Training Models with Regression and Gradient Descent

COMP 4630 | Winter 2025

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Overview

- Linear Regression and the Normal Equation
- Gradient Descent and its various flavours
- References and suggested reading:
    - Scikit-learn book:
        - Chapter 4: Training Models
    - Deep Learning Book
        - Section 5.1.4: Linear Regression

Linear Regression

Unlike most models, linear regression has a **closed-form** solution called the **Normal Equation**:

$$\hat{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

where

- $\hat{\theta}$ are the weights of the model minimizing the **cost function**
- $\mathbf{y}$ is the vector of target values
- $\mathbf{X}$ is the **design matrix** of feature values

> *As usual, different sources use different notation, e.g.* $\mathbf{w}$ *or* ϕ *instead of* θ.

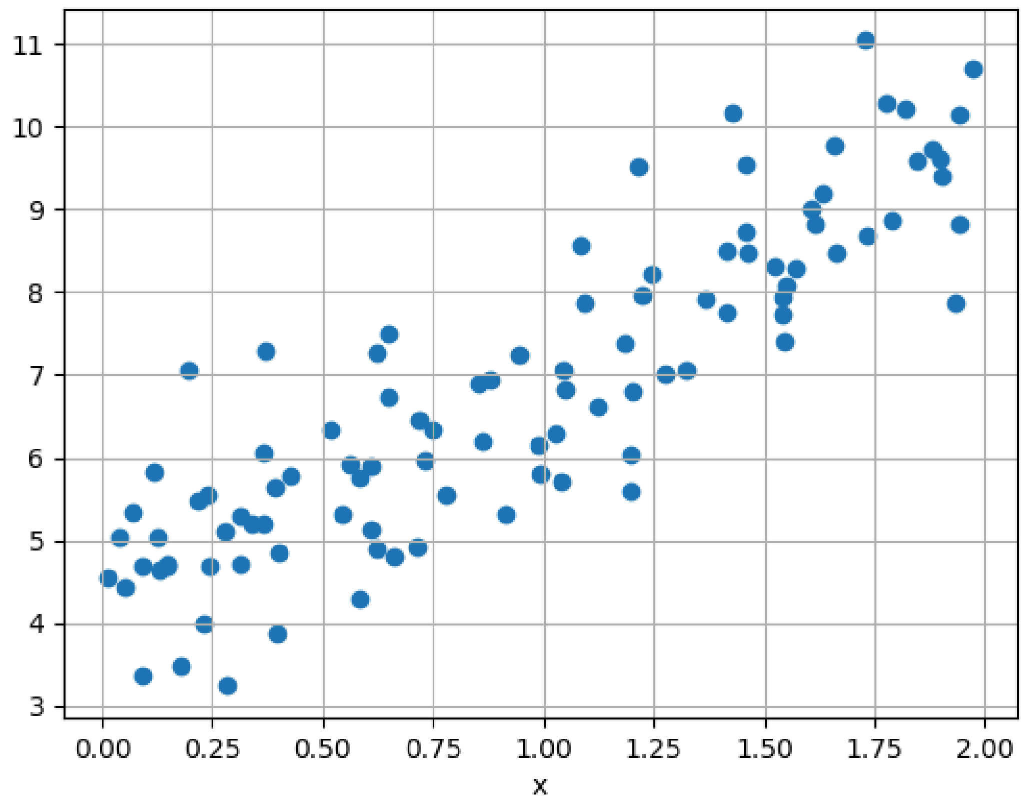
Consider the 1-d case:

$$\hat{y} = \theta_0 + \theta_1 x$$

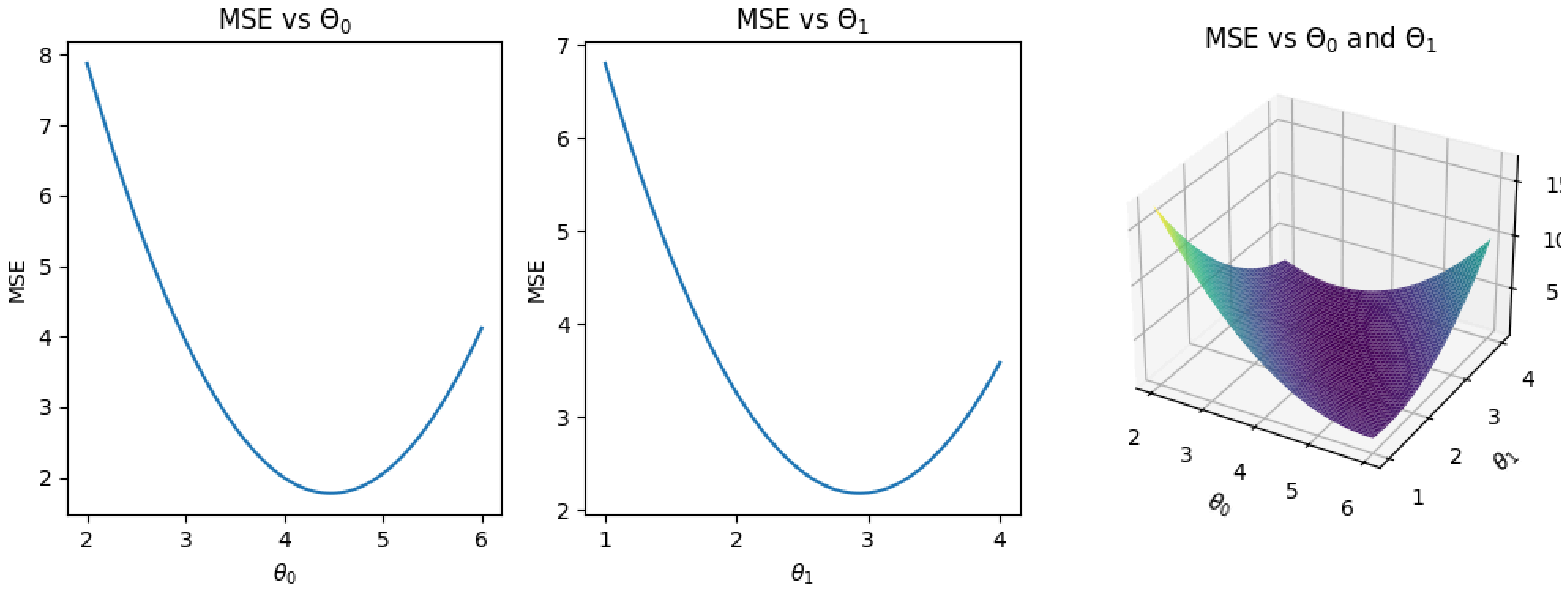
we want the values of θ_0 and θ_1 that minimize the **Mean Square Error** between the actual and predicted y values:

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y} - y_i)^2$$

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\theta_0 + \theta_1 x_i - y_i)^2$$



Solving for θ_0 and θ_1

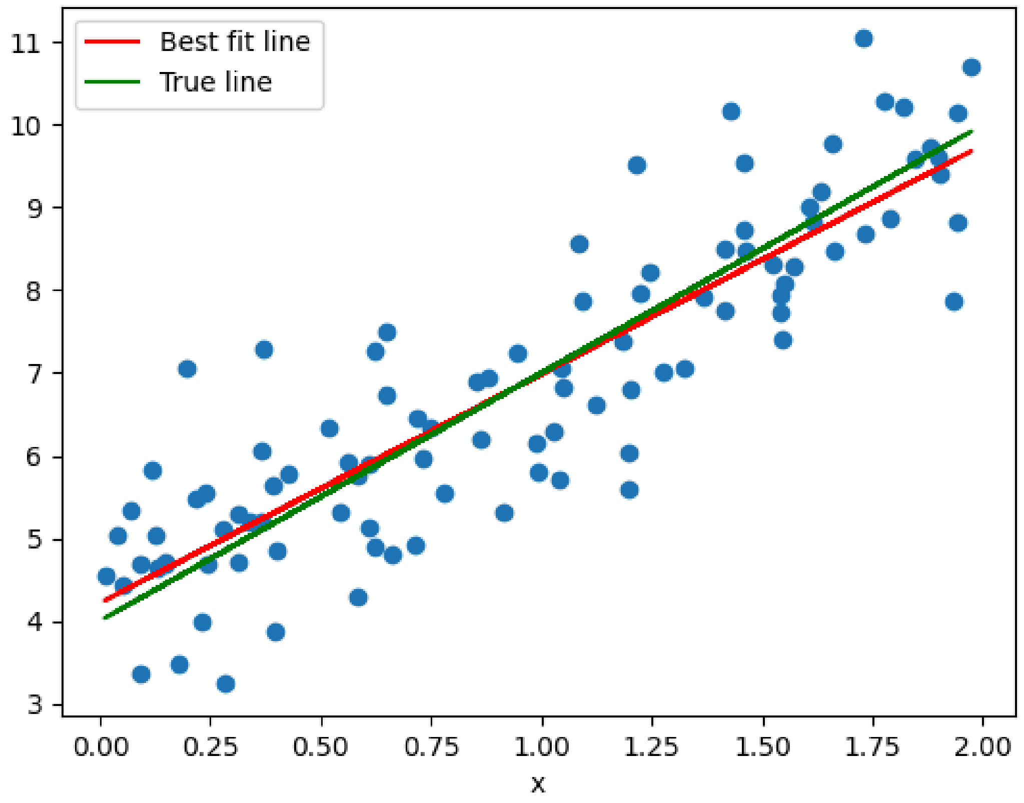


Solving for θ_0 and θ_1

After some algebraic gymnastics, we get:

$$\theta_1 = \frac{\mu_y \sum_m x_i - \sum_m x_i y_i}{\mu_x \sum_m x_i - \sum_m x_i^2}$$
$$\theta_0 = \mu_y - \theta_1 \mu_x$$

where μ_x and μ_y are the means of the x and y values, respectively.



Expanding to matrix form

Instead of the scalar x or even vector $\mathbf{x}$, we can use a **design matrix** $\mathbf{X}$ to represent the feature values:

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}$$

where each row is an instance (sample) and each column is a feature.

> *It is common for the first column to be all ones, representing the bias term*

Back to the linear regression problem...

- We can rewrite the estimate in matrix notation:

$$\hat{\mathbf{y}} = \mathbf{X}\theta$$

- The MSE can be written as:

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2 = \frac{1}{m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y})$$

  where we've used the trick of substituting $\mathbf{a}^T\mathbf{a} = \sum_i a_i^2$

- 🧮 Find the gradient of the MSE w.r.t θ, set it to zero, and solve for θ

Properties of matrices and their transpose

The following properties are useful for solving linear algebra problems:

- $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$
- $(\mathbf{A}+\mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$
- $(\mathbf{A}^{\mathbf{-1}})^T = (\mathbf{A}^T)^{-1}$
- $(\mathbf{A}^{\mathbf{T}})^T = \mathbf{A}$

Additionally, any matrix or vector multiplied by $\mathbf{I}$ is unchanged.

The Normal Equation

We made it! The **Normal Equation** is again:

$$\hat{\theta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- No optimization is required to find the optimal θ
- Limitations:
  - $\mathbf{X}^T\mathbf{X}$ must be invertible and small enough to fit in memory
  - The computational complexity is (at least) $O(n^3)$
- Even in linear regression problems, it is common to use **gradient descent** instead due to these limitations

Gradient Descent

The goal of gradient descent is still to minimize the cost function, but it follows an iterative process:

1. Start with a random θ
2. Calculate the gradient ∇_θ for the current θ
3. Update θ as $\theta = \theta - \eta\nabla_\theta$
4. Repeat 2-3 until some stopping criterion is met

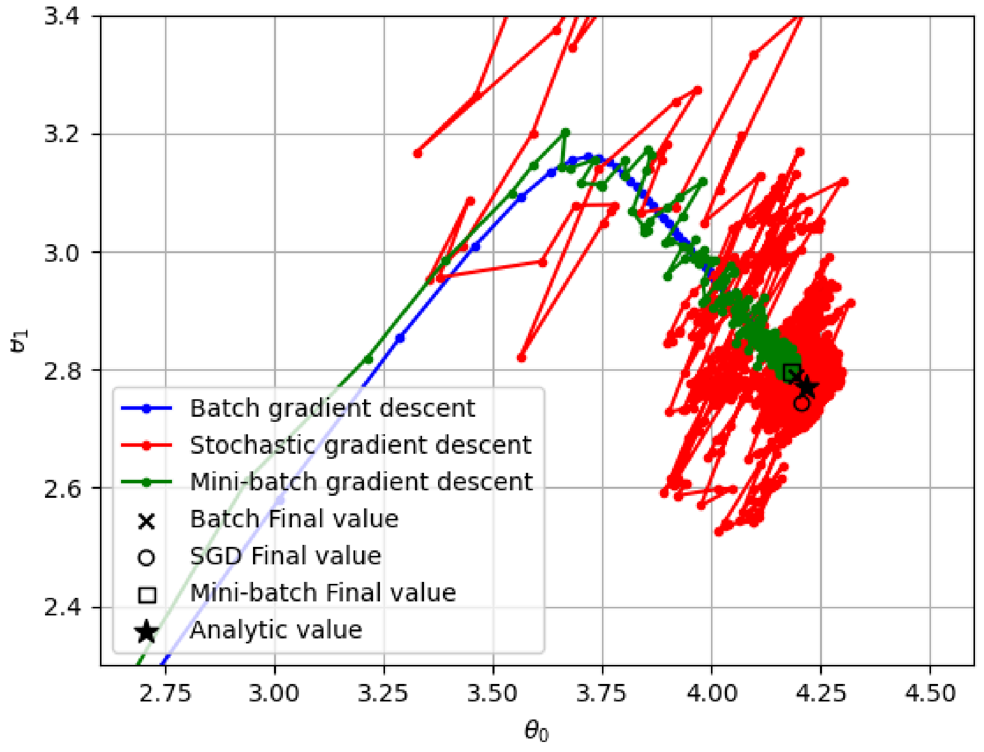
   where η is the **learning rate**, or the size of step to take in the direction opposite the gradient.

Stochastic Gradient Descent

- Standard or **batch** gradient descent uses the entire training set to calculate the gradient for each instance at every step
- **Stochastic Gradient Descent** uses a single random instance at each step:
    i. Start with a random θ
    ii. Pick a random instance $\mathbf{x}_i$ (row in the design matrix)
    iii. Calculate the gradient ∇_θ for the current θ and $\mathbf{x}_i$
    iv. Update θ as $\theta = \theta - \eta\nabla_\theta$
    v. Repeat 2-4 until some stopping criterion is met

Mini-batch Gradient Descent

- **Mini-batch** gradient descent uses a random *subset* of the training set
- Less chaotic than stochastic, but faster than batch
- Most common type of gradient descent used in practice



Gradient Descent Hyperparameters

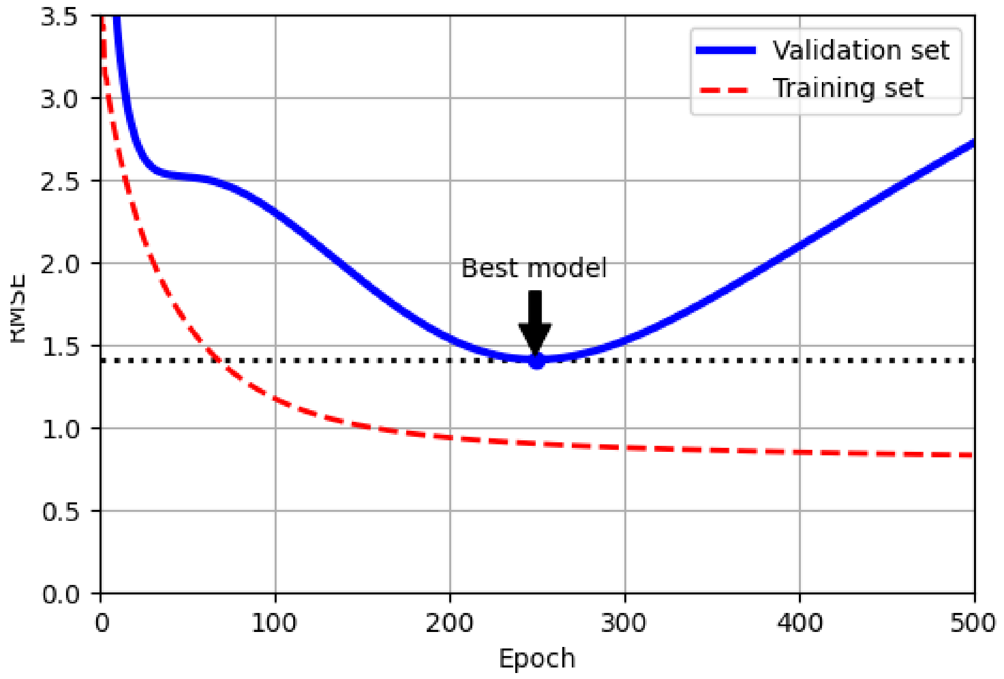
- The **learning rate** η - size of step taken
- No rule that it needs to be constant! A simple **learning schedule** is to decrease η over time, e.g.:

  $$\eta = \frac{t_0}{t + t_1}$$

  where t is the current iteration and t_0 and t_1 are hyper-parameters
- For mini-batch, the **batch size** is another hyper-parameter
- The number of **epochs**, or times to process the entire training set

Stopping Criteria

- The simplest stopping criterion is to set a maximum number of epochs
- **Early stopping** is another option:
  - Evaluate on a validation set at regular intervals
  - Stop when the validation error starts to increase
- The comparison between training and validation performance can also help prevent **overfitting**



Loss functions

- The **loss function** is the function being minimized by gradient descent
- MSE is **convex** and guaranteed to have a single global minimum, but many other loss functions have multiple local minima
- The relative scale of the features can affect the convergence:

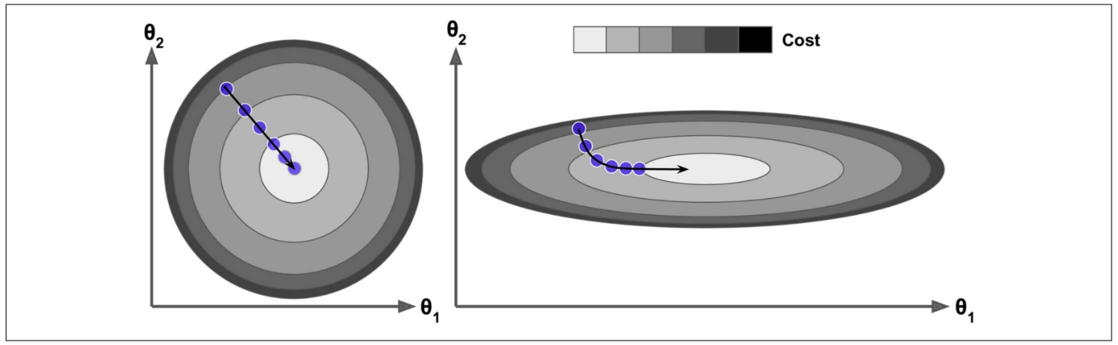


Figure 4-7. Gradient Descent with (left) and without (right) feature scaling

Figure from Scikit-Learn book

Higher-order Polynomials

- Higher order polynomials can be solved with the Normal Equation as well:

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^n$$

- Just include the higher order terms in $\mathbf{X}$
- This is still a linear regression problem because the coefficients are linear!
- Risk of **overfitting** the data
- Easy way to regularize: drop one or more of the higher order terms

Regularization

- If the model fits the training data *too* well, but doesn't generalize to new data, it is **overfitting**
- **Regularization** imposes additional constraints on the weights
- Example: **Ridge Regression** adds a term to the loss function:

$$J(\theta) = MSE(\theta) + \alpha\frac{1}{2}\sum_{i=1}^{n}\theta_i^2$$

  where α is the **regularization parameter**
- The regularization term is only added during training, not evaluation

> *Note: the term **cost** function is often used instead of **loss** function*

Logistic regression and beyond

Logistic regression is a binary classifier that uses the **logistic function** (aka **sigmoid function**) to map the output to a range of 0 to 1:

$$\sigma(t) = \frac{1}{1 + e^{-t}}$$

We can then minimize the **log loss** or **cross-entropy** loss function:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \left[y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i) \right]$$

where $\hat{p}_i = \sigma(\theta^T \mathbf{x}_i)$ is the probability that instance i is positive.

More on cross-entropy loss when we talk about classification models

The gradient of the log loss ends up being:

$$\nabla_\theta J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(\sigma(\theta^T\mathbf{x}_i) - y_i\right)\mathbf{x}_i$$

- There is no (known) analytical solution this time, but we can still use gradient descent!
- In this case it's still convex, so we don't have to worry about local minima
- In general, for a loss function to work with gradient descent, it must be:
  - **Continuous** and
  - **Differentiable**
  - ... at the locations where you evaluate it

Next up: Backpropagation!