

Extra Mathematical Notes for Lectures and Classes*

Parley Ruogu Yang[†]

This version: Friday 4th February, 2022

Abstract

This document consists of notes for Lectures (section 2) and Classes (section 3).

Contents

1	General notes	2
1.1	Notations	2
1.2	Activation functions	2
2	Lectures	3
2.1	Lectures 3 and 4: Various optimisation methods	3
2.1.1	Gradient Descent in general	3
2.1.2	Gradient Descent in the ERM framework	3
2.1.3	Stochastic Gradient Descent	3
2.1.4	Momentum	4
2.1.5	Adaptive Learning Rates	4
3	Classes	5
3.1	Class 1: Linear and logistic regressions	5
3.1.1	Linear regression and MSE loss	5
3.1.2	Gradient of linear regression with MSE loss	5
3.1.3	Logistic regression model and binary cross entropy	5
3.2	Class 2: Perceptron and the XOR Problem	6
3.2.1	Perceptron	6
3.2.2	The XOR Problem statement	6
3.2.3	Theoretical result	6
3.3	Class 3: Options Pricing	7
3.3.1	Background	7
3.3.2	Class 3 Notebook 1	7
3.3.3	Class 3 Notebook 2	7
3.3.4	Class 3 Homework	7

*Latest version: <https://parleyyang.github.io/ST456/index.html>

[†]Faculty of Mathematics, University of Cambridge

1 General notes

1.1 Notations

The default meaning of \mathbb{N} is the set of integers greater or equal to 1. For $n \in \mathbb{N}$, denote $[n] := \{1, 2, \dots, n-1, n\} = [1, n] \cap \mathbb{N}$. When $x \in \mathbb{R}^n$ is written, x_i stands for the i -th entry of x . If $\rho : \mathbb{R} \rightarrow \mathbb{R}$ is well-defined, then for $y \in \mathbb{R}^n$, $\rho(y) := (\rho(y_1), \dots, \rho(y_n))$, also known as element-wise operation.

$N(\mu, \sigma^2)$ refers to a normal distribution with mean μ and variance σ^2 , while a standard normal distribution refers to the case when $\mu = 0$ and $\sigma^2 = 1$.

Where ε or ε_i are written, the default meaning is that they are drawn from iid $N(0, \sigma^2)$ distribution with σ^2 unknown.

NN stands for Neural Networks

1.2 Activation functions

Let $\rho^{\text{sigmoid}} : \mathbb{R} \rightarrow \mathbb{R}$ be the sigmoid function, it is defined by

$$x \mapsto (1 + \exp(-x))^{-1} \quad (1.2.1)$$

Let $\rho^{\text{thr}} : \mathbb{R} \rightarrow \mathbb{R}$ be the threshold function, it is defined by

$$x \mapsto \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{else} \end{cases} \quad (1.2.2)$$

This function is also commonly written as $\mathbb{1}[x \geq 0]$

2 Lectures

2.1 Lectures 3 and 4: Various optimisation methods

2.1.1 Gradient Descent in general

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a differentiable function, a gradient descent sequence $\{x_n\}_{n=0}^\infty$ with learning rate scheduling $\{\eta_n\}_{n=0}^\infty$ and initialisation x_{ini} is defined as

$$x_0 = x_{ini} \quad (2.1.1)$$

$$x_n = x_{n-1} - \eta_{n-1} \nabla f(x_{n-1}) \quad \forall n \in \mathbb{N} \quad (2.1.2)$$

2.1.2 Gradient Descent in the ERM framework

In the framework of Empirical Risk Minimisation (ERM), we are in the business of solving

$$\min_f \mathbb{E}_{(x,y) \sim p_{data}} [L(f(x, \theta), y)] \quad (2.1.3)$$

where $f(x, \theta)$ is the predicted output when the input data is x . In parametric setting, we search over some parametric space $\theta \in \Theta$ (often $\Theta = \mathbb{R}^n$), but also note the minimisation over f applies in a more general setting, e.g. functional minimisation or hyper-parameter search. Write the (empirical) data as $D := \{(x_i, y_i) : i \in [M]\}$ where M is the sample size, and the distribution of empirical data as p_{data} . We note that $J(\theta)$ can be written as $M^{-1} \sum_{i \in [M]} L(f(x_i, \theta), y_i)$.

Let $\theta \in \mathbb{R}^n$ and $J(\theta) := \mathbb{E}_{(x,y) \sim p_{data}} [L(f(x, \theta), y)]$, then a batch / deterministic gradient descent method with learning rate scheduling $\{\eta_n\}_{n=0}^\infty$ and initialisation θ_{ini} is defined as

$$\theta_0 = \theta_{ini} \quad (2.1.4)$$

$$\theta_n = \theta_{n-1} - \eta_{n-1} \nabla_\theta J(\theta_{n-1}) \quad \forall n \in \mathbb{N} \quad (2.1.5)$$

2.1.3 Stochastic Gradient Descent

A Stochastic Gradient Descent (SGD) algorithm takes the average gradient on a minibatch of m examples drawn randomly from the data. Clearly, for m to make sense, we practically have $m \ll M$. On the other hand, when we have $m = M$, SGD is the same as GD.

A SGD algorithm with batch size m , learning rate scheduling $\{\eta_n\}_{n=0}^\infty$, and initialisation θ_{ini} is defined as

$$\theta_0 = \theta_{ini} \quad (2.1.6)$$

$$\theta_n = \theta_{n-1} - \eta_{n-1} m^{-1} \nabla_\theta \sum_{j \in [m]} L(f(\tilde{x}_j, \theta_{n-1}), \tilde{y}_j) \quad \forall n \in \mathbb{N} \quad (2.1.7)$$

where, $\forall n \in \mathbb{N}$, a set of data $\{(\tilde{x}_j, \tilde{y}_j) : j \in [m]\}$ is sampled from p_{data} uniformly.

Larger m provides a more accurate estimate of the gradient, but more computational costs¹ Training with small m may require a small learning rate may require a small learning rate to maintain stability due to high variance in the estimation of gradient.

¹In case of parallel computing, then memory scales with m , in case of sequential computing, the computational time scales with m .

2.1.4 Momentum

Based on subsection 2.1.3, we rewrite Equation 2.1.7 into the following two lines:

$$v_n = \eta_{n-1} m^{-1} \nabla_{\theta} \sum_{j \in [m]} L(f(\tilde{x}_j, \theta_{n-1}), \tilde{y}_j) \quad (2.1.8)$$

$$\theta_n = \theta_{n-1} - v_n \quad (2.1.9)$$

Now, a momentum method with initial velocity v_0 and momentum parameter α varies the above into

$$v_n = \alpha v_{n-1} - \eta_{n-1} m^{-1} \nabla_{\theta} \sum_{j \in [m]} L(f(\tilde{x}_j, \theta_{n-1}), \tilde{y}_j) \quad (2.1.10)$$

$$\theta_n = \theta_{n-1} + v_n \quad (2.1.11)$$

2.1.5 Adaptive Learning Rates

General idea: adapt a separate learning rate (or momentum for Adam) for each parameter.

- Adagrad
- RMSProp
- Adam

3 Classes

3.1 Class 1: Linear and logistic regressions

3.1.1 Linear regression and MSE loss

Let $x \in \mathbb{R}^m$ be the input variable. Let $y \in \mathbb{R}$ be the output variable.

We consider $y = f(x) + \varepsilon$ where $f(x) = x^T w + b$

If we have data $\{(x_i, y_i) : i \in [n]\}$, the MSE loss takes the following form:

$$l(w, b) = n^{-1} \sum_{i \in [n]} (y_i - f(x_i))^2 = n^{-1} \sum_{i \in [n]} (y_i - x_i^T w - b)^2 \quad (3.1.1)$$

3.1.2 Gradient of linear regression with MSE loss

It will be useful later in subsection 2.1 to have the gradient ∇l in hand. In particular:

$$\nabla_w l(w, b) = n^{-1} \sum_{i \in [n]} (2x_i)(f(x_i) - y_i) \quad (3.1.2)$$

$$\nabla_b l(w, b) = n^{-1} \sum_{i \in [n]} 2(f(x_i) - y_i) \quad (3.1.3)$$

3.1.3 Logistic regression model and binary cross entropy

Let ρ be the sigmoid function, then we consider $y = f(x) + \varepsilon$ where $f(x) = \rho(x^T w + b)$

In the event of binary classification problem, in which $y \in \{0, 1\}$, we clearly do not have ε as a Normally distributed error. In this occasion, with data $\{(x_i, y_i) : i \in [n]\}$, we consider the binary cross entropy as

$$l(f) = -n^{-1} \left(\sum_{i \in [n]} y_i \log(f(x_i)) + (1 - y_i) \log(1 - f(x_i)) \right) \quad (3.1.4)$$

3.2 Class 2: Perceptron and the XOR Problem

3.2.1 Perceptron

With an activation function $\rho : \mathbb{R} \rightarrow \mathbb{R}$ and a feature engineering ϕ , we have a single-layer NN as $x \mapsto \rho(\phi(x)^T w + b)$

For the rest of the class (as well as in the lecture), we ignore ϕ , or equivalently replace it by an identity map. A feed-forward NN with depth L can be written as

$$y = h_L \circ h_{L-1} \circ \dots \circ h_1(x) \quad (3.2.1)$$

where $h_l(x) = a_l(W^{(l-1)}x + b^{(l-1)})$ for all $l \leq L-1$ and $h_L(x) = W^{L-1}x + b^{L-1}$.

3.2.2 The XOR Problem statement

Consider $x \in \mathbb{R}^2$ and $y \in \mathbb{R}$, in particular, our data is as follows:

$$D = \{((-1, -1), -1), ((-1, 1), 1), ((1, -1), 1), ((1, 1), -1)\} \quad (3.2.2)$$

The objective is to separate the points, mathematically one uses

$$L(f) = \sum_{i \in [4]} \max(-y_i f(x_i), 0) \quad (3.2.3)$$

3.2.3 Theoretical result

Theorem 1 (Failure of linear functions compared against two-layer NN). *Let \mathcal{L} be the class of all non-zero linear functions $\mathbb{R}^2 \rightarrow \mathbb{R}$ and let*

$$\mathcal{N}(\rho) = \{f : \mathbb{R}^2 \rightarrow \mathbb{R} : f(x) = \rho(w_1 x + b_1)^T w_2 + b_2, w_1 \in \mathbb{R}^{2 \times 2}, w_2, b_1 \in \mathbb{R}^2, b_2 \in \mathbb{R}\} \quad (3.2.4)$$

where ρ is the threshold function. Then

$$\min_{f \in \mathcal{L}} L(f) > 0 = \min_{f \in \mathcal{N}(\rho)} L(f) \quad (3.2.5)$$

Proof. The left hand side can be proved by a 2-D diagram, or analytically via the diagram-induced geometry. The right hand side can be proved by showing an element $f \in \mathcal{N}(\rho)$ satisfies $L(f) = 0$, which is equivalent to show $y_i = f(x_i) \forall i$. Consider

$$b_1 = (0, 0), b_2 = -1, w_2 = (-2, 2) \\ w_1 = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$$

which offers one specification that works. □

Remarks:

1. $\mathcal{N}(\rho)$ can also be thought as the class of all two-layer NNs with architecture as $(2, 2, 1)$ and activation function as the threshold function.
2. Note that the loss function can be 0 if $f(x_i) = 0 \forall i$. This is a bug of the loss function, hence when considering linear function, we restrict to the non-linear ones.

3.3 Class 3: Options Pricing

3.3.1 Background

A (European) call option at maturity T gives the owner the right to buy an underlying asset at strike price K . This price of such an option is denoted as $V(S_t, t; K)$ at time $t \in [0, T]$, where S_t is the price of the underlying asset at time t . It is natural to relate this to various parameters in the market: in the Black-Scholes model, we relate this to the interest rate r and volatility σ . A PDE expression is provided as

$$\partial_t V + rS\partial_S V + \frac{1}{2}\sigma^2 S^2 \partial_S^2 V = rV \quad (3.3.1)$$

The solution of this is complicated and non-linear:

$$V(S_t, t; K) = S_t N(d_1) - K e^{r(T-t)} N(d_2) \quad (3.3.2)$$

where $d_1 = (\sigma\sqrt{T-t})^{-1}(\log(S_t K^{-1}) + (r + \frac{\sigma^2}{2})(T-t))$ and $d_2 = d_1 - \sigma\sqrt{T-t}$

3.3.2 Class 3 Notebook 1

In this notebook, we keep other parameters the same and study the relationship between strike price K and the associated price of call option V . In particular, we select a number of strike prices, denoted $x_1, \dots, x_n \in \mathbb{R}$ and generate the call option prices $y_1, \dots, y_n \in \mathbb{R}$ in accordance with Equation 3.3.2. The dataset is hence $\{(x_i, y_i) : i \in [n]\}$ and that we would like to approximate a function $f : \mathbb{R} \rightarrow \mathbb{R}$ as we generate our data $y_i = f(x_i) \quad \forall i$

3.3.3 Class 3 Notebook 2

In practice, one would be asked for the implied volatility σ given the data they receive — in this notebook, we fix 16 different strike prices and collect their corresponding call prices: for now, assume no noise. Then, for each $y_i = \sigma_i \in \mathbb{R}$, we have a 16-dimensional data $x_i \in \mathbb{R}^{16}$, so the dataset is $\{(x_i, y_i) : i \in [n]\}$ and that we would like to approximate a function $f : \mathbb{R}^{16} \rightarrow \mathbb{R}$ as we generate our data $y_i = f(x_i) \quad \forall i$

3.3.4 Class 3 Homework

Realistically, the data contains noise. In the Homework, we will work with noisy data, in particular, we consider the same function $f : \mathbb{R}^{16} \rightarrow \mathbb{R}$ as was in Notebook 2, but that we generate $\varepsilon_i \sim N(0_{16}, \sigma^2 I_{16 \times 16}) \forall i \in [n]$, and observe $\tilde{x}_i = \max\{x_i + \varepsilon_i, 0\}$ instead of x_i . The maximum is in place because the practical world would not accept a negative prices on an option — so whilst there are noises, there is an obvious truncation.

So, we are still in the business of approximating f , but this time we have data $\{(\tilde{x}_i, y_i) : i \in [n]\}$.