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b.$$

- A design matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ contains one row for each observation and one column for each feature, so that

$$\mathbf{X} = \begin{bmatrix} {\mathbf{x}^{(1)}}^T \\ {\mathbf{x}^{(2)}}^T \\ \vdots \\ {\mathbf{x}^{(n)}}^T \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \ldots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \ldots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \\ x_1^{(n)} & x_2^{(n)} & \ldots & x_d^{(n)} \end{bmatrix}.$$

- A target vector $\mathbf{y}$ is composed of one element for each target, so that $\mathbf{y} = [y^{(1)}, y^{(2)}, \ldots, y^{(n)}]$.
- Using this notation, we may compute a prediction vector $\hat{\mathbf{y}}$ given by

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} + b,$$

where the constant b is added elementwise to the vector $\mathbf{X}\mathbf{w}$ (which results from a matrix-vector multiplication).

- Together, the weights $\mathbf{w}$ and bias b define a *model*.
- Given a training dataset defined by a design matrix $\mathbf{X}$ and a target vector $\mathbf{y}$, our goal is to find a model (weights $\mathbf{w}$ and bias b) that makes good predictions for new observations.
- In this particular example, it is appropriate to look for a model that performs as well as possible in the training dataset.
- We need to define what it means to perform well on the training dataset.
- We also need a procedure to find the best model.

4 Loss Function

- A *loss function* measures the disparity between *actual* and *predicted* targets for a given model.
- A loss function for a given model is zero if and only if the model makes perfect predictions in the training dataset.

- A model is considered better than another model if its loss is smaller.
- For a regression task, we may define the (halved squared error) loss function $l^{(i)}$ for the i-the example as

$$l^{(i)}(\mathbf{w}, b) = \frac{1}{2}\left(\hat{y}^{(i)} - y^{(i)}\right)^2,$$

where $\hat{y}^{(i)}$ is the prediction for the i-th observation and $y^{(i)}$ is the target for the i-th observation.

- Note that the model (weights $\mathbf{w}$ and bias b) affects the loss for the i-th example through the prediction $\hat{y}^{(i)}$
- When $d = 1$, the linear model corresponds to the line defined by the equation $\hat{y} = w_1 x + b$, so that the difference between actual and predicted targets can be visualized as follows:
- Large differences between $\hat{y}^{(i)}$ and $y^{(i)}$ lead to a large loss for the i-th observation.

5 Loss Function

- In order to measure the performance of a model on a dataset composed of n examples, we may average the individual loss functions to obtain a loss function L given by:

$$L(\mathbf{w}, b) = \frac{1}{n}\sum_{i=1}^{n} l^{(i)}(\mathbf{w}, b) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{2}\left(\mathbf{w}^T\mathbf{x}^{(i)} + b - y^{(i)}\right)^2,$$

where we used the fact that the prediction $\hat{y}^{(i)}$ is given by $\hat{y}^{(i)} = \mathbf{w}^T\mathbf{x}^{(i)} + b$.

- *Training* is the process of solving the following optimization problem: find parameters $(\mathbf{w}^*, b^*)$ such that

$$L(\mathbf{w}^*, b^*) = \min_{\mathbf{w}, b} L(\mathbf{w}, b).$$

6 Analytic Solution

- It is possible to solve the optimization problem stated above analytically (that is, there is a formula to compute $\mathbf{w}^*$ and b^*).
- First, consider an extended design matrix $\mathbf{X}$ where we include an additional column filled with ones, so that

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \dots & x_d^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \dots & x_d^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \\ 1 & x_1^{(n)} & x_2^{(n)} & \dots & x_d^{(n)} \end{bmatrix}.$$

- If we let $\mathbf{w} = [w_0, w_1, w_2, \dots, w_d]^T$ denote the corresponding extended weights, note that there is no longer need for a bias term b, since w_0 acts as a bias as long as the prediction $\hat{y}^{(i)}$ for the i-th observation is redefined as

$$\hat{y}^{(i)} = w_0 + w_1 x_1^{(i)} + \cdots + w_d x_d^{(i)}.$$

- With these new definitions, we only need to find weights $\mathbf{w} = [w_0, w_1, w_2, \dots, w_d]^T$ that perform as well as possible in the training dataset.
- If $\|\cdot\|$ denotes the L_2-norm, we may redefine the corresponding loss function L as

$$L(\mathbf{w}) = \frac{1}{2n}||\mathbf{y} - \mathbf{X}\mathbf{w}||^2.$$

- In other words, $L(\mathbf{w})$ is the squared Euclidean distance between the target vector and the prediction vector divided by $2n$.
- By computing the gradient of the loss function L and setting it to zero, we find that if $\mathbf{w}^*$ exists then it must be equal to

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.$$

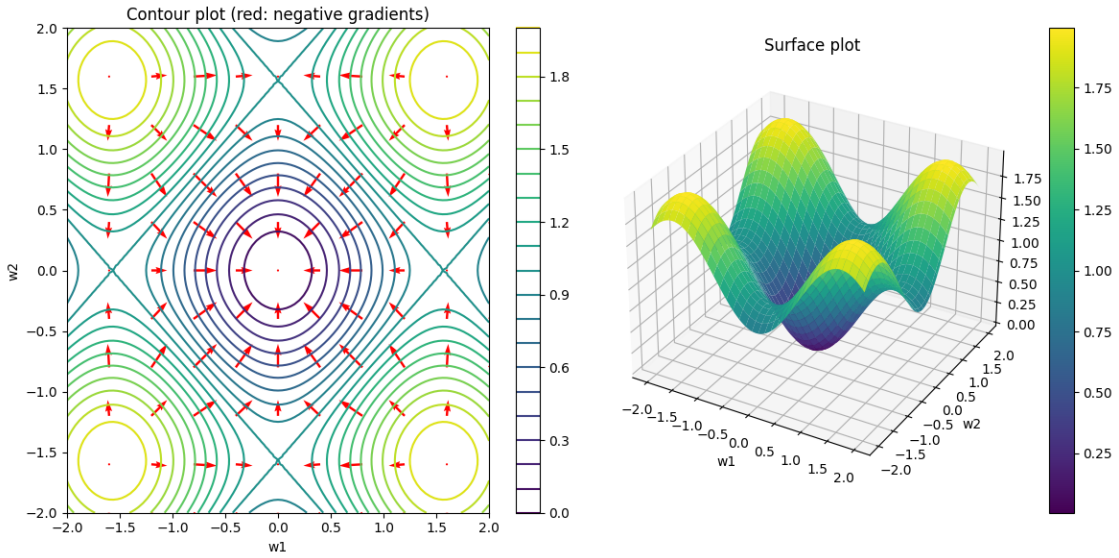
- Computing $\mathbf{w}^*$ only requires being able to invert and multiply matrices. The matrix $\mathbf{X}^T\mathbf{X}$ is invertible whenever the columns in $\mathbf{X}$ are linearly independent.
- When we use neural networks for regression, we will not be able to solve the corresponding optimization problem analytically, which is why we need optimization methods such as gradient descent.

7 Gradient Descent

- Consider a differentiable loss function $L : \mathbb{R}^d \to \mathbb{R}$. The gradient $\nabla L(\mathbf{w})$ has the following intuitive interpretation:
  - $\nabla L(\mathbf{w})$ gives the direction in which a *very small* change in $\mathbf{w}$ would **increase** $L(\mathbf{w})$ the most.
  - $-\nabla L(\mathbf{w})$ gives the direction in which a *very small* change in $\mathbf{w}$ would **decrease** $L(\mathbf{w})$ the most.
- The following code illustrates this interpretation of $-\nabla L(\mathbf{w})$. You do not need to understand the code, just observe the results.

[2]:
```
# You do not need to understand the code, just observe the results.
import numpy as np
import matplotlib.pyplot as plt

# A simple "loss function" `l`
def l(w1, w2):
    return np.sin(w1)**2 + np.sin(w2)**2

# Partial derivative of `l` with respect to `w1`
def dldw1(w1, w2):
    return 2 * np.sin(w1) * np.cos(w1)

# Partial derivative of `l` with respect to `w2`
def dldw2(w1, w2):
    return 2 * np.sin(w2) * np.cos(w2)
```

```
w1s = np.linspace(-2, 2, 101)
w2s = np.linspace(-2, 2, 101)

W1, W2 = np.meshgrid(w1s, w2s)

L = l(W1, W2)
dLdW1 = dldw1(W1, W2)
dLdW2 = dldw2(W1, W2)

plt.figure(figsize=(12, 6))

# Contour plot
plt.subplot(1, 2, 1)
contour = plt.contour(W1, W2, L, 20, cmap='viridis')
k = 10
plt.quiver(W1[::k, ::k], W2[::k, ::k], -dLdW1[::k, ::k], -dLdW2[::k, ::k],␣
 ↪color='red')
plt.colorbar(contour)
plt.title('Contour plot (red: negative gradients)')
plt.xlabel('w1')
plt.ylabel('w2')

# Surface plot
ax = plt.subplot(1, 2, 2, projection='3d')
surface = ax.plot_surface(W1, W2, L, cmap='viridis')
plt.colorbar(surface)
ax.set_title('Surface plot')
ax.set_xlabel('w1')
ax.set_ylabel('w2')

plt.tight_layout()
plt.show()
```



- Gradient descent is a minimization technique that exploits this property by starting at arbitrary weights $\mathbf{w}$ and updating them using $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla L(\mathbf{w})$, where $\eta > 0$ is a small constant called **learning rate**.
- Gradient descent can try to minimize any loss function L as long as the gradient $\nabla L(\mathbf{w})$ can be computed for any given $\mathbf{w}$.

8 Minibatch Stochastic Gradient Descent

- Let $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(n)}, y^{(n)})$ denote a dataset with n examples, where each observation $\mathbf{x}^{(i)}$ corresponds to the target $y^{(i)}$.
- Let $l^{(i)}$ denote the loss function for the i-th example, so that the loss function L is given by

$$L(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} l^{(i)}(\mathbf{w}).$$

- The gradient ∇L of the loss function L is given by

$$\nabla L(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} \nabla l^{(i)}(\mathbf{w}).$$

- If the dataset has many examples (if n is large), computing $\nabla L(\mathbf{w})$ can be expensive.
- Minibatch stochastic gradient descent approximates ∇L using a random subset of examples in the dataset:

  0. Initialize the weights $\mathbf{w}$ arbitrarily.
  1. Sample a random set of indices $\mathcal{B}$ (minibatch), each between 1 and n.
  2. Compute the gradient of the loss function for the i-th example $\nabla l^{(i)}(\mathbf{w})$, for each $i \in \mathcal{B}$.

3. Compute the average of these gradients to obtain an approximation of $\nabla L(\mathbf{w})$.
4. Multiply the resulting vector by a small positive constant (learning rate) and then subtract it from the current weights $\mathbf{w}$ to obtain new weights $\mathbf{w}$:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla l^{(i)}(\mathbf{w}).$$

5. Return to Step 1.

9 Minibatch Stochastic Gradient Descent for Linear Regression

- In linear regression, the gradient of the loss function for the i-the example $\nabla l^{(i)}(\mathbf{w})$ is given by

$$\nabla l^{(i)}(\mathbf{w}) = \nabla \left[\frac{1}{2} \left(\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)} \right)^2 \right] = (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}.$$

- Therefore, the minibatch stochastic gradient descent update is given by

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\eta}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} (\mathbf{w}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}.$$

10 Hyperparameters

- The weights of a linear model are considered *parameters*.
- In minibatch stochastic gradient descent, the batch size and the learning rate need to be fixed before training a model. This makes them *hyperparameters*.
- Hyperparameter tuning is the process of choosing hyperparameters based on their performance on a *validation set*.
  - A training set is used to train a model for a specific set of hyperparameters.
  - A validation dataset is used to compare the performance of different models, each of which comes from a different set of hyperparameters.
- The number of updates performed by minibatch stochastic gradient descent is also a hyperparameter.
- After this number is reached (or until some other stopping criterion is met), we need to record the weights $\hat{\mathbf{w}}$ of the final model.
- The final weights $\hat{\mathbf{w}}$ will typically not minimize the loss function L, because minibatch stochastic gradient descent is not guaranteed to converge to a (local/global) minimum in a finite number of steps.

11 Predicting using the Learned Model

- Given the final weights $\hat{\mathbf{w}} = [\hat{w}_0, \hat{w}_1, \ldots, \hat{w}_d]^T$, we can compute a prediction $\hat{y}$ for a new observation $\mathbf{x}$ as $\hat{y} = \hat{\mathbf{w}}^T \mathbf{x}$.

- If an observation $\mathbf{x} = [1, \text{area}, \text{age}]^T$ represents the features of a house, our prediction $\hat{y}$ would be given by

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot \text{area} + \hat{w}_2 \cdot \text{age}.$$

- While the process of minimizing a loss function for a given dataset is called **training**, the process of computing predictions for new observations is called **inference**.

12 From Linear Regression to Neural Networks

- We can think of a linear model as a very simple neural network:
- An observation $\mathbf{x} = [x_1, \dots, x_d]^T$ is the input layer, which has d dimensions.
- Each element of the input layer is connected to the output layer through a weighted connection: the k-th arrow has a corresponding weight w_k.
- The output o_1 is given by $o_1 = \sum_{k=1}^{d} w_k x_k$, which corresponds to weighing each of its inputs and then adding the results.
- The *number of layers* in the neural network above is 1.

13 Recommended reading

- Dive into Deep Learning: Chapters 3.1, 3.2, and 3.3.

14 [Storing this notebook as a pdf]

- In order to store this notebook as a pdf, you will need to hide the images included in the previous cells using the following syntax:
  - `<!--- ![Image caption.](https://link.to.image) --->`

[3]:
```
from google.colab import drive
drive.mount('/content/gdrive', force_remount=True)

!sudo apt-get install texlive-xetex texlive-fonts-recommended␣
 ↪texlive-plain-generic

# Set the path to this notebook below (add \ before spaces). The output `pdf`␣
 ↪will be stored in the corresponding folder.
!jupyter nbconvert --to pdf /content/gdrive/My\ Drive/Colab\ Notebooks/nndl/
 ↪week_03/lecture/01_Linear_Regression.ipynb

# If having issues, save this notebook (File > Save) and restart the session␣
 ↪(Runtime > Restart session) before running this cell. To debug, remove the␣
 ↪first line (`%%capture`).
```