Chapter 2

Machine Learning with Shallow Neural Networks

"Simplicity is the ultimate sophistication."—Leonardo da Vinci

2.1 Introduction

Conventional machine learning often uses optimization and gradient-descent methods for learning parameterized models. Examples of such models include linear regression, support vector machines, logistic regression, dimensionality reduction, and matrix factorization. Neural networks are also parameterized models that are learned with continuous optimization methods. This chapter will show that a wide variety of optimization-centric methods in machine learning can be captured with *very simple* neural network architectures containing one or two layers. In fact, neural networks can be viewed as more powerful versions of these simple models, with this power being achieved by combining the basic models into a comprehensive neural architecture (i.e., computational graph). It is useful to show these parallels early on, as this allows the understanding of the design of a deep network as a composition of the basic units that one often uses in machine learning. Furthermore, showing this relationship provides an appreciation of the specific way in which traditional machine learning is different from neural networks, and of the cases in which one can hope to do better with neural networks. In many cases, minor variations of these simple neural network architectures (corresponding to traditional machine learning methods) provide useful variations of machine learning models that have not been studied elsewhere. In a sense, the number of ways in which one can combine the different elements of a computational graph is far greater than what is studied in traditional machine learning, even when shallow models are used.

Complex or deep neural architectures are often an overkill in instances where only a small amount of data are available. Additionally, it is easier to optimize traditional machine

C. C. Aggarwal, *Neural Networks and Deep Learning*,
https://doi.org/10.1007/978-3-319-94463-0_2

learning models in data-lean settings as these models are more interpretable. On the other hand, as the amount of data increases, neural networks have an advantage because they retain the flexibility to model more complex functions with the addition of neurons to the computational graph. Figure 2.1 illustrates this point.

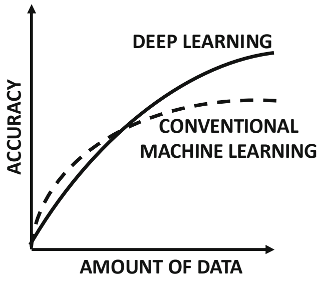


Figure 2.1: Re-visiting Figure 1.2: The effect of increased data availability on accuracy.

One way of viewing deep learning models is as a stacking of simpler models like logistic or linear regression. The coupling of a linear neuron with the sigmoid activation leads to *logistic regression*, which will be discussed in detail in this chapter. The coupling of a linear unit with sigmoid activation is also used[1] extensively for building complex neural networks. Therefore, it is natural to ask the following question [312]:

> *Is deep learning simply a stacking of simpler models like logistic or linear regression?*

Although many neural networks can be viewed in this way, this point of view does not fully capture the complexity and the style of thinking involved in deep learning models. For example, several models (such as recurrent neural networks or convolutional neural networks) perform this stacking in a particular way with a *domain-specific understanding* of the input data. Furthermore, the parameters of different units are sometimes shared in order to force the solution to obey specific types of properties. The ability to put together the basic units in a clever way is a key architectural skill required by practitioners in deep learning. Nevertheless, it is also important to learn the properties of the basic models in machine learning, since they are used repeatedly in deep learning as elementary units of computation. This chapter will, therefore, explore these basic models.

It is noteworthy that there are close relationships between some of the earliest neural networks (e.g., perceptron and Widrow-Hoff learning) and traditional machine learning models (e.g., support vector machine and Fisher discriminant). In some cases, these relationships remained unnoticed for several years, as these models were proposed independently by different communities. As a specific example, the loss function of the L_2-support vector machine was proposed by Hinton [190] in the context of a neural architecture in 1989. When used with regularization, the resulting neural network would behave identically to an L_2-support vector machine. In comparison, Cortes and Vapnik's paper on the support vector machine [82] appeared several years later with an L_1-loss function. These relationships are not surprising because the best way to define a shallow neural network is often closely related to a known machine learning algorithm. Therefore, it is important to explore these basic neural models in order to develop an integrated view of neural networks and traditional machine learning.

[1] In recent years, the sigmoid unit has fallen out of favor compared to the ReLU.

This chapter will primarily discuss two classes of models for machine learning:

1. *Supervised models:* The supervised models discussed in this chapter primarily correspond to linear models and their variants. These include methods like least-squares regression, support vector machines, and logistic regression. Multiclass variants of these models will also be studied.

2. *Unsupervised models:* The unsupervised models discussed in this chapter primarily correspond to dimensionality reduction and matrix factorization. Traditional methods like principal component analysis can also be presented as simple neural network architectures. Minor variations of these models can provide reductions of vastly different properties, which will be discussed later. The neural network framework also provides a way of understanding the relationships between widely different unsupervised methods like linear dimensionality reduction, nonlinear dimensionality reduction, and sparse feature learning, thereby providing an integrated view of traditional machine learning algorithms.

This chapter assumes that the reader has a basic familiarity with the classical machine learning models. Nevertheless, a brief overview of each model will also be provided to the uninitiated reader.

Chapter Organization

The next section will discuss some basic models for classification and regression, such as least-squares regression, binary Fisher discriminant, support vector machine, and logistic regression. The multiway variants of these models will be discussed in Section 2.3. Feature selection methods for neural networks are discussed in Section 2.4. The use of autoencoders for matrix factorization is discussed in Section 2.5. As a specific application of simple neural architectures, the *word2vec* method is discussed in Section 2.6. Simple methods for creating node embeddings in graphs are introduced in Section 2.7. A summary is given in Section 2.8.

2.2 Neural Architectures for Binary Classification Models

In this section, we will discuss some basic architectures for machine learning models such as least-squares regression and classification. As we will see, the corresponding neural architectures are minor variations of the perceptron model in machine learning. The main difference is in the choice of the activation function used in the final layer, and the loss function used on these outputs. This will be a recurring theme throughout this chapter, where we will see that small changes in neural architectures can result in distinct models from traditional machine learning. Presenting traditional machine learning models in the form of neural architectures also helps one appreciate the true closeness among various machine learning models.

Throughout this section, we will work with a single-layer network with d input nodes and a single output node. The coefficients of the connections from the d input nodes to the output node are denoted by $\overline{W} = (w_1 \dots w_d)$. Furthermore, the bias will not be explicitly shown because it can be seamlessly modeled as the coefficient of an additional dummy input with a constant value of 1.

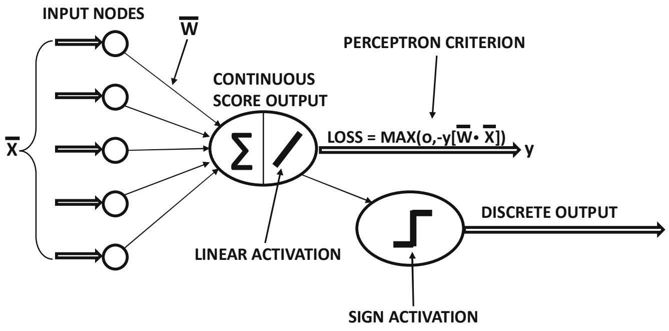


Figure 2.2: An extended architecture of the perceptron with both discrete and continuous predictions

2.2.1 Revisiting the Perceptron

Let $(\overline{X_i}, y_i)$ be a training instance, in which the observed value y_i is predicted from the feature variables $\overline{X_i}$ using the following relationship:

$$\hat{y}_i = \text{sign}(\overline{W} \cdot \overline{X_i}) \tag{2.1}$$

Here, $\overline{W}$ is the d-dimensional coefficient vector learned by the perceptron. Note the circumflex on top of $\hat{y}_i$ to indicate that it is a predicted value rather than an observed value. In general, the goal of training is to ensure that the prediction $\hat{y}_i$ is as close as possible to the observed value y_i. The gradient-descent steps of the perceptron are focused on reducing the number of misclassifications, and therefore the updates are proportional to the difference $(y_i - \hat{y}_i)$ between the observed and predicted values based on Equation 1.33 of Chapter 1:

$$\overline{W} \Leftarrow \overline{W}(1 - \alpha\lambda) + \alpha(y_i - \hat{y}_i)\overline{X_i} \tag{2.2}$$

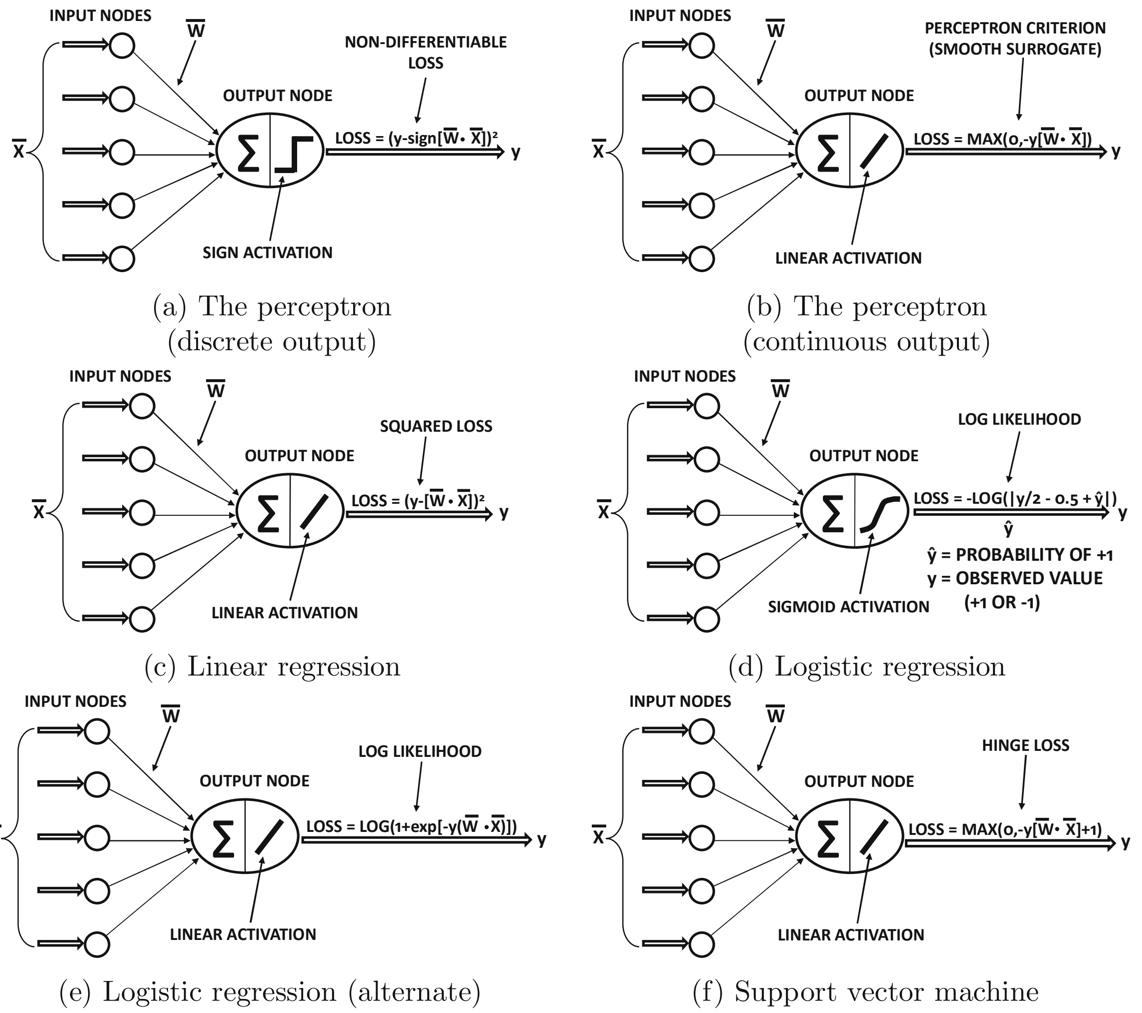
A gradient-descent update that is proportional to the difference between the observed and predicted values is naturally caused by a squared loss function such as $(y_i - \hat{y}_i)^2$. Therefore, one possibility is to consider the squared loss between the predicted and observed values as the loss function. This architecture is shown in Figure 2.3(a), and the output is a discrete value. However, the problem is that this loss function is discrete because it takes on the value of either 0 or 4. Such a loss function is not differentiable because of its staircase-like jumps.

The perceptron is one of the few learning models in which the gradient-descent updates were proposed historically before the loss function was proposed. What *differentiable* objective function does the perceptron really optimize? The answer to this question may be found in Section 1.2.1.1 of Chapter 1 by observing that the updates are performed only for misclassified training instances (i.e., $y_i\hat{y}_i < 0$), and may be written using the indicator function $I(\cdot) \in \{0, 1\}$ that takes on 1 when the condition in its argument is satisfied:

$$\overline{W} \Leftarrow \overline{W}(1 - \alpha\lambda) + \alpha y_i \overline{X_i}\,[I(y_i\hat{y}_i < 0)] \tag{2.3}$$

This rewrite from Equation 2.2 to Equation 2.3 uses the fact that $y_i = (y_i - \hat{y}_i)/2$ for misclassified points, and one can absorb a constant factor of 2 within the learning rate. This update can be shown to be consistent with the loss function L_i (specific to the ith training example) as follows:

$$L_i = \max\{0, -y_i(\overline{W} \cdot \overline{X_i})\} \tag{2.4}$$



(a) The perceptron (discrete output)

(b) The perceptron (continuous output)

(c) Linear regression

(d) Logistic regression

(e) Logistic regression (alternate)

(f) Support vector machine

Figure 2.3: Different variants of the perceptron

This loss function is referred to as the *perceptron criterion*, which is correspondingly reflected in Figure 2.3(b). Note that Figure 2.3(b) uses *linear* activations to compute the continuous loss function, although it still uses sign activations to compute the discrete predictions for a given test instance. In many discrete variable prediction settings, the output is often a predicted score (e.g., probability of class or the value of $\overline{W} \cdot \overline{X_i}$), which is then converted into a discrete prediction. Nevertheless, the final prediction need not always be converted into a discrete value, and one can simply output the relevant score for the class (which is often used for computing the loss function anyway). The sign activation is rarely used in most neural-network implementations, as most class-variable predictions of neural-network implementations are continuous scores. One can, in fact, create an extended architecture for the perceptron (cf. Figure 2.2), in which both discrete and continuous values are output. However, since the discrete part is not relevant to the loss computation and most outputs are reported as scores anyway, one rarely uses this type of extended representation. Therefore, throughout the remainder of this book, the activation in the output node is based on the score output (and how the loss function is computed), rather than on how a test instance is predicted as a discrete value.

2.2.2 Least-Squares Regression

In least-squares regression, the training data contains n different training pairs $(\overline{X_1}, y_1) \ldots (\overline{X_n}, y_n)$, where each $\overline{X_i}$ is a d-dimensional representation of the data points, and each y_i is a *real-valued* target. The fact that the target is real-valued is important, because the underlying problem is then referred to as *regression* rather than *classification.* Least-squares regression is the oldest of all learning problems, and the gradient-descent methods proposed by Tikhonov and Arsenin in the 1970s [499] are very closely related to the gradient-descent updates of Rosenblatt [405] for the perceptron algorithm. In fact, as we will see later, one can also use least-squares regression on binary targets by "pretending" that these targets are real-valued. The resulting approach is equivalent to the Widrow-Hoff learning algorithm, which is famous in the neural network literature as the second learning algorithm proposed after the perceptron.

In least-squares regression, the target variable is related to the feature variables using the following relationship:

$$\hat{y}_i = \overline{W} \cdot \overline{X_i} \tag{2.5}$$

Note the presence of the circumflex on top of $\hat{y}_i$ to indicate that it is a predicted value. The bias is missing in the relationship of Equation 2.5. Throughout this section, it will be assumed that one of the features in the training data has a constant value of 1, and the coefficient of this dummy feature is the bias. This is a standard feature engineering trick borrowed from conventional machine learning. In neural networks, the bias is often represented with the use of a bias neuron (cf. Section 1.2.1 of Chapter 1) with a constant output of 1. Although the bias neuron is almost always used in real settings, we avoid showing it explicitly throughout this book in order to maintain simplicity in presentation.

The error of the prediction, e_i, is given by $e_i = (y_i - \hat{y}_i)$. Here, $\overline{W} = (w_1 \ldots w_d)$ is a d-dimensional coefficient vector that needs to be learned so as to minimize the total squared error on the training data, which is $\sum_{i=1}^{n} e_i^2$. The portion of the loss that is specific to the ith training instance is given by the following:

$$L_i = e_i^2 = (y_i - \hat{y}_i)^2 \tag{2.6}$$

This loss can be simulated with the use of an architecture similar to the perceptron except that the squared loss is paired with the identity activation function. This architecture is shown in Figure 2.3(c), whereas the perceptron architecture is shown in Figure 2.3(a). Both the perceptron and least-squares regression have the same goal of minimizing the prediction error. However, since the loss function in classification is inherently discrete, the perceptron algorithm uses a smooth approximation of the desired goal. This results in the smoothed *perceptron criterion* shown in Figure 2.3(b). As we will see below, the gradient-descent update in least-squares regression is very similar to that in the perceptron, with the main difference being that real-valued errors are used in regression rather than discrete errors drawn from $\{-2, +2\}$.

As in the perceptron algorithm, the stochastic gradient-descent steps are determined by computing the gradient of e_i^2 with respect to $\overline{W}$, when the training pair $(\overline{X_i}, y_i)$ is presented to the neural network. This gradient can be computed as follows:

$$\frac{\partial e_i^2}{\partial \overline{W}} = -e_i \overline{X_i} \tag{2.7}$$

Therefore, the gradient-descent updates for $\overline{W}$ are computed using the above gradient and step-size α:

$$\overline{W} \Leftarrow \overline{W} + \alpha e_i \overline{X}$$

One can rewrite the above update as follows:

$$\overline{W} \Leftarrow \overline{W} + \alpha(y_i - \hat{y}_i)\overline{X} \tag{2.8}$$

It is possible to modify the gradient-descent updates of least-squares regression to incorporate forgetting factors. Adding regularization is equivalent to penalizing the loss function of least-squares classification with the additional term proportional to $\lambda \cdot ||\overline{W}||^2$, where $\lambda > 0$ is the regularization parameter. With regularization, the update can be written as follows:

$$\overline{W} \Leftarrow \overline{W}(1 - \alpha \cdot \lambda) + \alpha(y_i - \hat{y}_i)\overline{X} \tag{2.9}$$

Note that the update above looks identical to the perceptron update of Equation 2.2. The updates are, however, not exactly identical because of how the predicted value $\hat{y}_i$ is computed in the two cases. In the case of the perceptron, the sign function is applied to $\overline{W} \cdot \overline{X_i}$ in order to compute the binary value $\hat{y}_i$ and therefore the error $(y_i - \hat{y}_i)$ can only be drawn from $\{-2, +2\}$. In least-squares regression, the prediction $\hat{y}_i$ is a real value without the application of the sign function.

This observation naturally leads to the following question; what if we applied least-squares regression directly to minimize the squared distance of the *real-valued* prediction $\hat{y}_i$ from the observed binary targets $y_i \in \{-1, +1\}$? The direct application of least-squares regression to binary targets is referred to as *least-squares classification.* The gradient-descent update is the same as the one shown in Equation 2.9, which *looks* identical to that of the perceptron. However, the least-squares classification method does not yield the same result as the perceptron algorithm, because the *real-valued* training errors $(y_i - \hat{y}_i)$ in least-squares classification are computed differently from the *integer* error $(y_i - \hat{y}_i)$ in the perceptron. This direct application of least-squares regression to binary targets is referred to as *Widrow-Hoff learning.*

2.2.2.1 Widrow-Hoff Learning

Following the perceptron, the Widrow-Hoff learning rule was proposed in 1960. However, the method was not a fundamentally new one, as it is a direct application of least-squares regression to binary targets. Although the sign function is applied to the real-valued prediction *of unseen test instances* to convert them to binary predictions, the error of training instances is computed directly using real-valued predictions (unlike the perceptron). Therefore, it is also referred to as *least-squares classification* or *linear least-squares method* [6]. Remarkably, a seemingly unrelated method proposed in 1936, known as the Fisher discriminant, also reduces to Widrow-Hoff learning in the special case of binary targets.

The Fisher discriminant is formally defined as a direction $\overline{W}$ along which the ratio of inter-class variance to the intra-class variance is maximized in the projected data. By choosing a scalar b in order to define the hyperplane $\overline{W} \cdot \overline{X} = b$, it is possible to model the separation between the two classes. This hyperplane is used for classification. Although the definition of the Fisher discriminant seems quite different from least-squares regression/classification at first sight, a remarkable result is that the Fisher discriminant for binary targets is identical to the least-squares regression as applied to binary targets (i.e., least-squares classification). Both the data and the targets need to be mean-centered, which allows the bias variable b to be set to 0. Several proofs of this result are available in the literature [3, 6, 40, 41].

The neural architecture for classification with the Widrow-Hoff method is illustrated in Figure 2.3(c). The gradient-descent steps in both the perceptron and the Widrow-Hoff would be given by Equation 2.8, except for differences in how $(y_i - \hat{y}_i)$ is computed. In the case of the perceptron, this value will always be drawn from $\{-2, +2\}$. In the case of Widrow-Hoff, these errors can be arbitrary real values, since $\hat{y}_i$ is set to $\overline{W} \cdot \overline{X_i}$ without using the sign function. This difference is important because the perceptron algorithm never penalizes a positive class point for $\overline{W} \cdot \overline{X_i}$ being "too correct" (i.e., larger than 1), whereas using real-valued predictions to compute the error has the unfortunate effect of penalizing such points. The inappropriate penalization of over-performance is the Achilles heel of Widrow-Hoff learning and the Fisher discriminant [6].

It is noteworthy that least-squares regression/classification, Widrow-Hoff learning, and the Fisher discriminant were proposed independently in very different eras and by different communities of researchers. Indeed, the Fisher discriminant, which is oldest of these methods and dates back to 1936, is often viewed as a method for finding class-sensitive directions rather than as a classifier. It can, however, also be used as a classifier by using the resulting direction $\overline{W}$ to create a linear prediction. The completely different origins and seemingly different motives of all these methods make the equivalence in their solutions all the more noticeable. The Widrow-Hoff learning rule is also referred to as *Adaline*, which is short for *adaptive linear neuron*. It is also referred to as the *delta rule*. To recap, the learning rule of Equation 2.8, when applied to binary targets in $\{-1, +1\}$, can be alternatively referred to as least-squares classification, least mean-squares algorithm (LMS), Fisher[2] discriminant classifier, the Widrow-Hoff learning rule, delta rule, or Adaline. Therefore, the family of least-squares classification methods has been rediscovered several times in the literature under different names and with different motivations.

The loss function of the Widrow-Hoff method can be rewritten slightly from least-squares regression because of its binary responses:

$$\begin{aligned} L_i &= (y_i - \hat{y}_i)^2 = \underbrace{y_i^2}_{1}(y_i - \hat{y}_i)^2 \\ &= (\underbrace{y_i^2}_{1} - \hat{y}_i y_i)^2 = (1 - \hat{y}_i y_i)^2 \end{aligned}$$

This type of encoding is possible when the target variable y_i is drawn from $\{-1, +1\}$ because we can use $y_i^2 = 1$. It is helpful to convert the Widrow-Hoff objective function to this form because it can be more easily related to other objective functions like the perceptron and the support vector machine. For example, the loss function of the support vector machine is obtained by "repairing" the above loss so that over-performance is not penalized. One can repair the loss function by changing the objective function to $[\max\{(1 - \hat{y}_i y_i), 0\}]^2$, which was Hinton's L_2-loss support vector machine (SVM) [190]. Almost all the binary classification models discussed in this chapter can be shown to be closely related to the Widrow-Hoff loss function by using different ways of repairing the loss, so that over-performance is not penalized.

The gradient-descent updates (cf. Equation 2.9) of least-squares regression can be rewritten slightly for Widrow-Hoff learning because of binary response variables:

$$\begin{aligned} \overline{W} &\Leftarrow \overline{W}(1 - \alpha \cdot \lambda) + \alpha(y_i - \hat{y}_i)\overline{X} \quad \text{[For numeric as well as binary responses]} \\ &= \overline{W}(1 - \alpha \cdot \lambda) + \alpha y_i (1 - y_i \hat{y}_i)\overline{X} \quad \text{[Only for binary responses, since } y_i^2 = 1\text{]} \end{aligned}$$

[2] In order to obtain exactly the same direction as the Fisher method with Equation 2.8, it is important to mean-center both the feature variables and the binary targets. Therefore, each binary target will be one of two real values with different signs. The real values will contain the fraction of instances belonging to the other class. Alternatively, one can use a bias neuron to absorb the constant offsets.

The second form of the update is helpful in relating it to perceptron and SVM updates, in each of which $(1 - y_i \hat{y}_i)$ is replaced with an indicator variable that is a function of $y_i \hat{y}_i$. This point will be discussed in a later section.

2.2.2.2 Closed Form Solutions

The special case of least-squares regression and classification is solvable in closed form (without gradient-descent) by using the *pseudo-inverse* of the $n \times d$ training data matrix D, whose rows are $\overline{X_1} \ldots \overline{X_n}$. Let the n-dimensional column vector of dependent variables be denoted by $\overline{y} = [y_1 \ldots y_n]^T$. The pseudo-inverse of matrix D is defined as follows:

$$D^+ = (D^T D)^{-1} D^T \tag{2.10}$$

Then, the row-vector $\overline{W}$ is defined by the following relationship:

$$\overline{W}^T = D^+ \overline{y} \tag{2.11}$$

If regularization is incorporated, the coefficient vector $\overline{W}$ is given by the following:

$$\overline{W}^T = (D^T D + \lambda I)^{-1} D^T \overline{y} \tag{2.12}$$

Here, $\lambda > 0$ is the regularization parameter. However, inverting a matrix like $(D^T D + \lambda I)$ is typically done using numerical methods that require gradient descent anyway. One rarely inverts large matrices like $D^T D$. In fact, the Widrow-Hoff updates provide a very efficient way of solving the problem without using the closed-form solution.

2.2.3 Logistic Regression

Logistic regression is a probabilistic model that classifies the instances in terms of probabilities. Because the classification is probabilistic, a natural approach for optimizing the parameters is to ensure that the predicted probability of the observed class for each training instance is as large as possible. This goal is achieved by using the notion of *maximum-likelihood estimation* in order to learn the parameters of the model. The likelihood of the training data is defined as the product of the probabilities of the observed labels of each training instance. Clearly, larger values of this objective function are better. By using the negative logarithm of this value, one obtains an a loss function in minimization form. Therefore, the output node uses the negative *log-likelihood* as a loss function. This loss function replaces the squared error used in the Widrow-Hoff method. The output layer can be formulated with the sigmoid activation function, which is very common in neural network design.

Let $(\overline{X_1}, y_1), (\overline{X_2}, y_2), \ldots (\overline{X_n}, y_n)$ be a set of n training pairs in which $\overline{X_i}$ contains the d-dimensional features and $y_i \in \{-1, +1\}$ is a binary class variable. As in the case of a perceptron, a single-layer architecture with weights $\overline{W} = (w_1 \ldots w_d)$ is used. Instead of using the hard sign activation on $\overline{W} \cdot \overline{X_i}$ to predict y_i, logistic regression applies the soft sigmoid function to $\overline{W} \cdot \overline{X_i}$ in order to estimate the *probability* that y_i is 1:

$$\hat{y}_i = P(y_i = 1) = \frac{1}{1 + \exp(-\overline{W} \cdot \overline{X_i})} \tag{2.13}$$

For a test instance, it can be predicted to the class whose predicted probability is greater than 0.5. Note that $P(y_i = 1)$ is 0.5 when $\overline{W} \cdot \overline{X_i} = 0$, and $\overline{X_i}$ lies on the separating hyperplane. Moving $\overline{X_i}$ in either direction from the hyperplane results in different signs of $\overline{W} \cdot \overline{X_i}$ and corresponding movements in the probability values. Therefore, the sign of $\overline{W} \cdot \overline{X_i}$ also yields the same prediction as picking the class with probability larger than 0.5.

We will now describe how the loss function corresponding to likelihood estimation is set up. This methodology is important because it is used widely in many neural models. For positive samples in the training data, we want to maximize $P(y_i = 1)$ and for negative samples, we want to maximize $P(y_i = -1)$. For positive samples satisfying $y_i = 1$, one wants to maximize $\hat{y}_i$ and for negative samples satisfying $y_i = -1$, one wants to maximize $1 - \hat{y}_i$. One can write this casewise maximization in the form of a consolidated expression of always maximizing $|y_i/2 - 0.5 + \hat{y}_i|$. The products of these probabilities must be maximized over all training instances to maximize the likelihood $\mathcal{L}$:

$$\mathcal{L} = \prod_{i=1}^{n} |y_i/2 - 0.5 + \hat{y}_i| \tag{2.14}$$

Therefore, the loss function is set to $L_i = -\log(|y_i/2 - 0.5 + \hat{y}_i|)$ for each training instance, so that the product-wise maximization is converted to additive minimization over training instances.

$$\mathcal{LL} = -\log(\mathcal{L}) = \sum_{i=1}^{n} \underbrace{-\log(|y_i/2 - 0.5 + \hat{y}_i|)}_{L_i} \tag{2.15}$$

Additive forms of the objective function are particularly convenient for the types of stochastic gradient updates that are common in neural networks. The overall architecture and loss function is illustrated in Figure 2.3(d). For each training instance, the predicted probability $\hat{y}_i$ is computed by passing it through the neural network, and the loss is used to determine the gradient for each training instance.

Let the loss for the ith training instance be denoted by L_i, which is also annotated in Equation 2.15. Then, the gradient of L_i with respect to the weights in $\overline{W}$ can be computed as follows:

$$\begin{aligned}
\frac{\partial L_i}{\partial \overline{W}} &= -\frac{\text{sign}(y_i/2 - 0.5 + \hat{y}_i)}{|y_i/2 - 0.5 + \hat{y}_i|} \cdot \frac{\partial \hat{y}_i}{\partial \overline{W}} \\
&= -\frac{\text{sign}(y_i/2 - 0.5 + \hat{y}_i)}{|y_i/2 - 0.5 + \hat{y}_i|} \cdot \frac{\overline{X_i}}{1 + \exp(-\overline{W} \cdot \overline{X_i})} \cdot \frac{1}{1 + \exp(\overline{W} \cdot \overline{X_i})} \\
&= \begin{cases} -\frac{\overline{X_i}}{1+\exp(\overline{W}\cdot\overline{X_i})} & \text{if } y_i = 1 \\ \frac{\overline{X_i}}{1+\exp(-\overline{W}\cdot\overline{X_i})} & \text{if } y_i = -1 \end{cases}
\end{aligned}$$

Note that one can concisely write the above gradient as follows:

$$\frac{\partial L_i}{\partial \overline{W}} = -\frac{y_i\overline{X_i}}{1 + \exp(y_i\overline{W} \cdot \overline{X_i})} = -\left[\text{Probability of mistake on } (\overline{X_i}, y_i)\right] (y_i\overline{X_i}) \tag{2.16}$$

Therefore, the gradient-descent updates of logistic regression are given by the following (including regularization):

$$\overline{W} \Leftarrow \overline{W}(1 - \alpha\lambda) + \alpha\frac{y_i\overline{X_i}}{1 + \exp[y_i(\overline{W} \cdot \overline{X_i})]} \tag{2.17}$$

Just as the perceptron and the Widrow-Hoff algorithms use the *magnitudes* of the mistakes to make updates, the logistic regression method uses the *probabilities* of the mistakes to make updates. This is a natural extension of the probabilistic nature of the loss function to the update.

2.2.3.1 Alternative Choices of Activation and Loss

It is possible to implement the same model by using different choices of activation and loss in the output node as long as they combine to yield the same result. Instead of using sigmoid activation to create the output $\hat{y}_i \in (0, 1)$, it is also possible to use identity activation to create the output $\hat{y}_i \in (-\infty, +\infty)$, and then apply the following loss function:

$$L_i = \log(1 + \exp(-y_i \cdot \hat{y}_i)) \tag{2.18}$$

The alternative architecture for logistic regression is shown in Figure 2.3(e). For the final prediction of the test instance, the sign function can be applied to $\hat{y}_i$, which is equivalent to predicting it to the class for which its probability is greater than 0.5. This example shows that it is possible to implement the same model using different combinations of activation and loss functions, as long as they combine to yield the same result.

One desirable property of using the identity activation to define $\hat{y}_i$ is that it is consistent with how the loss functions of other models like the perceptron and Widrow-Hoff learning are defined. Furthermore, the loss function of Equation 2.18 contains the product of y_i and $\hat{y}_i$ as in other models. This makes it possible to directly compare the loss functions of various models, which will be explored later in this chapter.

2.2.4 Support Vector Machines

The loss function in support vector machines is closely related to that in logistic regression. However, instead of using a smooth loss function (like that in Equation 2.18), the *hinge-loss* is used instead.

Consider the training data set of n instances denoted by $(\overline{X_1}, y_1)$, $(\overline{X_2}, y_2)$, $\ldots (\overline{X_n}, y_n)$. The neural architecture of the support-vector machine is identical to that of least-squares classification (Widrow-Hoff). The main difference is in the choice of loss function. As in the case of least-squares classification, the prediction $\hat{y}_i$ for the training point $\overline{X_i}$ is obtained by applying the identity activation function on $\overline{W} \cdot \overline{X_i}$. Here, $\overline{W} = (w_1, \ldots w_d)$ contains the vector of d weights for the d different inputs into the single-layer network. Therefore, the output of the neural network is $\hat{y}_i = \overline{W} \cdot \overline{X_i}$ for computing the loss function, although a test instance is predicted by applying the sign function to the output.

The loss function L_i for the ith training instance in the support-vector machine is defined as follows:

$$L_i = \max\{0, 1 - y_i \hat{y}_i\} \tag{2.19}$$

This loss is referred to as the *hinge-loss*, and the corresponding neural architecture is illustrated in Figure 2.3(f). The overall idea behind this loss function is that a positive training instance is only penalized for being less than 1, and a negative training instance is only penalized for being greater than −1. In both cases, the penalty is linear, and abruptly flattens out at the aforementioned thresholds. It is helpful to compare this loss function with the Widrow-Hoff loss value of $(1 - y_i \hat{y}_i)^2$, in which predictions are penalized for being *different* from the target values. As we will see later, this difference is an important advantage for the support vector machine over the Widrow-Hoff loss function.

In order to explain the difference in loss functions between the perceptron, Widrow-Hoff, logistic regression, and the support vector machine, we have shown the loss for a single *positive* training instance at different values of $\hat{y}_i = \overline{W} \cdot \overline{X_i}$ in Figure 2.4. In the case of the perceptron, only the smoothed *surrogate* loss function (cf. Section 1.2.1.1 of Chapter 1) is shown. Since the target value is +1, the loss function shows diminishing improvement by increasing $\overline{W} \cdot \overline{X_i}$ beyond +1 in the case of logistic regression. In the case of the support-vector machine the hinge-loss function flattens out beyond this point. In other words, only misclassified points or points that are too close to the decision boundary $\overline{W} \cdot \overline{X} = 0$ are penalized. The perceptron criterion is identical in shape to the hinge loss, except that it is shifted by one unit to the left. The Widrow-Hoff method is the only case in which a positive training point is penalized for having too large a positive value of $\overline{W} \cdot \overline{X_i}$. In other words, the Widrow-Hoff method penalizes points for being properly classified in a very strong way. This is a potential problem with the Widrow-Hoff objective function, in which well-separated points cause problems in training.

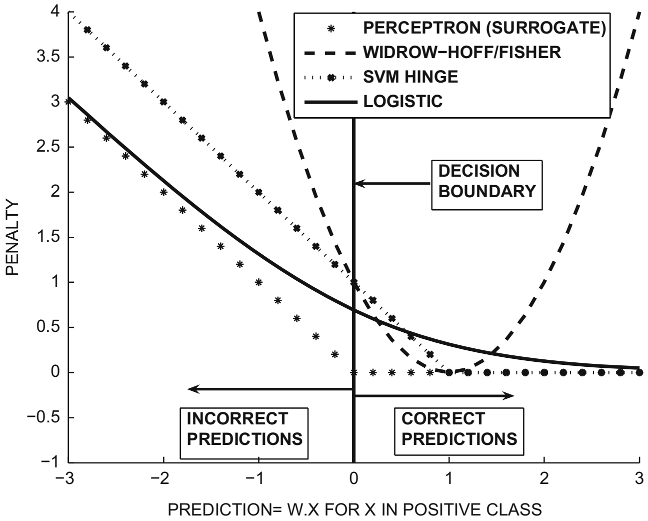


Figure 2.4: The loss functions of different variants of the perceptron. Key observations: (i) The SVM loss is shifted from the perceptron (surrogate) loss by exactly one unit to the right; (ii) the logistic loss is a smooth variant of the SVM loss; (iii) the Widrow-Hoff/Fisher loss is the only case in which points are increasingly penalized for classifying points "too correctly" (i.e., increasing $\overline{W} \cdot \overline{X}$ beyond +1 for $\overline{X}$ in positive class). Repairing the Widrow-Hoff loss function by setting it to 0 for $\overline{W} \cdot \overline{X} > 1$ yields the *quadratic loss* SVM [190].

The stochastic gradient-descent method computes the partial derivative of the point-wise loss function L_i with respect to the elements in $\overline{W}$. The gradient is computed as follows:

$$\frac{\partial L_i}{\partial \overline{W}} = \begin{cases} -y_i \overline{X_i} & \text{if } y_i \hat{y}_i < 1 \\ 0 & \text{otherwise} \end{cases} \tag{2.20}$$

Therefore, the stochastic gradient method samples a point and checks whether $y_i \hat{y}_i < 1$. If this is the case, an update is performed that is proportional to $y_i \overline{X_i}$:

$$\overline{W} \Leftarrow \overline{W}(1 - \alpha\lambda) + \alpha y_i \overline{X_i} \left[I(y_i \hat{y}_i < 1) \right] \tag{2.21}$$

Here, $I(\cdot) \in \{0, 1\}$ is the indicator function that takes on the value of 1 when the condition in its argument is satisfied. This approach is the simplest version of the primal update for

SVMs [448]. The reader should also convince herself is that this update is *identical* to that of a (regularized) perceptron (cf. Equation 2.3), except that the condition for making this update in the perceptron is $y_i \hat{y}_i < 0$. Therefore, a perceptron makes the update only when a point is misclassified, whereas the support vector machine also makes updates for points that are classified correctly, albeit not very confidently. This neat relationship is because the loss function of the perceptron criterion shown in Figure 2.4 is shifted from the hinge-loss in the SVM.

To emphasize the similarities and differences in the loss functions used by the different methods, we tabulate the loss functions below:

Model	**Loss function** L_i **for** $(\overline{X_i}, y_i)$
Perceptron (Smoothed surrogate)	$\max\{0, -y_i \cdot (\overline{W} \cdot \overline{X_i})\}$
Widrow-Hoff/Fisher	$(y_i - \overline{W} \cdot \overline{X_i})^2 = \{1 - y_i \cdot (\overline{W} \cdot \overline{X_i})\}^2$
Logistic Regression	$\log(1 + \exp[-y_i(\overline{W} \cdot \overline{X_i})])$
Support vector machine (Hinge)	$\max\{0, 1 - y_i \cdot (\overline{W} \cdot \overline{X_i})\}$
Support vector machine (Hinton's L_2-Loss) [190]	$[\max\{0, 1 - y_i \cdot (\overline{W} \cdot \overline{X_i})\}]^2$

It is noteworthy that all the derived updates in this section typically correspond to stochastic gradient-descent updates that are encountered both in traditional machine learning and in neural networks. The updates are the same whether or not we use a neural architecture to represent the models for these algorithms. Our main point in going through this exercise is to show that rudimentary special cases of neural networks are instantiations of well-known algorithms in the machine learning literature. The key point is that with greater availability of data one can incorporate additional nodes and depth to increase the model's capacity, explaining the superior behavior of neural networks with larger data sets (cf. Figure 2.1).

2.3 Neural Architectures for Multiclass Models

All the models discussed so far in this chapter are designed for binary classification. In this section, we will discuss how one can design multiway classification models by changing the architecture of the perceptron slightly, and allowing multiple output nodes.

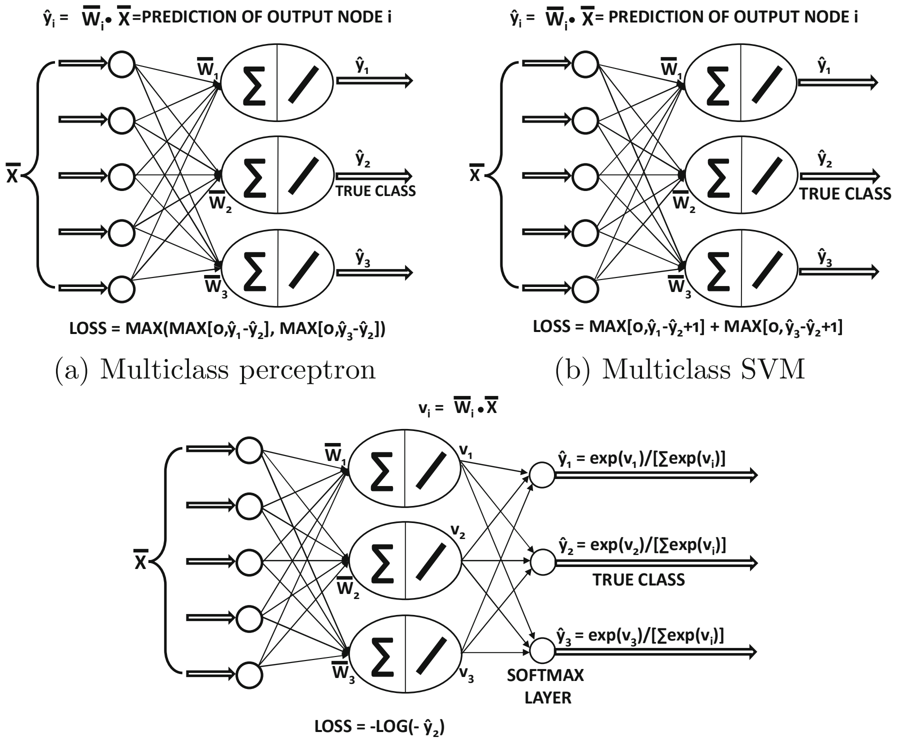
2.3.1 Multiclass Perceptron

Consider a setting with k different classes. Each training instance $(\overline{X_i}, c(i))$ contains a d-dimensional feature vector $\overline{X_i}$ and the index $c(i) \in \{1 \ldots k\}$ of its observed class. In such a case, we would like to find k different linear separators $\overline{W_1} \ldots \overline{W_k}$ simultaneously so that the value of $\overline{W_{c(i)}} \cdot \overline{X_i}$ is larger than $\overline{W_r} \cdot \overline{X_i}$ for each $r \neq c(i)$. This is because one always predicts a data instance $\overline{X_i}$ to the class r with the largest value of $\overline{W_r} \cdot \overline{X_i}$. Therefore, the loss function for the ith training instance in the case of the multiclass perceptron is defined as follows:

$$L_i = \max_{r:r \neq c(i)} \max(\overline{W_r} \cdot \overline{X_i} - \overline{W_{c(i)}} \cdot \overline{X_i}, 0) \tag{2.22}$$

The multiclass perceptron is illustrated in Figure 2.5(a). As in all neural network models, one can use gradient-descent in order to determine the updates. For a correctly classified instance, the gradient is always 0, and there are no updates. For a misclassified instance, the gradients are as follows:

$$\frac{\partial L_i}{\partial \overline{W_r}} = \begin{cases} -\overline{X_i} & \text{if } r = c(i) \\ \overline{X_i} & \text{if } r \neq c(i) \text{ is most misclassified prediction} \\ 0 & \text{otherwise} \end{cases} \tag{2.23}$$


$\hat{y}_i = \overline{W_i} \cdot \overline{X}$=PREDICTION OF OUTPUT NODE i
$\overline{X}$
$\overline{W_1}$
$\overline{W_2}$
$\overline{W_3}$
Σ
$\hat{y}_1$
$\hat{y}_2$
TRUE CLASS
$\hat{y}_3$
LOSS = MAX(MAX[o,$\hat{y}_1$-$\hat{y}_2$], MAX[o,$\hat{y}_3$-$\hat{y}_2$])
$\hat{y}_i = \overline{W_i} \cdot \overline{X}$= PREDICTION OF OUTPUT NODE i
$\overline{X}$
$\overline{W_1}$
$\overline{W_2}$
$\overline{W_3}$
Σ
$\hat{y}_1$
$\hat{y}_2$
TRUE CLASS
$\hat{y}_3$
LOSS = MAX[o,$\hat{y}_1$-$\hat{y}_2$+1] + MAX[o,$\hat{y}_3$-$\hat{y}_2$+1]
$v_i = \overline{W_i} \cdot \overline{X}$
$\overline{X}$
$\overline{W_1}$
$\overline{W_2}$
$\overline{W_3}$
Σ
v_1
v_2
v_3
$\hat{y}_1$ = exp(v_1)/[∑exp(v_i)]
$\hat{y}_2$ = exp(v_2)/[∑exp(v_i)]
TRUE CLASS
$\hat{y}_3$ = exp(v_3)/[∑exp(v_i)]
SOFTMAX
LAYER
LOSS = -LOG(- $\hat{y}_2$)

(a) Multiclass perceptron

(b) Multiclass SVM

(c) Multinomial logistic regression

Figure 2.5: Multiclass models: In each case, class 2 is assumed to be the ground-truth class.

Therefore, the stochastic gradient-descent method is applied as follows. Each training instance is fed into the network. If the correct class $r = c(i)$ receives the largest of output $\overline{W_r} \cdot \overline{X_i}$, then no update needs to be executed. Otherwise, the following update is made to each separator $\overline{W_r}$ for learning rate $\alpha > 0$:

$$\overline{W_r} \Leftarrow \overline{W_r} + \begin{cases} \alpha\overline{X_i} & \text{if } r = c(i) \\ -\alpha\overline{X_i} & \text{if } r \neq c(i) \text{ is most misclassified prediction} \\ 0 & \text{otherwise} \end{cases} \tag{2.24}$$

Only two of the separators are always updated at a given time. In the special case that $k = 2$, these gradient updates reduce to the perceptron because both the separators $\overline{W_1}$ and $\overline{W_2}$ will be related as $\overline{W_1} = -\overline{W_2}$ if the descent is started at $\overline{W_1} = \overline{W_2} = 0$. Another quirk that is specific to the unregularized perceptron is that it is possible to use a learning rate of $\alpha = 1$ without affecting the learning because the value of α only has the effect of scaling the weight when starting with $\overline{W_j} = 0$ (see Exercise 2). This property is, however, not true for other linear models in which the value of α does affect the learning.

2.3.2 Weston-Watkins SVM

The Weston-Watkins SVM [529] varies on the multiclass perceptron in two ways:

1. The multiclass perceptron only updates the linear separator of a class that is predicted *most* incorrectly along with the linear separator of the true class. On the other hand, the Weston-Watkins SVM updates the separator of *any* class that is predicted more favorably than the true class. In both cases, the separator of the observed class is updated by the same aggregate amount as the incorrect classes (but in the opposite direction).

2. Not only does the Weston-Watkins SVM update the separator in the case of misclassification, it updates the separators in cases where an incorrect class gets a prediction that is "uncomfortably close" to the true class. This is based on the notion of margin.

As in the case of the multiclass perceptron, it is assumed that the ith training instance is denoted by $(\overline{X_i}, c(i))$, where $\overline{X_i}$ contains the d-dimensional feature variables, and $c(i)$ contains the class index drawn from $\{1, \ldots, k\}$. One wants to learn d-dimensional coefficients $\overline{W_1} \ldots \overline{W_k}$ of the k linear separators so that the class index r with the largest value of $\overline{W_r} \cdot \overline{X_i}$ is predicted to be the correct class $c(i)$. The loss function L_i for the ith training instance $(\overline{X_i}, c(i))$ in the Weston-Watkins SVM is as follows:

$$L_i = \sum_{r:r \neq c(i)} \max(\overline{W_r} \cdot \overline{X_i} - \overline{W}_{c(i)} \cdot \overline{X_i} + 1, 0) \tag{2.25}$$

The neural architecture of the Weston-Watkins SVM is illustrated in Figure 2.5(b). It is instructive to compare the objective function of the Weston-Watkins SVM (Equation 2.25) with that of the multiclass perceptron (Equation 2.22). First, for each class $r \neq c(i)$, if the prediction $\overline{W_r} \cdot \overline{X_i}$ lags behind that of the true class by less than a margin amount of 1, then a loss is incurred for that class. Furthermore, the losses over all such classes $r \neq c(i)$ are *added*, rather than taking the maximum of the losses. These two differences accomplish the two intuitive goals discussed above.

In order to determine the gradient-descent updates, one can find the gradient of the loss function with respect to each $\overline{W_r}$. In the event that the loss function L_i is 0, the gradient of the loss function is 0 as well. Therefore, no update is required when the training instance is classified correctly with sufficient margin with respect to the second-best class. However, if the loss function is non-zero we have either a misclassified or a "barely correct" prediction in which the second-best and best class prediction are not sufficiently separated. In such cases, the gradient of the loss is non-zero. The loss function of Equation 2.25 is created by adding up the contributions of the $(k-1)$ separators belonging to the incorrect classes. Let $\delta(r, \overline{X_i})$ be a 0/1 indicator function, which is 1 when the rth class separator contributes positively to the loss function in Equation 2.25. In such a case, the gradient of the loss function is as follows:

$$\frac{\partial L_i}{\partial \overline{W_r}} = \begin{cases} -\overline{X_i}[\sum_{j \neq r} \delta(j, \overline{X_i})] & \text{if } r = c(i) \\ \overline{X_i}[\delta(r, \overline{X_i})] & \text{if } r \neq c(i) \end{cases} \tag{2.26}$$

This results in the following stochastic gradient-descent step for the rth separator $\overline{W_r}$ at learning rate α:

$$\overline{W_r} \Leftarrow \overline{W_r}(1 - \alpha\lambda) + \alpha \begin{cases} \overline{X_i}[\sum_{j \neq r} \delta(j, \overline{X_i})] & \text{if } r = c(i) \\ -\overline{X_i}[\delta(r, \overline{X_i})] & \text{if } r \neq c(i) \end{cases} \tag{2.27}$$

For training instances $\overline{X_i}$ in which the loss L_i is zero, the above update can be shown to simplify to a regularization update of each hyperplane $\overline{W_r}$:

$$\overline{W_r} \Leftarrow \overline{W_r}(1 - \alpha\lambda) \tag{2.28}$$

The regularization uses the parameter $\lambda > 0$. Regularization is considered essential to the proper functioning of a support vector machine.

2.3.3 Multinomial Logistic Regression (Softmax Classifier)

Multinomial logistic regression can be considered the multi-way generalization of logistic regression, just as the Weston-Watkins SVM is the multiway generalization of the binary SVM. Multinomial logistic regression uses negative log-likelihood loss, and is therefore a probabilistic model. As in the case of the multiclass perceptron, it is assumed that the input to the model is a training data set containing pairs of the form $(\overline{X_i}, c(i))$, where $c(i) \in \{1 \ldots k\}$ is the index of the class of d-dimensional data point $\overline{X_i}$. As in the case of the previous two models, the class r with the largest value of $\overline{W_r} \cdot \overline{X_i}$ is predicted to be the label of the data point $\overline{X_i}$. However, in this case, there is an additional probabilistic interpretation of $\overline{W_r} \cdot \overline{X_i}$ in terms of the posterior probability $P(r|\overline{X_i})$ that the data point $\overline{X_i}$ takes on the label r. This estimation can be naturally accomplished with the softmax activation function:

$$P(r|\overline{X_i}) = \frac{\exp(\overline{W_r} \cdot \overline{X_i})}{\sum_{j=1}^{k} \exp(\overline{W_j} \cdot \overline{X_i})} \tag{2.29}$$

In other words, the model predicts the class membership in terms of probabilities. The loss function L_i for the ith training instance is defined by the cross-entropy, which is the negative logarithm of the probability of the true class. The neural architecture of the softmax classifier is illustrated in Figure 2.5(c).

The cross-entropy loss may be expressed in terms of either the input features or in terms of the softmax pre-activation values $v_r = \overline{W_r} \cdot \overline{X_i}$ as follows:

$$\begin{aligned} L_i &= -\log[P(c(i)|\overline{X_i})] && (2.30)\\ &= -\overline{W}_{c(i)} \cdot \overline{X_i} + \log[\sum_{j=1}^{k} \exp(\overline{W_j} \cdot \overline{X_i})] && (2.31)\\ &= -v_{c(i)} + \log[\sum_{j=1}^{k} \exp(v_j)] && (2.32) \end{aligned}$$

Therefore, the partial derivative of L_i with respect to v_r can be computed as follows:

$$\begin{aligned} \frac{\partial L_i}{\partial v_r} &= \begin{cases} -\left(1 - \frac{\exp(v_r)}{\sum_{j=1}^{k} \exp(v_j)}\right) & \text{if } r = c(i) \\ \left(\frac{\exp(v_r)}{\sum_{j=1}^{k} \exp(v_j)}\right) & \text{if } r \neq c(i) \end{cases} && (2.33)\\ &= \begin{cases} -(1 - P(r|\overline{X_i})) & \text{if } r = c(i) \\ P(r|\overline{X_i}) & \text{if } r \neq c(i) \end{cases} && (2.34) \end{aligned}$$

The gradient of the loss of the ith training instance with respect to the separator of the rth class is computed by using the chain rule of differential calculus in terms of its pre-activation value $v_j = \overline{W_j} \cdot \overline{X_i}$:

$$\frac{\partial L_i}{\partial \overline{W_r}} = \sum_j \left(\frac{\partial L_i}{\partial v_j}\right)\left(\frac{\partial v_j}{\partial \overline{W_r}}\right) = \frac{\partial L_i}{\partial v_r} \underbrace{\frac{\partial v_r}{\partial \overline{W_r}}}_{\overline{X_i}} \tag{2.35}$$

In the above simplification, we used the fact that v_j has a zero gradient with respect to $\overline{W_r}$ for $j \neq r$. The value of $\frac{\partial L_i}{\partial v_r}$ in Equation 2.35 can be substituted from Equation 2.34 to obtain the following result:

$$\frac{\partial L_i}{\partial \overline{W_r}} = \begin{cases} -\overline{X_i}(1 - P(r|\overline{X_i})) & \text{if } r = c(i) \\ \overline{X_i}\, P(r|\overline{X_i}) & \text{if } r \neq c(i) \end{cases} \tag{2.36}$$

Note that we have expressed the gradient indirectly using probabilities (based on Equation 2.29) both for brevity and for intuitive understanding of how the gradient is related to the probability of making different types of mistakes. Each of the terms $[1 - P(r|\overline{X_i})]$ and $P(r|\overline{X_i})$ is the probability of making a mistake for an instance with label $c(i)$ with respect to the predictions for the rth class. After including similar regularization impact as other models, the separator for the rth class is updated as follows:

$$\overline{W_r} \Leftarrow \overline{W_r}(1 - \alpha\lambda) + \alpha \begin{cases} \overline{X_i} \cdot (1 - P(r|\overline{X_i})) & \text{if } r = c(i) \\ -\overline{X_i} \cdot P(r|\overline{X_i}) & \text{if } r \neq c(i) \end{cases} \tag{2.37}$$

Here, α is the learning rate, and λ is the regularization parameter. The softmax classifier updates all the k separators for each training instance, unlike the multiclass perceptron and the Weston-Watkins SVM, each of which updates only a small subset of separators (or no separator) for each training instance. This is a consequence of probabilistic modeling, in which correctness is defined in a soft way.

2.3.4 Hierarchical Softmax for Many Classes

Consider a classification problem in which we have an extremely large number of classes. In such a case, learning becomes too slow, because of the large number of separators that need to be updated for each training instance. This situation can occur in applications like text mining, where the prediction is a target word. Predicting target words is particularly common in *neural language models*, which try to predict the next word given the immediate history of previous words. The cardinality of the number of classes will typically be larger than 10^5 in such cases. Hierarchical softmax is a way of improving learning efficiency by decomposing the classification problem hierarchically. The idea is to group the classes hierarchically into a binary tree-like structure, and then perform $\log_2(k)$ binary classifications from the root to the leaf for k-way classification. Although the hierarchical classification can compromise the accuracy to some extent, the efficiency improvements can be significant.

How is the hierarchy of classes obtained? The naïve approach is to create a random hierarchy. However, the specific grouping of classes has an effect on performance. Grouping similar classes tends to improve performance. It is possible to use domain-specific insights to improve the quality of the hierarchy. For example, if the prediction is a target word, one can use the *WordNet* hierarchy [329] to guide the grouping. Further reorganization may be needed [344] because the *WordNet* hierarchy is not exactly a binary tree. Another option is to use Huffman encoding in order to create the binary tree [325, 327]. Refer to the bibliographic notes for more pointers.

2.4 Backpropagated Saliency for Interpretability and Feature Selection

One of the common refrains about neural networks has been their lack of interpretability [97]. However, it turns out that one can use backpropagation in order to determine the features that contribute the most to the classification of a particular test instance. This provides the analyst with an understanding of the relevance of each feature to classification. This approach also has the useful property that it can be used for feature selection [406].

Consider a test instance $\overline{X} = (x_1, \ldots x_d)$, for which the multilabel output scores of the neural network are $o_1 \ldots o_k$. Furthermore, let the output of the winning class among the k outputs be o_m, where $m \in \{1 \ldots k\}$. Our goal is to identify the features that are most relevant to the classification of this test instance. In general, for each attribute x_i, we would like to determine the sensitivity of the output o_m to x_i. Features with large *absolute* magnitudes of this sensitivity are obviously relevant to the classification of this test instance. In order to achieve this goal, we would like to compute the absolute magnitude of $\frac{\partial o_m}{\partial x_i}$. The features with the largest absolute value of the partial derivative have the greatest influence on the classification to the winning class. The sign of this derivative also tells us whether increasing x_i slightly from its current value increases or decreases the score of the winning class. For classes other than the winning class, the derivative also provides some understanding of the sensitivity, but this is less important, particularly when the number of classes is large. The value of $\frac{\partial o_m}{\partial x_i}$ can be computed by a straightforward application of the backpropagation algorithm, in which one does not stop backpropagating at the first hidden layer but applies the process all the way to the input layer.

One can also use this approach for feature selection by aggregating the absolute value of the gradient over all classes and all correctly classified training instances. The features with the largest aggregate sensitivity over the whole training data are the most relevant. Strictly speaking, one does not need to aggregate this value over all classes, but one can simply use only the winning class for correctly classified training instances. However, the original work in [406] aggregates this value over all classes and all instances.

Similar methods for interpreting the effects of different portions of the input are also used in computer vision with convolutional neural networks [466]. A discussion of some of these methods is provided in Section 8.5.1 of Chapter 8. In the case of computer vision, the visual effects of this type of saliency analysis are sometimes spectacular. For example, for an image of a dog, the analysis will tell us which features (i.e., pixels) results in the image being considered a dog. As a result, we can create a black-and-white saliency image in which the portion corresponding to a dog is emphasized in light color against a dark background (cf. Figure 8.12 of Chapter 8).

2.5 Matrix Factorization with Autoencoders

Autoencoders represent a fundamental architecture that is used for various types of unsupervised learning, including matrix factorization, principal component analysis, and dimensionality reduction. Natural architectural variations of the autoencoder can also be used for matrix factorization of incomplete data to create recommender systems. Furthermore, some recent feature engineering methods in the natural language domain like *word2vec* can also be viewed as variations of autoencoders, which perform nonlinear matrix factorizations of word-context matrices. The nonlinearity is achieved with the activation function in the output layer, which is usually not available with traditional matrix factorization. Therefore, one of our goals will be to demonstrate how small changes to the underlying building blocks of the neural network can be used to implement sophisticated variations of a given family of methods. This is particularly convenient for the analyst, who only has to experiment with small variations of the architecture to test different types of models. Such variations would require more effort to construct in traditional machine learning, because one does not have the benefit of learning abstractions like backpropagation. First, we begin with a simple simulation of a traditional matrix factorization method with a shallow neural architecture. Then, we discuss how this basic setup provides the path to generalizations to nonlinear dimensionality reduction methods by adding layers and/or nonlinear activation functions. Therefore, the goal of this section is to show two things:

1. Classical dimensionality reduction methods like singular value decomposition and principal component analysis are special cases of neural architectures.

2. By adding different types of complexities to the basic architecture, one can generate complex nonlinear embeddings of the data. While nonlinear embeddings are also available in machine learning, neural architectures provide unprecedented flexibility in controlling the properties of the embedding by making various types of architectural changes (and allowing backpropagation to take care of the changes in the underlying learning algorithms).

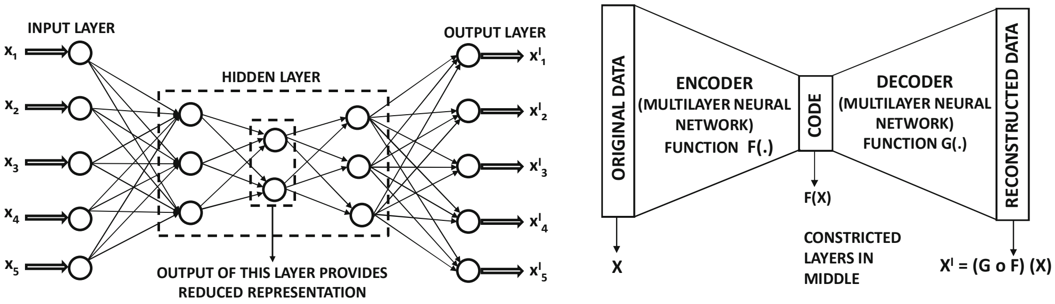
We will also discuss a number of applications such as recommender systems and outlier detection.

2.5.1 Autoencoder: Basic Principles

The basic idea of an autoencoder is to have an output layer with the same dimensionality as the inputs. The idea is to try to reconstruct each dimension exactly by passing it through the network. An autoencoder *replicates* the data from the input to the output, and is therefore sometimes referred to as a *replicator neural network*. Although reconstructing the data might seem like a trivial matter by simply copying the data forward from one layer to another, this is not possible when the number of units in the middle are *constricted*. In other words, the number of units in each middle layer is typically fewer than that in the input (or output). As a result, these units hold a reduced representation of the data, and the final layer can no longer reconstruct the data exactly. Therefore, this type of reconstruction is inherently *lossy*. The loss function of this neural network uses the sum-of-squared differences between the input and the output in order to force the output to be as similar as possible to the input. This general representation of the autoencoder is given in Figure 2.6(a), where an architecture is shown with three constricted layers. It is noteworthy that the representation of the innermost hidden layer will be hierarchically related to those in the two outer hidden layers. Therefore, an autoencoder is capable of performing hierarchical data reduction.

It is common (but not necessary) for an M-layer autoencoder to have a symmetric architecture between the input and output, where the number of units in the kth layer is the same as that in the $(M - k + 1)$th layer. Furthermore, the value of M is often odd, as a result of which the $(M + 1)/2$th layer is often the most constricted layer. Here, we are counting the (non-computational) input layer as the first layer, and therefore the minimum number of layers in an autoencoder would be three, corresponding to the input layer, constricted layer, and the output layer. As we will see later, this simplest form of the autoencoder is used in traditional machine learning for singular value decomposition. The symmetry in the architecture often extends to the fact that the weights outgoing from the

kth layer are tied to those incoming to the $(M-k)$th layer in many architectures. For now, we will not make this assumption for simplicity in presentation. Furthermore, the symmetry is never absolute because of the effect of nonlinear activation functions. For example, if a nonlinear activation function is used in the output layer, there is no way to symmetrically mirror that fact in the (non-computational) input layer.


INPUT LAYER
x_1
x_2
x_3
x_4
x_5
HIDDEN LAYER
OUTPUT LAYER
x'_1
x'_2
x'_3
x'_4
x'_5
OUTPUT OF THIS LAYER PROVIDES REDUCED REPRESENTATION
ORIGINAL DATA
ENCODER (MULTILAYER NEURAL NETWORK) FUNCTION F(.)
CODE
DECODER (MULTILAYER NEURAL NETWORK) FUNCTION G(.)
RECONSTRUCTED DATA
X
F(X)
CONSTRICTED LAYERS IN MIDDLE
X' = (G o F) (X)

(a) Three hidden layers

(b) General schematic

Figure 2.6: The basic schematic of the autoencoder

The reduced representation of the data is also sometimes referred to as the *code*, and the number of units in this layer is the dimensionality of the reduction. The initial part of the neural architecture before the bottleneck is referred to as the *encoder* (because it creates a reduced code), and the final part of the architecture is referred to as the *decoder* (because it reconstructs from the code). The general schematic of the autoencoder is shown in Figure 2.6(b).

2.5.1.1 Autoencoder with a Single Hidden Layer

In the following, we describe the simplest version of an autoencoder, which is used for matrix factorization. This autoencoder only has a single hidden layer of $k \ll d$ units between the input and output layers of d units each. For the purpose of discussion, assume that we have an $n \times d$ matrix denoted by D, which we would like to factorize into an $n \times k$ matrix U and a $d \times k$ matrix V:

$$D \approx UV^T \tag{2.38}$$

Here, k is the rank of the factorization. The matrix U contains the reduced representation of the data, and the matrix V contains the basis vectors. Matrix factorization is one of the most widely studied problems in supervised learning, and it is used for dimensionality reduction, clustering, and predictive modeling in recommender systems.

In traditional machine learning, this problem is solved by minimizing the *Frobenius norm* of the *residual matrix* denoted by $(D - UV^T)$. The squared Frobenius norm of a matrix is the sum of the squares of the entries in the matrix. Therefore, one can write the objective function of the optimization problem as follows:

$$\text{Minimize } J = ||D - UV^T||_F^2$$

Here, the notation $|| \cdot ||_F$ indicates the Frobenius norm. The parameter matrices U and V need to be learned in order to optimize the aforementioned error. This objective function has an infinite number of optima, one of which has mutually orthogonal basis vectors. That particular solution is referred to as *truncated singular value decomposition*. Although it is relatively easy to derive the gradient-descent steps [6] for this optimization problem (without worrying about neural networks at all), our goal here is to capture this optimization problem within a neural architecture. Going through this exercise helps us show that SVD is a special case of an autoencoder architecture, which sets the stage for understanding the gains obtained with more complex autoencoders.

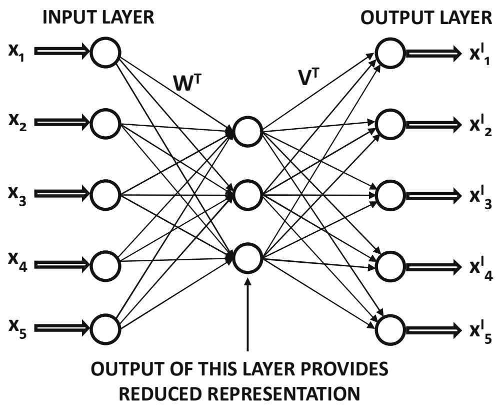


Figure 2.7: A basic autoencoder with a single layer

This neural architecture for SVD is illustrated in Figure 2.7, where the hidden layer contains k units. The rows of D are input into the autoencoder, whereas the k-dimensional rows of U are the activations of the hidden layer. The $k \times d$ matrix of weights in the decoder is V^T. As we discussed in the introduction to the multilayer neural network in Chapter 1, the vector of values in a particular layer of the network can be obtained by multiplying the vector of values in the previous layer with the matrix of weights connecting the two layers (with linear activation). Since the activations of the hidden layer are U and the decoder weights contain the matrix V^T, it follows that the reconstructed output contains the rows of UV^T. The autoencoder minimizes the sum-of-squared differences between the input and the output, which is equivalent to minimizing $||D - UV^T||^2$. Therefore, the same problem is being solved as singular value decomposition.

Note that one can use this approach to provide the reduced representation of *out-of-sample* instances that were not included in the original matrix D. One simply has to feed these out-of-sample rows as the input, and the activations of the hidden layer will provide the reduced representation. Reducing out-of-sample instances is particularly useful for nonlinear dimensionality-reduction methods, as it is more difficult for traditional machine learning methods to fold in new instances.

Encoder Weights

As shown in Figure 2.7, the encoder weights are contained in the $k \times d$ matrix denoted by W. How is this matrix related to U and V? Note that the autoencoder creates the reconstructed representation DW^TV^T of the original data matrix. Therefore, it tries to optimize the problem of minimizing $||DW^TV^T - D||^2$. The optimal solution to this problem is obtained when the matrix W contains the *pseudo-inverse* of V, which is defined as follows:

$$W = (V^TV)^{-1}V^T \tag{2.39}$$

This result is easy to show at least for non-degenerate cases in which the rows of matrix D span the full rank of d dimensions (see Exercise 14). Of course, the final solution found by the training algorithm of the autoencoder might deviate from this condition because it might not solve the problem precisely or because the matrix D might be of smaller rank.

By the definition of the pseudo-inverse, it follows that $WV = I$ and $V^T W^T = I$, where I is a $k \times k$ identity matrix. Post-multiplying Equation 2.38 with W^T we obtain the following:

$$DW^T \approx U \underbrace{(V^T W^T)}_{I} = U \tag{2.40}$$

In other words, multiplying each row of the matrix D with the $d \times k$ matrix W^T yields the reduced representation of that instance, which is the corresponding row in U. Furthermore, multiplying that row of U again with V^T yields the reconstructed version of the original data matrix D.

Note that there are many alternate optima for W and V, but in order for reconstruction to occur (i.e., minimization of loss function), the learned matrix W will always be (approximately) related to V as its pseudo-inverse and the columns of V will always span[3] a particular k-dimensional subspace defined by the SVD optimization problem.

2.5.1.2 Connections with Singular Value Decomposition

The single-layer autoencoder architecture is closely connected with singular value decomposition (SVD). Singular value decomposition finds a factorization UV^T in which the columns of V are orthonormal. The loss function of this neural network is identical to that of singular value decomposition, and a solution V in which the columns of V are orthonormal will always be one of the *possible* optima obtained by training the neural network. However, since this loss function allows alternative optima, it is possible to find an optimal solution in which the columns of V are not necessarily mutually orthogonal or scaled to unit norm. SVD is defined by an orthonormal basis system. Nevertheless, the subspace spanned by the k columns of V will be the same as that spanned by the top-k basis vectors of SVD. Principal component analysis is identical to singular value decomposition, except that it is applied to a mean-centered matrix D. Therefore, the approach can also be used to find the subspace spanned by the top-k principal components. However, each column of D needs to be mean-centered up front by subtracting its mean. One can achieve an orthonormal basis system, which is even closer to SVD and PCA by sharing some of the weights in the encoder and decoder. This approach is discussed in the next section.

2.5.1.3 Sharing Weights in Encoder and Decoder

There are many possible alternate solutions for W and V in the above discussion, in which W is the pseudo-inverse of V. One can, therefore, reduce the parameter footprint further without significant[4] loss in reconstruction accuracy. A common practice that is used in the autoencoder construction is to share some of the weights between the encoder and the

[3] This subspace is defined by the top-k singular vectors of singular value decomposition. However, the optimization problem does not impose orthogonality constraints, and therefore the columns of V might use a different non-orthogonal basis system to represent this subspace.

[4] There is no loss in reconstruction accuracy in several special cases like the single-layer case discussed here, even on the training data. In other cases, the loss of accuracy is only on the training data, but the autoencoder tends to better reconstruct out-of-sample data because of the regularization effects of parameter footprint reduction.

decoder. This is also referred to as *tying the weights*. In particular, the autoencoder has an inherently symmetric structure, in which the weights of the encoder and decoder are forced to be the same in symmetrically matching layers. In the shallow case, the encoder and decoder weights are shared by using the following relationship:

$$W = V^T \tag{2.41}$$

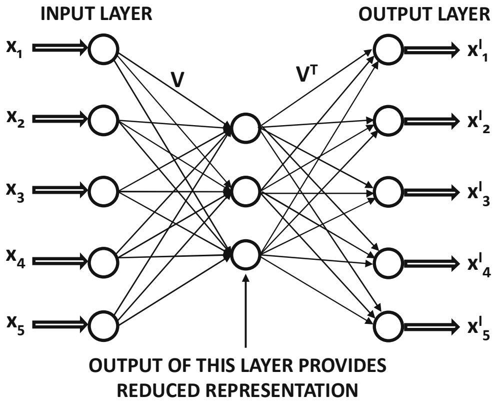


Figure 2.8: Basic autoencoder with a single layer; note tied weights (unlike the autoencoder shown in Figure 2.7).

This architecture is shown in Figure 2.8, and it is identical to the architecture of Figure 2.7 except for the presence of tied weights. In other words, the $d \times k$ matrix V of weights is first used to transform the d-dimensional data point $\overline{X}$ into a k-dimensional representation. Then, the matrix V^T of weights is used to reconstruct the data to its original representation.

The tying of the weights effectively means that V^T is the pseudo-inverse of V (see Exercise 14). In other words, we have $V^T V = I$, and therefore the columns of V are mutually orthogonal. As a result, by tying the weights, it is now possible to *exactly* simulate SVD, in which the different basis vectors need to be mutually orthogonal.

In this particular example of an architecture with a single hidden layer, the tying of weights is done only for a pair of weight matrices. In general, one would have an odd number of hidden layers and an even number of weight matrices. It is a common practice to match up the weight matrices in a symmetric way about the middle. In such a case, the symmetrically arranged hidden layers would need to have the same numbers of units. Even though it is not necessary to share weights between the encoder and decoder portions of the architecture, it reduces the number of parameters by a factor of 2. This is beneficial from the point of view of reducing overfitting. In other words, the approach would better reconstruct out-of-sample data. Another benefit of tying the weight matrices in the encoder and the decoder is that it automatically normalizes the columns of V to similar values. For example, if we do not tie the weight matrices in the encoder and the decoder, it is possible for the different columns of V to have very different norms. At least in the case of linear activations, tying the weight matrices forces all columns of V to have similar norms. This is also useful from the perspective of providing better normalization of the embedded representation. The normalization and orthogonality properties no longer hold exactly when nonlinear activations are used in the computational layers. However, there are considerable benefits in tying the weights even in these cases in terms of better conditioning of the solution.

The sharing of weights does require some changes to the backpropagation algorithm during training. However, these modifications are not very difficult. All that one has to do is to perform normal backpropagation by pretending that the weights are not tied in order to compute the gradients. Then, the gradients across different copies of the same weight are added in order to compute the gradient-descent steps. The logic for handing shared weights in this way is discussed in Section 3.2.9 of Chapter 3.

2.5.1.4 Other Matrix Factorization Methods

It is possible to modify the simple three-layer autoencoder to simulate other types of matrix factorization methods such as non-negative matrix factorization, probabilistic latent semantic analysis, and logistic matrix factorization methods. Different methods for logistic matrix factorization will be discussed in the next section, in Section 2.6.3, and in Exercise 8. Methods for non-negative matrix factorization and probabilistic latent semantic analysis are discussed in Exercises 9 and 10. It is instructive to examine the relationships between these different variations, because it shows how one can vary on simple neural architectures in order to get results with vastly different properties.

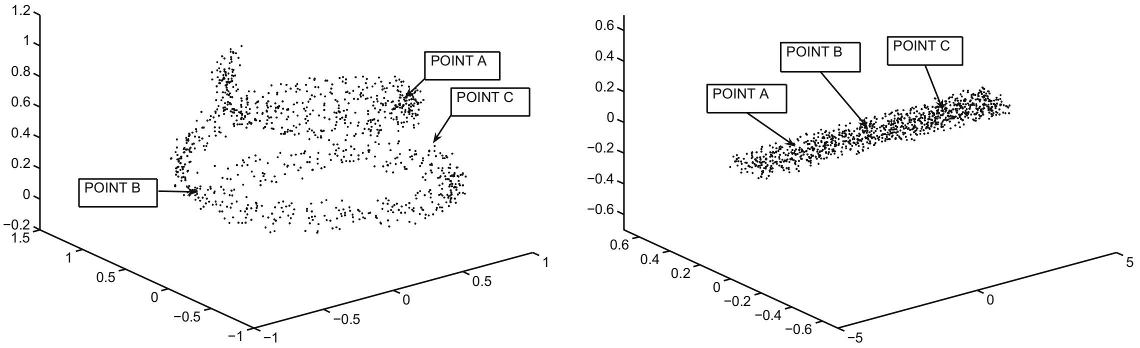
2.5.2 Nonlinear Activations

So far, the discussion has focussed on simulating singular value decomposition using a neural architecture. Clearly, this does not seem to achieve much because many off-the-shelf tools exist for singular value decomposition. However, the real power of autoencoders is realized when one starts using nonlinear activations and multiple layers. For example, consider a situation in which the matrix D is binary. In such a case, one can use the same neural architecture as shown in Figure 2.7, but one can also use a sigmoid function in the final layer to predict the output. This sigmoid layer is combined with negative log loss. Therefore, for a binary matrix $B = [b_{ij}]$, the model assumes the following:

$$B \sim \text{sigmoid}(UV^T) \tag{2.42}$$

Here, the sigmoid function is applied in element-wise fashion. Note the use of $\sim$ instead of $\approx$ in the above expression, which indicates that the binary matrix B is an instantiation of random draws from Bernoulli distributions with corresponding parameters contained in sigmoid(UV^T). The resulting factorization can be shown to be equivalent to *logistic matrix factorization*. The basic idea is that the (i, j)th element of UV^T is the parameter of a Bernoulli distribution, and the binary entry b_{ij} is generated from a Bernoulli distribution with these parameters. Therefore, U and V are learned using the log-likelihood loss of this *generative* model. The log-likelihood loss implicitly tries to find parameter matrices U and V so that the probability of the matrix B being generated by these parameters is maximized.

Logistic matrix factorization has only recently been proposed [224] as a sophisticated matrix factorization method for binary data, which is useful for recommender systems with *implicit feedback* ratings. Implicit feedback refers to the binary actions of users such as buying or not buying specific items. The solution methodology of this recent work on logistic matrix factorization [224] seems to be vastly different from SVD, and it is not based on a neural network approach. However, for a neural network practitioner, the change from the SVD model to that of logistic matrix factorization is a relatively small one, where only the final layer of the neural network needs to be changed. It is this modular nature of neural networks that makes them so attractive to engineers and encourages all types of experimentation. In fact, one of the variants of the popular *word2vec* neural approach [325, 327] for text feature engineering is a logistic matrix factorization method, when one examines it more closely. Interestingly, *word2vec* was proposed earlier than logistic matrix factorization in traditional machine learning [224], although the equivalence of the two methods was not shown in the original work. The equivalence was first shown in [6], and a proof of this result is also provided later in this chapter. Indeed, for multilayer variants of the autoencoder, an exact counterpart does not even exist in traditional machine learning. All this seems to suggest that it is often more natural to discover sophisticated machine learning algorithms when working with the modular approach of constructing multilayer neural networks. Note that one can even use this approach to factorize real-valued matrix entries drawn from $[0, 1]$, as long as the log-loss is suitably modified to handle fractional values (see Exercise 8). Logistic matrix factorization is a type of *kernel matrix factorization*.



(a) A nonlinear pattern in three dimensions (b) A reduced data set in two dimensions

Figure 2.9: The effect of nonlinear dimensionality reduction. This figure is drawn for illustrative purposes only.

One can also use non-linear activations in the hidden layer rather than (or in addition to) the output layer. By using the non-linearity in the hidden layer to impose non-negativity, one can simulate non-negative matrix factorization (cf. Exercises 9 and 10). Furthermore, consider an autoencoder with a single hidden layer in which sigmoid units are used in the hidden layer, and the output layer is linear. Furthermore, the input-to-hidden and the hidden-to-output matrices are denoted by W^T and V^T, respectively. In this case, the matrix W will no longer be the pseudo-inverse of V because of the non-linear activation in the hidden layer.

If U is the output of the hidden layer in which the nonlinear activation $\Phi(\cdot)$ is applied, we have:

$$U = \Phi(DW^T) \tag{2.43}$$

If the output layer is linear, the overall factorization is still of the following form:

$$D \approx UV^T \tag{2.44}$$

Note, however, that we can write $U' = DW^T$, which is a linear projection of the original matrix D. Then, the factorization can be written as follows:

$$D \approx \Phi(U')V^T \tag{2.45}$$

Here, U' is a linear projection of D. This is a different type of nonlinear matrix factorization [521, 558]. Although the specific form of the nonlinearity (e.g., sigmoid) might seem simplistic compared to what is considered typical in kernel methods, in reality multiple hidden layers are used to learn more complex forms of nonlinear dimensionality reduction. Nonlinearity can also be combined in the hidden layers and in the output layer. Nonlinear dimensionality reduction methods can map the data into much lower dimensional spaces (with good reconstruction characteristics) than would be possible with methods like PCA. An example of a data set, which is distributed on a nonlinear spiral, is shown in Figure 2.9(a). This data set cannot be reduced to lower dimensionality using PCA (without causing significant reconstruction error). However, the use of nonlinear dimensionality reduction methods can flatten out the nonlinear spiral into a 2-dimensional representation. This representation is shown in Figure 2.9(b).

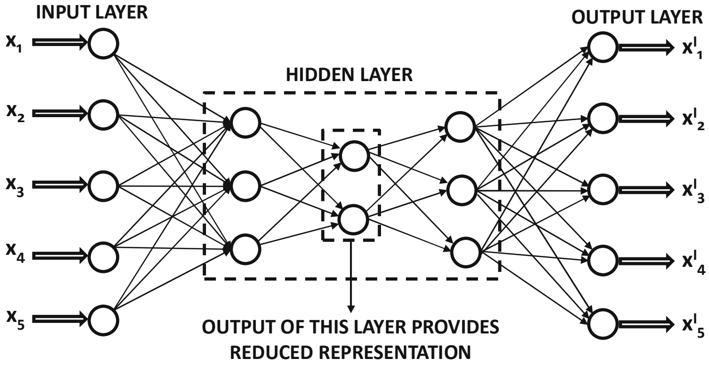


Figure 2.10: An example of an autoencoder with three hidden layers. Combining nonlinear activations with multiple hidden layers increases the representation power of the network.

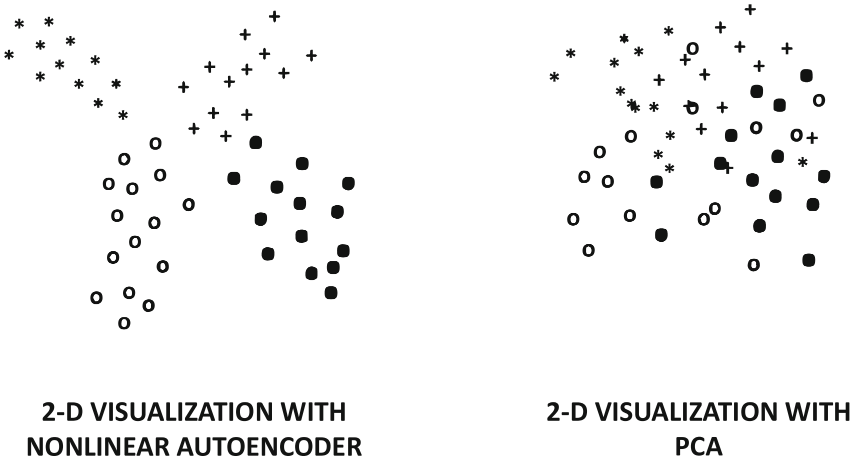
Nonlinear dimensionality-reduction methods often require deeper networks due to the more complex transformations possible with the combination of nonlinear units. The benefits of depth will be discussed in the next section.

2.5.3 Deep Autoencoders

The real power of autoencoders in the neural network domain is realized when deeper variants are used. For example, an autoencoder with three hidden layers is shown in Figure 2.10. One can increase the number of intermediate layers in order to further increase the representation power of the neural network. It is noteworthy that it is essential for some of the layers of the deep autoencoder to use a nonlinear activation function to increase its representation power. As shown in Lemma 1.5.1 of Chapter 1, no additional power is gained by a multilayer network when only linear activations are used. Although this result was shown in Chapter 1 for the classification problem, it is broadly true for any type of multilayer neural network (including an autoencoder).

Deep networks with multiple layers provide an extraordinary amount of representation power. The multiple layers of this network provide *hierarchically* reduced representations of the data. For some data domains like images, hierarchically reduced representations are particularly natural. Note that there is no precise analog of this type of model in traditional machine learning, and the backpropagation approach rescues us from the challenges associated in computing the complicated gradient-descent steps. A nonlinear dimensionality reduction might map a manifold of arbitrary shape into a reduced representation. Although several methods for nonlinear dimensionality reduction are known in machine learning, neural networks have some advantages over these methods:

1. Many nonlinear dimensionality reduction methods have a very hard time mapping out-of-sample data points to reduced representations, unless these points are included in the training data up front. On the other hand, it is a relatively simple matter to compute the reduced representation of an out-of-sample point by passing it through the network.


2-D VISUALIZATION WITH NONLINEAR AUTOENCODER

2-D VISUALIZATION WITH PCA

Figure 2.11: A depiction of the typical difference between the embeddings created by nonlinear autoencoders and principal component analysis (PCA). Nonlinear and deep autoencoders are often able to separate out the entangled class structures in the underlying data, which is not possible within the constraints of linear transformations like PCA. This occurs because individual classes are often populated on curved manifolds in the original space, which would appear mixed when looking at a data in any 2-dimensional cross-section unless one is willing to warp the space itself. The figure above is drawn for illustrative purposes only and does not represent a specific data set.

2. Neural networks allow more power and flexibility in the nonlinear data reduction by varying on the number and type of layers used in intermediate stages. Furthermore, by choosing specific types of activation functions in particular layers, one can engineer the nature of the reduction to the properties of the data. For example, it makes sense to use a logistic output layer with logarithmic loss for a binary data set.

It is possible to achieve extraordinarily compact reductions by using this approach. For example, the work in [198] shows how one can convert a 784-dimensional representation of the pixels of an image into a 6-dimensional reduction with the use of deep autoencoders. Greater reduction is always achieved by using nonlinear units, which implicitly map warped manifolds into linear hyperplanes. The superior reduction in these cases is because it is easier to thread a warped surface (as opposed to a linear surface) through a larger number of points. This property of nonlinear autoencoders is often used for 2-dimensional visualizations of the data by creating a deep autoencoder in which the most compact hidden layer has only two dimensions. These two dimensions can then be mapped on a plane to visualize the points. In many cases, the class structure of the data is exposed in terms of well-separated clusters.

An illustrative example of the typical behavior of real data distributions is shown in Figure 2.11, in which the 2-dimensional mapping created by a deep autoencoder seems to clearly separate out the different classes. On the other hand, the mapping created by PCA does not seem to separate the classes well. Figure 2.9, which provides a nonlinear spiral mapped to a linear hyperplane, clarifies the reason for this behavior. In many cases, the data may contain heavily entangled spirals (or other shapes) that belong to different classes. Linear dimensionality reduction methods cannot attain clear separation because nonlinearly entangled shapes are not linearly separable. On the other hand, deep autoencoders with nonlinearity are far more powerful and able to disentangle such shapes. Deep autoencoders can sometimes be used as alternatives to other robust visualization methods like t-distributed stochastic neighbor embedding (t-SNE) [305]. Although t-SNE can often provide better performance[5] for visualization (because it is specifically designed for visualization rather than dimensionality reduction), the advantage of an autoencoder over t-SNE is that it is easier to generalize to out-of-sample data. When new data points are received, they can simply be passed through the encoder portion of the autoencoder in order to add them to the current set of visualized points. A specific example of a visualization of a high-dimensional document collection with an autoencoder is provided in [198].

It is, however, possible to go too far and create representations that are not useful. For example, one can compress a very high-dimensional data point into a single dimension, which reconstructs a point from the training data very well but gives high reconstruction error for test data. In other words, the neural network has found a way to memorize the data set without sufficient ability to create reduced representations of unseen points. Therefore, even for unsupervised problems like dimensionality reduction, it is important to keep aside some points as a *validation set*. The points in the validation set are not used during training. One can then quantify the difference in reconstruction error between the training and validation data. Large differences in reconstruction error between the training and validation data are indicative of overfitting. Another issue is that deep networks are harder to train, and therefore tricks like *pretraining* are important. These tricks will be discussed in Chapters 3 and 4.

2.5.4 Application to Outlier Detection

Dimensionality reduction is closely related to outlier detection, because outlier points are hard to encode and decode without losing substantial information. It is a well-known fact that if a matrix D is factorized as $D \approx D' = UV^T$, then the low-rank matrix D' is a de-noised representative of the data. After all, the compressed representation U captures only the regularities in the data, and is unable to capture the unusual variations in specific points. As a result, reconstruction to D' misses all these unusual variations.

The absolute values of the entries of $(D - D')$ represent the outlier scores of the matrix entries. Therefore, one can use this approach to find outlier entries, or add the squared scores of the entries in each row of D to find the outlier score of that row. Therefore, one can identify outlier data points. Furthermore, by adding the squared scores in each column of D, one can find outlier features. This is useful for applications like feature selection in clustering, where a feature with a large outlier score can be removed because it adds noise to the clustering. Although we have provided the description above with the use of matrix factorization, any type of autoencoder can be used. In fact, the construction of de-noising autoencoders is a vibrant field in its own right. Refer to the bibliographic notes.

[5] The t-SNE method works on the principle is that it is impossible to preserve all pairwise similarities and dissimilarities with the same level of accuracy in a low-dimensional embedding. Therefore, unlike dimensionality reduction or autoencoders that try to faithfully reconstruct the data, it has an asymmetric loss function in terms of how similarity is treated versus dissimilarity. This type of asymmetric loss function is particularly helpful for separating out different manifolds during visualization. Therefore, t-SNE might perform better than autoencoders at visualization.

2.5.5 When the Hidden Layer Is Broader than the Input Layer

So far, we have only discussed cases in which the hidden layer has fewer units than the input layer. It makes sense for the hidden layer to have fewer units than the input layer when one is looking for a compressed representation of the data. A constricted hidden layer forces dimensionality reduction, and the loss function is designed to avoid information loss. Such representations are referred to as *undercomplete representations*, and they correspond to the traditional use-case of autoencoders.

What about the case when the number of hidden units is greater than the input dimensionality? This situation corresponds to the case of *over-complete representations.* Increasing the number of hidden units beyond the number of input units makes it possible for the hidden layer to simply learn the identity function (with zero loss). Simply copying the input across the layers does not seem to be particularly useful. However, this does not occur in practice (while learning weights), especially if certain types of regularization and *sparsity constraints* are imposed on the hidden layer. Even if no sparsity constraints are imposed, and stochastic gradient descent is used for learning, the probabilistic regularization caused by stochastic gradient descent is sufficient to ensure that the hidden representation will always scramble the input before reconstructing it at the output. This is because stochastic gradient descent is a type of noise addition to the learning process, and therefore it will not be possible to learn weights that simply copy input to output as identity functions across layers. Furthermore, because of some peculiarities of the training process, a neural network almost never uses its full modeling ability, which leads to dependencies among the weights [94]. Rather, an over-complete representation may be created, although it may not have the property of sparsity (which needs to be explicitly encouraged). The next section will discuss ways of encouraging sparsity.

2.5.5.1 Sparse Feature Learning

When explicit sparsity constraints are imposed, the resulting autoencoder is referred to as a *sparse autoencoder.* A sparse representation of a d-dimensional point is a k-dimensional point in which $k \gg d$ and most of the values in the sparse representation are 0s. Sparse feature learning has tremendous applicability to many settings like image data, where the learned features are often intuitively more interpretable from an application-specific perspective. Furthermore, points with a variable amount of information will be naturally represented by having varying numbers of nonzero feature values. This type of property is naturally true in some *input* representations like documents; documents with more information will have more non-zero features (word frequencies) when represented in multidimensional format. However, if the available input is not sparse to begin with, there are often benefits in creating a sparse transformation where such a flexibility of representation exists. Sparse representations also enable the effective use of particular types of efficient algorithms that are highly dependent on sparsity. There are many ways in which constraints might be enforced on the hidden layer to create sparsity. One approach is to add biases to the hidden layer, so that many units are encouraged to be zeros. Some examples are as follows:

1. One can impose an L_1-penalty on the activations in the hidden layer to force sparse activations. The notion of L_1-penalties for creating sparse solutions (in terms of either weights or hidden units) is discussed in Sections 4.4.2 and 4.4.4 of Chapter 4. In such a case, backpropagation must also propagate the gradient of this penalty in the backwards direction. Surprisingly, this natural alternative is rarely used.

2. One can allow only the top-r activations in the hidden layer to be nonzero for $r \leq k$. In such a case, backpropagation only backpropagates through the activated units. This approach is referred to as the r-sparse autoencoder [309].

3. Another approach is the *winner-take-all* autoencoder [310], in which only a fraction f of the activations of *each* hidden unit are allowed over the *whole training data*. In this case, the top activations are computed across training examples, whereas in the previous case the top activations are computed across a hidden layer for a single training example. Therefore node-specific thresholds need to be estimated using the statistics of a minibatch. The backpropagation algorithm needs to propagate the gradient only through the activated units.

Note that the implementations of the competitive mechanisms are almost like ReLU activations with adaptive thresholds. Refer to the bibliographic notes for pointers and more details of these algorithms.

2.5.6 Other Applications

Autoencoders form the workhorse of unsupervised learning in the neural network domain. They are used for a host of applications, which will be discussed later in the book. After training an autoencoder, it is not necessary to use both the encoder and decoder portions. For example, when using the approach for dimensionality reduction, one can use the encoder portion in order to create the reduced representations of the data. The reconstructions of the decoder might not be required at all.

Although an autoencoder naturally removes noise (like almost any dimensionality reduction method), one can enhance the ability of the autoencoder to remove specific types of noise. To perform the training of a *de-noising autoencoder*, a special type of training is used. First, some noise is added to the training data before passing it through the neural network. The distribution of the added noise reflects the analyst's understanding of the natural types of noise in that particular data domain. However, the loss is computed with respect to the *original* training data instances rather than their corrupted versions. The original training data are relatively clean, although one expects the test instances to be corrupted. Therefore, the autoencoder learns to recover clean representations from corrupted data. A common approach to add noise is to randomly set a fraction f of the inputs to zeros [506]. This approach is especially effective when the inputs are binary. The value of f regulates the level of corruption in the inputs. One can either fix f or even allow f to randomly vary over different training instances. In some cases, when the input is real-valued, Gaussian noise is also used. More details of the de-noising autoencoder are provided in Section 4.10.2 of Chapter 4. A closely related autoencoder is the *contractive autoencoder*, which is discussed in Section 4.10.3.

Another interesting application of the autoencoder is one in which we use only the *decoder* portion of the network to create artistic renderings. This idea is based on the notion of *variational autoencoders* [242, 399], in which the loss function is modified to impose a specific structure on the hidden layer. For example, one might add a term to the loss function to enforce the fact that the hidden variables are drawn from a Gaussian distribution. Then, one might repeatedly draw samples from this Gaussian distribution and use only the decoder portion of the network in order to generate samples of the original data. The generated samples often represent realistic samples from the original data distribution.

A closely related model is that of *generative adversarial networks*, which have become increasingly popular in recent years. These models pair the learning of a decoding network with that of an adversarial discriminator in order to create generative samples of a data set. Generative adversarial networks are used frequently with image, video, and text data, and they generate artistic renderings of images and videos, which often have the flavor of an AI that is "dreaming." These methods can be used for image-to-image translation as well. The variational autoencoder is discussed in detail in Section 4.10.4 of Chapter 4. Generative adversarial networks are discussed in Section 10.4 of Chapter 10.

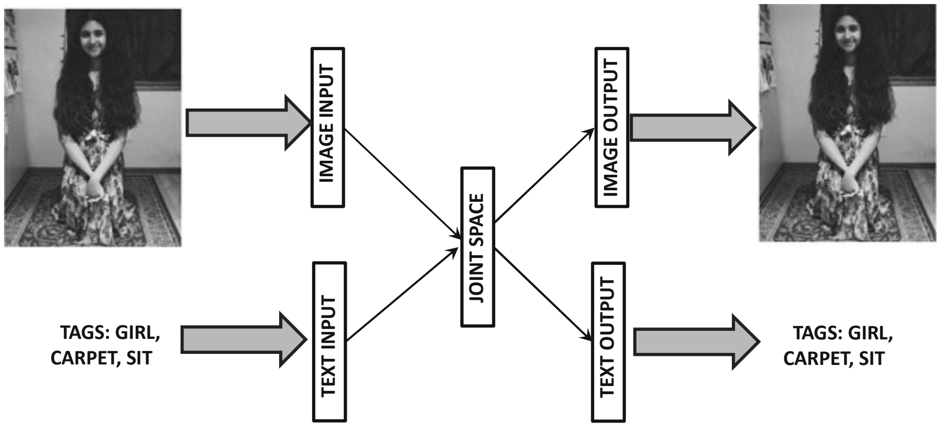


Figure 2.12: Multimodal embedding with autoencoders

One can use an autoencoder for embedding multimodal data in a joint latent space. Multimodal data is essentially data in which the input features are heterogeneous. For example, an image with descriptive tags can be considered multimodal data. Multimodal data pose challenges to mining applications because different features require different types of processing and treatment. By embedding the heterogeneous attributes in a unified space, one is removing this source of difficulty in the mining process. An autoencoder can be used to embed the heterogeneous data into a joint space. An example of such a setting is shown in Figure 2.12. This figure shows an autoencoder with only a single layer, although one might have multiple layers in general [357, 468]. Such joint spaces can be very useful in a variety of applications.

Finally, autoencoders are used to improve the learning process in neural networks. A specific example is that of *pretraining* in which an autoencoder is used to initialize the weights of a neural network. The basic idea is that learning the manifold structure of a data set is also useful for supervised learning applications like classification. This is because the features that define the manifold of a data set are often likely to be more informative in terms of their relationships to different classes. Pretraining methods are discussed in Section 4.7 of Chapter 4.

2.5.7 Recommender Systems: Row Index to Row Value Prediction

One of the most interesting applications of matrix factorization is the design of neural architectures for recommender systems. Consider an $n \times d$ ratings matrix D with n users and d items. The (i, j)th entry of the matrix is the rating of user i for item j. However, most entries in the matrix are not specified, which creates difficulties in using a traditional autoencoder architecture. This is because traditional autoencoders are designed for fully specified matrices, in which a single *row* of the matrix is input at one time. On the other hand, recommender systems are inherently suited to *elementwise* learning, in which a very small subset of ratings from a row may be available. As a practical matter, one might consider the input to a recommender system as a set of triplets of the following form:

$$\langle \text{RowId} \rangle,\ \langle \text{ ColumnId } \rangle,\ \langle \text{ Rating } \rangle$$

As in traditional forms of matrix factorization, the ratings matrix D is given by UV^T. However, the difference is that one must learn U and V using triplet-centric input because all entries of D are not observed. Therefore, a natural approach is to create an architecture in which the inputs are not affected by the missing entries and can be uniquely specified. The input layer contains n input units, which is the same as the number of rows (users). However, the input is a one-hot encoded index of the row identifier. Therefore, only one entry of the input takes on the value of 1, with the remaining entries taking on values of 0. The hidden layer contains k units, where k is the rank of the factorization. Finally, the output layer contains d units, where d is the number of columns (items). The output is a vector containing the d ratings (even though only a small subset of them are observed). The goal is to train the neural network with an incomplete data matrix D so that the network outputs all the ratings corresponding to a one-hot encoded row index after it is input. The approach is to be able to reconstruct the data by learning the ratings associated with each row index.

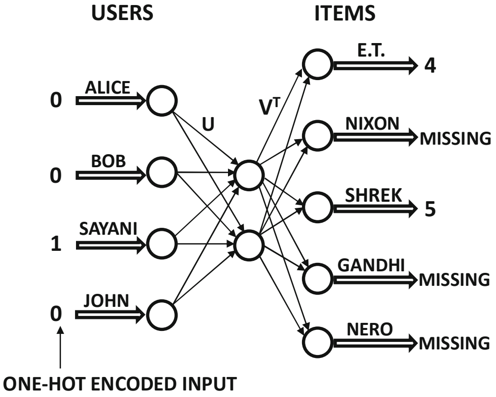


Figure 2.13: Row-index-to-value encoder for matrix factorization with missing values.

Consider a setting in which the $n \times k$ input-to-hidden matrix is U, and the $k \times d$ hidden-to-output matrix is V^T. The entries of the matrix U are denoted by u_{iq}, and those of the matrix V are denoted by v_{jq}. Assume that all activation functions are linear. Furthermore, let the one-hot encoded input (row) vector for the rth user be $\overline{e}_r$. This row vector contains n dimensions in which only the rth value is 1, and the remaining values are zeros. The loss function is the sum of the squares of the errors in the output layer. However, because of the missing entries, not all output nodes have an observed output value, and the updates are performed only with respect to entries that are known. The overall architecture of this neural network is illustrated in Figure 2.13. For any particular row-wise input we are really training on a neural network that is a subset of this base network, depending on which entries are specified. However, it is possible to give *predictions* for all outputs in the network (even though a loss function cannot be computed for missing entries). Since a neural network with linear activations performs matrix multiplications, it is easy to see that the vector of d outputs for the rth user is given by $\overline{e}_r UV^T$. In essence, pre-multiplication with $\overline{e}_r$ pulls out the rth row in the matrix UV^T. These values appear at the output layer and represent the item-wise ratings predictions for the rth user. Therefore, all feature values are reconstructed in one shot.

How is training performed? The main attraction of this architecture is that one can perform the training either in row-wise fashion or in element-wise fashion. When performing the training in row-wise fashion, the one-hot encoded index for that row is input, and all *specified* entries of that row are used to compute the loss. The backpropagation algorithm is done only starting at output nodes where the values are specified. From a theoretical point of view, each row is being trained on a slightly different neural network with a subset of the base output nodes (depending on which entries are observed), although the weights for the different neural networks are shared. This situation is shown in Figure 2.14, where the neural networks for the movie ratings of two different users, Bob and Sayani, are shown. For example, Bob is missing a rating for *Shrek*, as a result of which the corresponding output node is missing. However, since both users have specified a rating for $E.T.$, the k-dimensional hidden factors for this movie in matrix V will be updated during backpropagation when either Bob or Sayani is processed. This ability to train using only a subset of the output nodes is sometimes used as an efficiency optimization to reduce training time even in cases where all outputs are specified. Such situations occur often in binary recommendation data sets (referred to as *implicit feedback data sets*), where the vast majority of outputs are zeros. In such cases, only a subset of zeros is sampled for training in matrix factorization methods [4]. This technique is referred to as *negative sampling*. A specific example is that of neural models for natural language processing like *word2vec*.

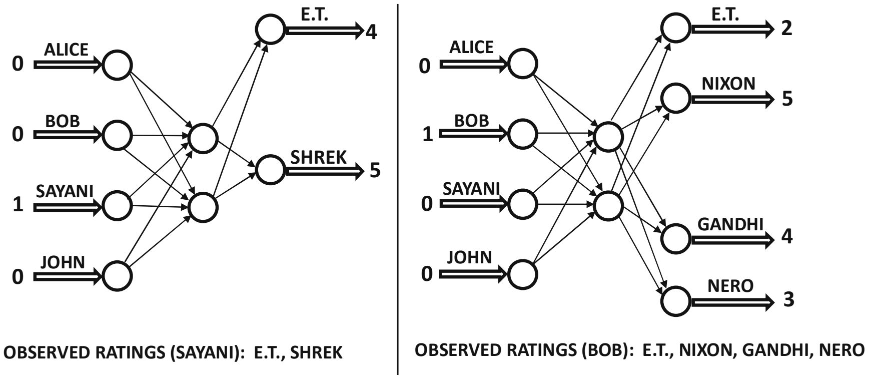

0
ALICE
0
BOB
1
SAYANI
0
JOHN
E.T.
4
SHREK
5
OBSERVED RATINGS (SAYANI): E.T., SHREK
0
ALICE
1
BOB
0
SAYANI
0
JOHN
E.T.
2
NIXON
5
GANDHI
4
NERO
3
OBSERVED RATINGS (BOB): E.T., NIXON, GANDHI, NERO

Figure 2.14: Dropping output nodes based on missing values. Output nodes are missing only at training time. At prediction time, all output nodes are materialized. One can achieve similar results with an RBM architecture as well (cf. Figure 6.5 of Chapter 6).

It is also possible to perform the training in element-wise fashion, where a single triplet is input. In such a case, the loss is computed only with respect to a single column index specified in the triplet. Consider the case where the row index is i, and the column index is j. In this specific case, and the single error computed at the output layer is $y - \hat{y} = e_{ij}$. the backpropagation algorithm essentially updates the weights on all the k paths from node j in the output layer to the node i in the input layer. These k paths pass through the k nodes in the hidden layer. It is easy to show that the update along the qth such path is as follows:

$$u_{iq} \Leftarrow u_{iq}(1 - \alpha\lambda) + \alpha e_{ij} v_{jq}$$
$$v_{jq} \Leftarrow v_{jq}(1 - \alpha\lambda) + \alpha e_{ij} u_{iq}$$

Here, α is the step-size, and λ is the regularization parameter. *These updates are identical to those used in stochastic gradient descent for matrix factorization in recommender systems.* However, an important advantage of the use of the neural architecture (over traditional matrix factorization) is that we can vary on it in so many different ways in order to enforce different properties. For example, for matrices with binary data, we can use a logistic layer in the output. This will result in *logistic matrix factorization*. We can incorporate multiple hidden layers to create more powerful models. For matrices with categorical entries (and count-centric weights attached to entries), one can use a softmax layer at the very end. This will result in *multinomial matrix factorization*. To date, we are not aware of a formal description of multinomial matrix factorization in traditional machine learning; yet, it is a simple modification of the neural architecture (implicitly) used by recommender systems. In general, it is often easy to stumble upon sophisticated models when working with neural architectures because of their modular structure. One does not need to relate the neural architecture to a conventional machine learning model, as long as empirical results establish its robustness. For example, two variations of the (highly successful) skip-gram model of *word2vec* [325, 327] correspond to logistic and multinomial matrix factorizations of word-context matrices; yet, this fact does not seem to be pointed[6] out by either by the original authors of *word2vec* [325, 327] or the broader community. In conventional machine learning, models like logistic matrix factorization are considered relatively esoteric techniques that have only recently been proposed [224]; yet, these sophisticated models represent relatively simple neural architectures. In general, the neural network abstraction brings practitioners (without too much mathematical training) much closer to sophisticated methods in machine learning, while being shielded from the details of optimization with the backpropagation framework.

2.5.8 Discussion

The main goal of this section was to show the benefits of the modular nature of neural networks in unsupervised learning. In our particular example, we started with a simple simulation of SVD, and then showed how minor changes to the neural architecture can achieve very different types of goals in intuitive settings. However, from an architectural point of view, the amount of effort required by the analyst to change from one architecture to the other is often a few lines of code. This is because modern softwares for building neural networks often provide templates for describing the architecture of the neural network, where each layer is specified independently. In a sense, the neural network is "built" with the well-known types of machine-learning units much like a child puts together building blocks of a toy. Backpropagation takes care of the details of optimization, while shielding the user from the complexities of the steps. Consider the significant mathematical differences between the specific details of SVD and logistic matrix factorization. Changing the output layer from linear to sigmoid (along with a change of loss function) can literally be a matter of changing a trivially small number of lines of code without affecting most of the remaining code (which usually isn't large anyway). This type of modularity is tremendously useful in application-centric settings. Autoencoders are also related to another type of unsupervised learning method, known as a Restricted Boltzmann Machines (RBM) (cf. Chapter 6). These methods can also be used for recommender systems, as discussed in Section 6.5.2 of Chapter 6.

[6] The work in [287] does point out a number of *implicit* relationships with matrix factorization, but not the more direct ones pointed out in this book. Some of these relationships are also pointed out in [6].

2.6 Word2vec: An Application of Simple Neural Architectures

Neural network methods have been used to learn word embeddings of text data. In general, one can create embeddings of both documents and words by using methods like SVD. In SVD, an $n \times d$ matrix of document-word counts is created. This matrix is then factorized as $D \approx UV$. Here, U and V are $n \times k$ and $k \times d$ matrices, respectively. The rows of U contain embeddings of documents and the columns of V contain embeddings of words. Note that we have changed the notation slightly from the previous section (by using UV instead of UV^T for factorization), because it is more convenient for this section.

SVD is, however, a method that treats a document as a bag of words. Here, we are interested in factorizations that use the sequential orderings among words to create embeddings. The focus here is to create *word* embeddings rather than *document* embeddings. The family of *word2vec* methods is well suited to creating word embeddings. The two variants of *word2vec* are as follows:

1. *Predicting target words from contexts:* This model tries to predict the ith word, w_i, in a sentence using a window of width t around the word. Therefore, the words $w_{i-t}w_{i-t+1}\ldots w_{i-1}w_{i+1}\ldots w_{i+t-1}w_{i+t}$ are used to predict the target word w_i. This model is also referred to as the *continuous bag-of-words (CBOW) model*.

2. *Predicting contexts from target words:* This model tries to predict the context $w_{i-t}w_{i-t+1}\ldots w_{i-1}w_{i+1}\ldots w_{i+t-1}w_{i+t}$ around word w_i, given the ith word in the sentence, denoted by w_i. This model is referred to as the *skip-gram model*. There are, however, two ways in which one can perform this prediction. The first technique is a *multinomial* model which predicts one word out of d outcomes. The second model is a Bernoulli model, which predicts whether or not each context is present for a particular word. The second model uses *negative sampling* of contexts for better efficiency and accuracy.

Each of these methods will be discussed in this section.

2.6.1 Neural Embedding with Continuous Bag of Words

In the continuous bag-of-words (CBOW) model, the training pairs are all context-word pairs in which a window of context words is input, and a single target word is predicted. The context contains $2 \cdot t$ words, corresponding to t words both before and after the target word. For notational ease, we will use the length $m = 2 \cdot t$ to define the length of the context. Therefore, the input to the system is a set of m words. Without loss of generality, let the subscripts of these words be numbered so that they are denoted by $w_1 \ldots w_m$, and let the target (output) word in the middle of the context window be denoted by w. Note that w can be viewed as a categorical variable with d possible values, where d is the size of the lexicon. The goal of the neural embedding is to compute the probability $P(w|w_1 w_2 \ldots w_m)$ and maximize the product of these probabilities over all training samples.

The overall architecture of this model is illustrated in Figure 2.15. In the architecture, we have a single input layer with $m \times d$ nodes, a hidden layer with p nodes, and an output layer with d nodes. The nodes in the input layer are clustered into m different groups, each of which has d units. Each group with d input units is the one-hot encoded input vector of one of the m context words being modeled by CBOW. Only one of these d inputs will be 1 and the remaining inputs will be 0. Therefore, one can represent an input x_{ij} with two indices corresponding to contextual position and word identifier. Specifically, the input $x_{ij} \in \{0, 1\}$ contains two indices i and j in the subscript, where $i \in \{1 \dots m\}$ is the position of the context, and $j \in \{1 \dots d\}$ is the identifier of the word.

The hidden layer contains p units, where p is the dimensionality of the hidden layer in *word2vec*. Let $h_1, h_2, \dots h_p$ be the outputs of the hidden layer nodes. Note that each of the d words in the lexicon has m different representatives in the input layer corresponding to the m different context words, but the weight of each of these m connections is the same. Such weights are referred to as shared. Sharing weights is a common trick used for regularization in neural networks, when one has specific insight about the domain at hand. Let the shared weight of each connection from the jth word in the lexicon to the qth hidden layer node be denoted by u_{jq}. Note that each of the m groups in the input layer has connections to the hidden layer that are defined by the same $d \times p$ weight matrix U. This situation is shown in Figure 2.15.

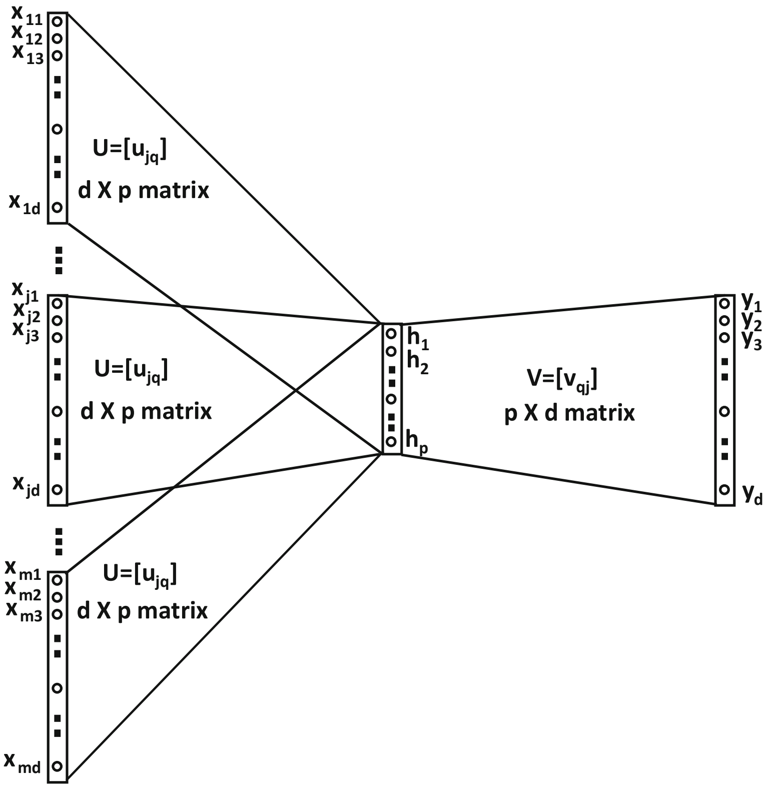


Figure 2.15: Word2vec: The CBOW model. Note the similarities and differences with Figure 2.13, which uses a single set of inputs with a linear output layer. One could also choose to collapse the m sets of d input nodes into a single set of d inputs, and aggregate the m one-hot encoded inputs in a single context window to achieve the same effect. In such a case, the input is no longer one-hot encoded.

It is noteworthy that $\overline{u}_j = (u_{j1}, u_{j2}, \dots u_{jp})$ can be viewed as the p-dimensional embedding of the jth input word over the entire corpus, and $\overline{h} = (h_1 \dots h_p)$ provides the embedding of a specific instantiation of an input context. Then, the output of the hidden layer is obtained by averaging the embeddings of the words present in the context. In other words, we have the following:

$$h_q = \sum_{i=1}^{m} \left[\sum_{j=1}^{d} u_{jq} x_{ij} \right] \quad \forall q \in \{1 \ldots p\} \tag{2.46}$$

Many expositions use an additional factor of m in the denominator on the right-hand side, although this type of multiplicative scaling (with a constant) is inconsequential. One can also write this relationship in vector form:

$$\overline{h} = \sum_{i=1}^{m} \sum_{j=1}^{d} \overline{u}_j x_{ij} \tag{2.47}$$

In essence, the one-hot encodings of the input words are aggregated, which implies that the ordering of the words within the window of size m does not affect the output of the model. This is the reason that the model is referred to as the continuous bag-of-words model. However, sequential information is still used by virtue of restricting the prediction to a context window.

The embedding $(h_1 \ldots h_p)$ is used to predict the probability that the target word is one of each of the d outputs with the use of the softmax function. The weights in the output layer are parameterized with a $p \times d$ matrix $V = [v_{qj}]$. The jth column of V is denoted by $\overline{v}_j$. The output after applying softmax creates d output values $\hat{y}_1 \ldots \hat{y}_d$, which are real values in $(0, 1)$. These real values sum to 1 because they can be interpreted as probabilities. The *ground-truth* value of only one of the outputs $y_1 \ldots y_d$ is 1 and the remaining values are 0 for a given training instance. One can write this condition as follows:

$$y_j = \begin{cases} 1 & \text{if the target word } w \text{ is the } j\text{th word} \\ 0 & \text{otherwise} \end{cases} \tag{2.48}$$

The softmax function computes the probability $P(w|w_1 \ldots w_m)$ of the one-hot encoded ground-truth outputs y_j as follows:

$$\hat{y}_j = P(y_j = 1|w_1 \ldots w_m) = \frac{\exp(\sum_{q=1}^{p} h_q v_{qj})}{\sum_{k=1}^{d} \exp(\sum_{q=1}^{p} h_q v_{qk})} \tag{2.49}$$

Note that this probabilistic form of the prediction is based on the softmax layer (cf. Section 1.2.1.4 of Chapter 1). For a particular target word $w = r \in \{1 \ldots d\}$, the loss function is given by $L = -\log[P(y_r = 1|w_1 \ldots w_m)] = -\log(\hat{y}_r)$. The use of the negative logarithm turns the multiplicative likelihoods over different training instances into an additive loss function using log-likelihoods.

The updates are defined by using the backpropagation algorithm, as training instances are passed through the neural network one by one. First, the derivative of the aforementioned loss function can be used to update the gradients of the weight matrix V in the output layer. Then, backpropagation can be used to update the weight matrix U between the input and hidden layer. The update equations with learning rate α are as follows:

$$\overline{u}_i \Leftarrow \overline{u}_i - \alpha \frac{\partial L}{\partial \overline{u}_i} \quad \forall i$$

$$\overline{v}_j \Leftarrow \overline{v}_j - \alpha \frac{\partial L}{\partial \overline{v}_j} \quad \forall j$$

One can compute the partial derivatives of this expression easily [325, 327, 404].

The probability of making a mistake in prediction on the jth word in the lexicon is defined by $|y_j - \hat{y}_j|$. However, we use *signed* mistakes ϵ_j, in which only the correct word with $y_j = 1$ is given a positive mistake value, while all the other words in the lexicon receive negative mistake values. This is achieved by dropping the modulus:

$$\epsilon_j = y_j - \hat{y}_j \tag{2.50}$$

Note that ϵ_j can also be shown to be equal to the negative of the derivative of the cross-entropy loss with respect to jth input into the softmax layer (which is $\overline{h} \cdot \overline{v}_j$). This result is shown in Section 3.2.5.1 of the next chapter and is useful in deriving the backpropagation updates. Then, the updates[7] for a particular input context and output word are as follows:

$$\begin{aligned}
\overline{u}_i &\Leftarrow \overline{u}_i + \alpha \sum_{j=1}^{d} \epsilon_j \overline{v}_j \quad [\forall \text{ words } i \text{ present in context window}] \\
\overline{v}_j &\Leftarrow \overline{v}_j + \alpha \epsilon_j \overline{h} \qquad [\forall j \text{ in lexicon}]
\end{aligned}$$

Here, $\alpha > 0$ is the learning rate. Repetitions of the same word i in the context window trigger multiple updates of $\overline{u}_i$. It is noteworthy that the input embeddings of the context words are aggregated in both updates, considering the fact that $\overline{h}$ aggregates input embeddings according to Equation 2.47. This type of aggregation has a smoothing effect on the CBOW model, which is particularly helpful with smaller data sets.

The training examples of context-target pairs are presented one by one, and the weights are trained to convergence. It is noteworthy that the *word2vec* model provides not one but two different embeddings corresponding to the p-dimensional rows of the matrix U and the p-dimensional columns of the matrix V. The former type of embedding of words is referred to as the *input* embedding, whereas the latter is referred to as the *output* embedding. In the CBOW model, the input embedding represents context, and therefore it makes sense to use the output embedding. However, the input embedding (or the sum/concatenation of input and output embeddings) can also be helpful for many tasks.

2.6.2 Neural Embedding with Skip-Gram Model

In the skip-gram model, the target words are used to predict the m context words. Therefore, we have one input word and m outputs. One issue with the CBOW model is that the averaging effect of the input words in the context window (which creates the hidden representation) has a (helpful) smoothing effect with less data, but fails to take full advantage of a larger amount of data. The skip-gram model is the technique of choice when a large amount of data is available.

The skip-gram model uses a single target word w as the input and outputs the m context words denoted by $w_1 \ldots w_m$. Therefore, the goal is to estimate $P(w_1, w_2 \ldots w_m | w)$, which is different from the quantity $P(w|w_1 \ldots w_m)$ estimated in the CBOW model. As in the case of the continuous bag-of-words model, we can use one-hot encoding of the (categorical) input and outputs in the skip-gram model. After such an encoding, the skip-gram model will have d binary inputs denoted by $x_1 \ldots x_d$ corresponding to the d possible values of the single input word. Similarly, the output of each training instance is encoded as $m \times d$ values $y_{ij} \in \{0, 1\}$, where i ranges from 1 to m (size of context window), and j ranges

[7] There is a slight abuse of notation in the updates adding $\overline{u}_i$ and $\overline{v}_j$. This is because $\overline{u}_i$ is a row vector and $\overline{v}_j$ is a column vector. Throughout this section, we omit the explicit transposition of one of these two vectors to avoid notational clutter, since the updates are intuitively clear.

from 1 to d (lexicon size). Each $y_{ij} \in \{0, 1\}$ indicates whether the ith contextual word takes on the jth possible value for that training instance. However, the (i, j)th output node only computes a soft probability value $\hat{y}_{ij} = P(y_{ij} = 1|w)$. Therefore, the probabilities $\hat{y}_{ij}$ in the output layer for fixed i and varying j sum to 1, since the ith contextual position takes on exactly one of the d words. The hidden layer contains p units, the outputs are denoted by $h_1 \ldots h_p$. Each input x_j is connected to all the hidden nodes with a $d \times p$ matrix U. Furthermore, the p hidden nodes are connected to each of the m groups of d output nodes with the same set of shared weights. This set of shared weights between the p hidden nodes and the d output nodes of each of the context words is defined by the $p \times d$ matrix V. Note that the input-output structure of the skip-gram model is an inverted version of the input-output structure of the CBOW model. The neural architecture of the skip-gram model is illustrated in Figure 2.16(a). However, in the case of the skip-gram model, one can collapse the m identical outputs into a single output, and achieve the same results simply by using a *particular type of mini-batching* during stochastic gradient descent. In particular, all elements of a single context window are always forced to belong to the same mini-batch. This architecture is shown in Figure 2.16(b). Since the value of m is small, this specific type of mini-batching has a very limited effect, and the simplified architecture of Figure 2.16(b) is sufficient to describe the model whether or not any specific type of mini-batching is used. For the purpose of further discussion, we will use the architecture of Figure 2.16(a).

The output of the hidden layer can be computed from the input layer using the $d \times p$ matrix of weights $U = [u_{jq}]$ between the input and hidden layer as follows:

$$h_q = \sum_{j=1}^{d} u_{jq} x_j \qquad \forall q \in \{1 \ldots p\} \tag{2.51}$$

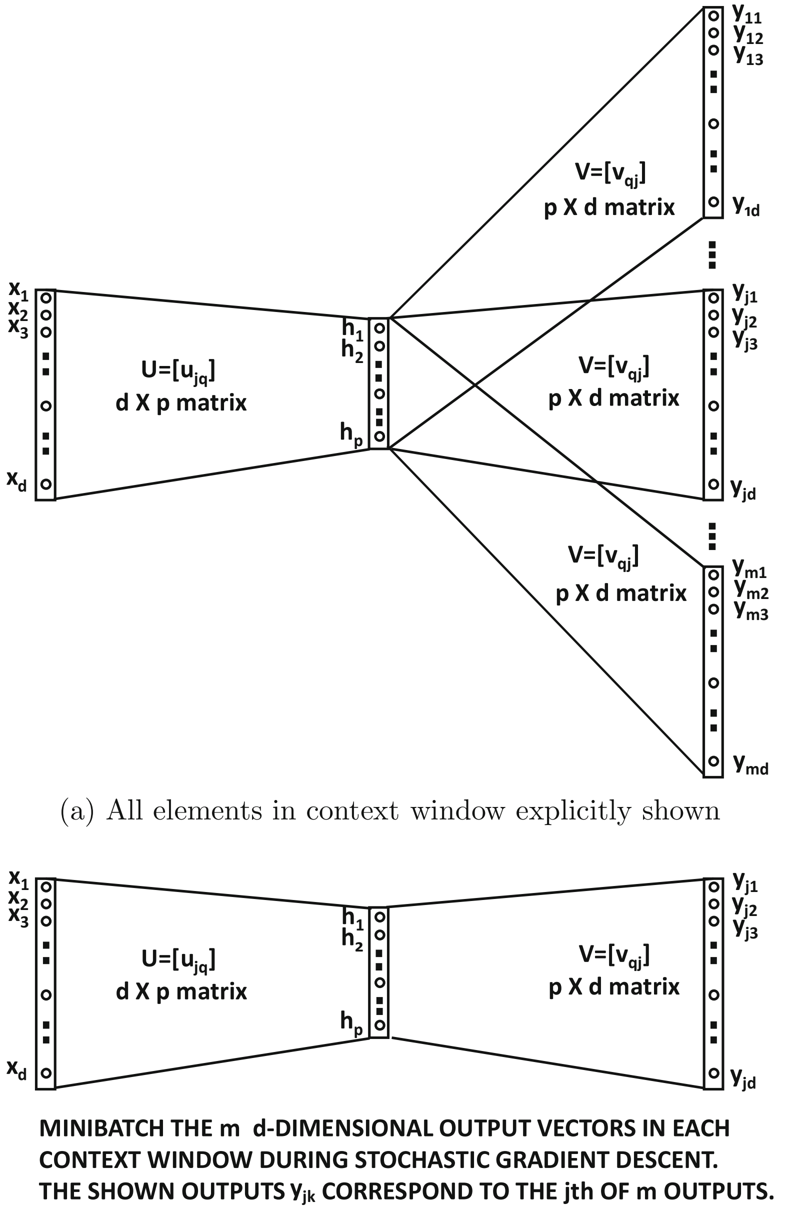
The above equation has a simple interpretation because of the one-hot encoding of the input word w in terms of $x_1 \ldots x_d$. If the input word w is the rth word, then one simply copies u_{rq} to the qth node of the hidden layer for each $q \in \{1 \ldots p\}$. In other words, the rth row $\overline{u}_r$ of U is copied to the hidden layer. As discussed above, the hidden layer is connected to m groups of d output nodes, each of which is connected to the hidden layer with a $p \times d$ matrix $V = [v_{qj}]$. Each of these m groups of d output nodes computes the probabilities of the various words for a particular context word. The jth column of V is denoted by $\overline{v}_j$ and represents the output embedding of the jth word. The output $\hat{y}_{ij}$ is the probability that the word in the ith context position takes on the jth word of the lexicon. However, since the same matrix V is shared by all groups, the neural network predicts the same multinomial distribution for each of the context words. Therefore, we have the following:

$$\hat{y}_{ij} = P(y_{ij} = 1|w) = \underbrace{\frac{\exp(\sum_{q=1}^{p} h_q v_{qj})}{\sum_{k=1}^{d} \exp(\sum_{q=1}^{p} h_q v_{qk})}}_{\text{Independent of context position } i} \qquad \forall i \in \{1 \ldots m\} \tag{2.52}$$

Note that the probability $\hat{y}_{ij}$ is the same for varying i and fixed j, since the right-hand side of the above equation does not depend on the exact location i in the context window.

The loss function for the backpropagation algorithm is the negative of the log-likelihood values of the ground truth $y_{ij} \in \{0, 1\}$ of a training instance. This loss function L is given by the following:

$$L = -\sum_{i=1}^{m} \sum_{j=1}^{d} y_{ij} \log(\hat{y}_{ij}) \tag{2.53}$$



(a) All elements in context window explicitly shown

(b) All elements in context window not explicitly shown

Figure 2.16: Word2vec: The skip-gram model. Note the similarity with Figure 2.13, which uses a single set of linear outputs. One could also choose to collapse the m sets of d output nodes in (a) into a single set of d outputs, and mini-batch the m instances in a single context window during stochastic gradient descent to achieve the same effect. All elements in the mini-batch are explicitly shown in (a), whereas the elements of the mini-batch are not explicitly shown in (b). However, both are equivalent as long as the nature of mini-batching is respected.

Note that the value outside the logarithm is a ground-truth binary value, whereas the value inside the logarithm is a predicted (probability) value. Since y_{ij} is one-hot encoded for fixed i and varying j, the objective function has only m non-zero terms. For each training instance, this loss function is used in combination with backpropagation to update the weights of the connections between the nodes. The update equations with learning rate α are as follows:

$$\overline{u}_i \Leftarrow \overline{u}_i - \alpha \frac{\partial L}{\partial \overline{u}_i} \quad \forall i$$
$$\overline{v}_j \Leftarrow \overline{v}_j - \alpha \frac{\partial L}{\partial \overline{v}_j} \quad \forall j$$

We state the details of the updates below after introducing some additional notations.

The probability of making a mistake in predicting the jth word in the lexicon for the ith context is defined by $|y_{ij} - \hat{y}_{ij}|$. However, we use *signed* mistakes ϵ_{ij} in which only the predicted words (positive examples) have a positive probability. This is achieved by dropping the modulus:

$$\epsilon_{ij} = y_{ij} - \hat{y}_{ij} \tag{2.54}$$

Then, the updates for a particular input word r and its output context are as follows:

$$\overline{u}_r \Leftarrow \overline{u}_r + \alpha \sum_{j=1}^{d} \left[\sum_{i=1}^{m} \epsilon_{ij} \right] \overline{v}_j \qquad \text{[Only for input word } r\text{]}$$
$$\overline{v}_j \Leftarrow \overline{v}_j + \alpha \left[\sum_{i=1}^{m} \epsilon_{ij} \right] \overline{h} \qquad \text{[For all words } j \text{ in lexicon]}$$

Here, $\alpha > 0$ is the learning rate. The p-dimensional rows of the matrix U are used as the embeddings of the words. In other words, the convention is to use the input embeddings in the rows of U rather than the output embeddings in the columns of V. It is stated in [288] that adding the input and output embeddings can help in some tasks (but hurt in others). The concatenation of the two can also be useful.

Practical Issues

Several practical issues are associated with the accuracy and efficiency of the *word2vec* framework. The embedding dimensionality, defined by the number of nodes in the hidden layer, provides the trade-off between bias and variance. Increasing the embedding dimensionality improves discrimination, but it requires a greater amount of data. In general, the typical embedding dimensionality is of the order of several hundred, although it is possible to choose dimensionalities in the thousands for very large collections. The size of the context window typically varies between 5 and 10, with larger window sizes being used for the skip-gram model as compared to the CBOW model. Using a random window size is a variant that has the implicit effect of giving greater weight to words that are placed close together. The skip-gram model is slower but it works better for infrequent words and for larger data sets.

Another issue is that the effect of frequent and less discriminative words (e.g., "*the*") can dominate the results. Therefore, a common approach is to downsample the frequent words, which improves both accuracy and efficiency. Note that downsampling frequent words has the implicit effect of increasing the context window size because dropping a word in the middle of two words brings the latter pair closer. The words that are very rare are misspellings, and it is hard to create a meaningful embedding for them without overfitting. Therefore, such words are ignored.

From a computational point of view, the updates of output embeddings are expensive. This is caused by applying the softmax over a lexicon of d words, which requires an update of each $\overline{v}_j$. Therefore, the softmax function is implemented hierarchically with *Huffman encoding* for better efficiency. We refer the reader to [325, 327, 404] for details.

Skip-Gram with Negative Sampling

An efficient alternative to the hierarchical softmax technique is a method known as *skip-gram with negative sampling (SGNS)* [327], in which both presence or absence of word-context pairs are used for training. As the name implies, the negative contexts are artificially generated by sampling words in proportion to their frequencies in the corpus (i.e., unigram distribution). This approach optimizes a different objective function from the skip-gram model, which is related to ideas from *noise contrastive estimation* [166, 333, 334].

The basic idea is that instead of directly predicting each of the m words in the context window, we try to predict whether or not each of the d words in the lexicon is present in the window. In other words, the final layer of Figure 2.16 is not a softmax prediction, but a Bernoulli layer of sigmoids. The output unit for each word at each context position in Figure 2.16 is a sigmoid providing a probability value that the position takes on that word. As the ground-truth values are also available, it is possible to use the logistic loss function over all the words. Therefore, in this point of view, even the prediction problem is defined differently. Of course, it is computationally inefficient to try to make binary predictions for all d words. Therefore, the SGNS approach uses all the positive words in a context window and a *sample* of negative words. The number of negative samples is k times the number of positive samples. Here, k is a parameter controlling the sampling rate. Negative sampling becomes essential in this modified prediction problem to avoid learning trivial weights that predict all examples to 1. In other words, we cannot choose to avoid negative samples entirely (i.e., we cannot set $k = 0$).

How does one generate the negative samples? The vanilla unigram distribution samples words in proportion to their relative frequencies $f_1 \ldots f_d$ in the corpus. Better results are obtained [327] by sampling words in proportion to $f_j^{3/4}$ rather than f_j. As in all *word2vec* models, let U be a $d \times p$ matrix representing the input embedding, and V be a $p \times d$ matrix representing the output embedding. Let $\overline{u}_i$ be the p-dimensional row of U (input embedding of ith word) and $\overline{v}_j$ be the p-dimensional column of V (output embedding of jth word). Let $\mathcal{P}$ be the set of positive target-context word pairs in a context window, and $\mathcal{N}$ be the set of negative target-context word pairs which are created by sampling. Therefore, the size of $\mathcal{P}$ is equal to the context window m, and that of $\mathcal{N}$ is $m \cdot k$. Then, the (minimization) objective function for each context window is obtained by summing up the logistic loss over the m positive samples and $m \cdot k$ negative samples:

$$O = -\sum_{(i,j)\in\mathcal{P}} \log(P[\text{Predict } (i,j) \text{ to } 1]) - \sum_{(i,j)\in\mathcal{N}} \log(P[\text{Predict } (i,j) \text{ to } 0]) \tag{2.55}$$

$$= -\sum_{(i,j)\in\mathcal{P}} \log\left(\frac{1}{1+\exp(-\overline{u}_i \cdot \overline{v}_j)}\right) - \sum_{(i,j)\in\mathcal{N}} \log\left(\frac{1}{1+\exp(\overline{u}_i \cdot \overline{v}_j)}\right) \tag{2.56}$$

This modified objective function is used in the skip-gram with negative sampling (SGNS) model in order to update the weights of U and V. SGNS is mathematically different from the basic skip-gram model discussed earlier. SGNS is not only efficient, but it also provides the best results among the different variants of skip-gram models.

What Is the Actual Neural Architecture of SGNS?

Even though the original *word2vec* paper seems to treat SGNS as an efficiency optimization of the skip-gram model, it is using a fundamentally different architecture in terms of the activation function used in the final layer. Unfortunately, the original *word2vec* paper does not explicitly point this out (and only provides the changed objective function), which causes confusion.

The modified neural architecture of SGNS is as follows. The softmax layer is no longer used in the SGNS implementation. Rather, each observed value y_{ij} in Figure 2.16 is *independently* treated as a *binary* outcome, rather than as a multinomial outcome in which the probabilistic predictions of different outcomes at a contextual position depend on one another. Instead of using softmax to create the prediction $\hat{y}_{ij}$, it uses the sigmoid activation to create probabilistic predictions $\hat{y}_{ij}$, whether each y_{ij} is 0 or 1. Then, one can add up the log loss of $\hat{y}_{ij}$ with respect to observed y_{ij} over all $m \cdot d$ possible values of (i, j) to create the full loss function of a context window. However, this is impractical because the number of zero values of y_{ij} is too large and zero values are noisy anyway. Therefore, SGNS uses negative sampling to approximate this *modified* objective function. This means that for each context window, we are backpropagating from only a subset of the $m \cdot d$ outputs in Figure 2.16. The size of this subset is $m + m \cdot k$. This is where efficiency is achieved. However, since the final layer uses binary predictions (with sigmoids), it makes the SGNS architecture fundamentally different from the vanilla skip-gram model even in terms of the basic neural network it uses (i.e., logistic instead of softmax activation). The difference between the SGNS model and the vanilla skip-gram model is analogous to the difference between the Bernoulli and multinomial models in naïve Bayes classification (with negative sampling applied only to the Bernoulli model). Obviously, one cannot be considered a direct efficiency optimization of the other.

2.6.3 Word2vec (SGNS) Is Logistic Matrix Factorization

Even though the work in [287] shows an *implicit* relationship between *word2vec* and matrix factorization, we provide a more direct relationship here. The architectures of the skip-gram models look suspiciously similar to those used in row index to value prediction in recommender systems (cf. Section 2.5.7). The use of a backpropagation from a subset of observed outputs is similar to the negative sampling idea, except that the dropping of outputs in negative sampling is performed for the purpose of efficiency. However, unlike the linear outputs of Figure 2.13 in Section 2.5.7, the SGNS model uses logistic outputs to model binary predictions. The SGNS model of *word2vec* can be simulated with logistic matrix factorization. To understand the similarity with the problem setting of Section 2.5.7, one can understand the predictions of a particular word-context window using the following triplets:

$$\langle \text{WordId} \rangle, \langle \text{Context WordId} \rangle, \langle 0/1 \rangle$$

Each context window produces $m \cdot d$ such triplets, although negative sampling only uses $m \cdot k + m$ of them, and *mini-batches* them during training. This mini-batching is another source of the difference between the architectures between Figures 2.13 and 2.16, wherein the latter has m different groups of outputs to accommodate m positive samples. However, these differences are relatively superficial, and one can still use logistic matrix factorization to represent the underlying model.

Let $B = [b_{ij}]$ be a binary matrix in which the (i,j)th value is 1 if word j occurs at least once in the context of word i in the data set, and 0 otherwise. The weight c_{ij} for any word (i,j) that occurs in the corpus is defined by the number of times word j occurs in the context of word i. The weights of the zero entries in B are defined as follows. For each row i in B we sample $k\sum_j b_{ij}$ different entries from row i, among the entries for which $b_{ij} = 0$, and the frequency with which the jth word is sampled is proportional to $f_j^{3/4}$. These are the negative samples, and one sets the weights c_{ij} for the negative samples (i.e., those for which $b_{ij} = 0$) to the number of times that each entry is sampled. As in *word2vec*, the p-dimensional embeddings of the ith word and jth context are denoted by $\overline{u}_i$ and $\overline{v}_j$, respectively. The simplest way of factorizing is to use *weighted* matrix factorization of B with the Frobenius norm:

$$\text{Minimize}_{U,V} \sum_{i,j} c_{ij}(b_{ij} - \overline{u}_i \cdot \overline{v}_j)^2 \tag{2.57}$$

Even though the matrix B is of size $O(d^2)$, this matrix factorization only has a limited number of nonzero terms in the objective function, which have $c_{ij} > 0$. These weights are dependent on co-occurrence counts, but some zero entries also have positive weight. Therefore, the stochastic gradient-descent steps only have to focus on entries with $c_{ij} > 0$. Each cycle of stochastic gradient-descent is *linear* in the number of non-zero entries, as in the SGNS implementation of *word2vec*.

However, this objective function also looks somewhat different from *word2vec*, which has a logistic form. Just as it is advisable to replace linear regression with logistic regression in supervised learning of binary targets, one can use the same trick in matrix factorization of binary matrices [224]. We can change the squared error term to the familiar likelihood term L_{ij}, which is used in logistic regression:

$$L_{ij} = \left| b_{ij} - \frac{1}{1 + \exp(\overline{u}_i \cdot \overline{v}_j)} \right| \tag{2.58}$$

The value of L_{ij} always lies in the range $(0,1)$, and higher values indicate greater likelihood (which results in a maximization objective). The modulus in the above expression flips the sign only for the negative samples in which $b_{ij} = 0$. Now, one can optimize the following objective function in minimization form:

$$\text{Minimize}_{U,V}\, J = -\sum_{i,j} c_{ij} \log(L_{ij}) \tag{2.59}$$

The main difference from the objective function (cf. Equation 2.56) of *word2vec* is that this is a global objective function over all matrix entries, rather than a local objective function over a particular context window. Using mini-batch stochastic gradient-descent in matrix factorization (with an appropriately chosen mini-batch) makes the approach almost identical to *word2vec*'s backpropagation updates.

How can one interpret this type of factorization? Instead of $B \approx UV$, we have $B \approx f(UV)$, where $f(\cdot)$ is the sigmoid function. More precisely, this is a *probabilistic* factorization in which one computes the product of matrices U and V, and then applies the sigmoid function to obtain the parameters of the Bernoulli distribution from which B is generated:

$$P(b_{ij} = 1) = \frac{1}{1 + \exp(-\overline{u}_i \cdot \overline{v}_j)} \qquad \text{[Matrix factorization analog of logistic regression]}$$

It is also easy to verify from Equation 2.58 that L_{ij} is $P(b_{ij} = 1)$ for positive samples and $P(b_{ij} = 0)$ for negative samples. Therefore, the objective function of the factorization is in the form of log-likelihood maximization. This type of logistic matrix factorization is commonly used [224] in recommender systems with binary data (e.g., user click-streams).

Gradient Descent

It is also helpful to examine the gradient-descent steps of the factorization. One can compute the derivative of J with respect to the input and output embeddings:

$$\begin{aligned}\frac{\partial J}{\partial \overline{u}_i} &= -\sum_{j:b_{ij}=1} \frac{c_{ij}\overline{v}_j}{1+\exp(\overline{u}_i \cdot \overline{v}_j)} + \sum_{j:b_{ij}=0} \frac{c_{ij}\overline{v}_j}{1+\exp(-\overline{u}_i \cdot \overline{v}_j)} \\ &= \underbrace{-\sum_{j:b_{ij}=1} c_{ij}P(b_{ij}=0)\overline{v}_j}_{\text{Positive Mistakes}} + \underbrace{\sum_{j:b_{ij}=0} c_{ij}P(b_{ij}=1)\overline{v}_j}_{\text{Negative Mistakes}}\end{aligned}$$

$$\begin{aligned}\frac{\partial J}{\partial \overline{v}_j} &= -\sum_{i:b_{ij}=1} \frac{c_{ij}\overline{u}_i}{1+\exp(\overline{u}_i \cdot \overline{v}_j)} + \sum_{i:b_{ij}=0} \frac{c_{ij}\overline{u}_i}{1+\exp(-\overline{u}_i \cdot \overline{v}_j)} \\ &= \underbrace{-\sum_{i:b_{ij}=1} c_{ij}P(b_{ij}=0)\overline{u}_i}_{\text{Positive Mistakes}} + \underbrace{\sum_{i:b_{ij}=0} c_{ij}P(b_{ij}=1)\overline{u}_i}_{\text{Negative Mistakes}}\end{aligned}$$

The optimization procedure uses gradient descent to convergence:

$$\begin{aligned}\overline{u}_i &\Leftarrow \overline{u}_i - \alpha\frac{\partial J}{\partial \overline{u}_i} \quad \forall i \\ \overline{v}_j &\Leftarrow \overline{v}_j - \alpha\frac{\partial J}{\partial \overline{v}_j} \quad \forall j\end{aligned}$$

It is noteworthy that the derivatives can be expressed in terms of the probabilities of making mistakes in predicting b_{ij}. This is common in gradient descent with log-likelihood optimization. It is also noteworthy that the derivative of the SGNS objective in Equation 2.56 yields a similar form of the gradient. The only difference is that the derivative of the SGNS objective is expressed over a smaller batch of instances, defined by a context window. We can also solve the probabilistic matrix factorization with mini-batch stochastic gradient descent. With an appropriate choice of the mini-batch, the stochastic gradient descent of matrix factorization becomes identical to the backpropagation update of SGNS. The only difference is that SGNS samples negative entries *for each set of updates* on the fly, whereas matrix factorization fixes the negative samples up front. Of course, on-the-fly sampling can also be used with matrix factorization updates. The similarity of SGNS to matrix factorization can also be inferred by observing that the architecture of Figure 2.16(b) is almost identical to the matrix factorization architecture for recommender systems in Figure 2.13. As in the case of recommender systems, SGNS has missing (negative) entries. This is caused by the fact the negative sampling uses only a subset of the zero values. The only difference between the two cases is that the architecture of SGNS caps the output layer with sigmoid units, whereas a linear layer is used for recommender systems. However, recommender systems with implicit feedback use *logistic matrix factorization* [224], which is similar to the *word2vec* setting.

2.6.4 Vanilla Skip-Gram Is Multinomial Matrix Factorization

Since we have already shown that the SGNS enhancement of the skip-gram model is logistic matrix factorization, a natural question arises as to whether we can also recast the original skip-gram model as a matrix factorization method. It turns out that one can also recast the vanilla skip-gram model as a *multinomial matrix factorization* model because of the use of the softmax layer at the very end.

Let $C = [c_{ij}]$ be a $d \times d$ word-context co-occurrence matrix in which the value of c_{ij} is the number of times that word j occurs in the context of word i. Let U be a $d \times p$ matrix containing the input embedding in its rows, and V be a $p \times d$ matrix containing the output embedding in its columns. *Then, the skip-gram model roughly creates a model in which the frequency vector of the rth row of C is an empirical instantiation of the probabilities obtained by applying the softmax to the rth row of UV.*

Let $\overline{u}_i$ be the p-dimensional vector corresponding to the ith row of U and $\overline{v}_j$ be the p-dimensional vector corresponding to the jth column of V. The loss function of the aforementioned factorization is as follows:

$$O = -\sum_{i=1}^{d}\sum_{j=1}^{d} c_{ij} \log \underbrace{\left(\frac{\exp(\overline{u}_i \cdot \overline{v}_j)}{\sum_{q=1}^{d} \exp(\overline{u}_i \cdot \overline{v}_q)} \right)}_{P(\text{word } j|\text{word } i)} \tag{2.60}$$

This loss function is written in minimization form. Note that this loss function is identical to the one used in the vanilla skip-gram model, except that the latter uses a mini-batch stochastic gradient descent in which the m words in a given context are grouped together. This type of specific mini-batch does not make a significant difference.

2.7 Simple Neural Architectures for Graph Embeddings

Large networks have become very common because of their ubiquity in many social- and Web-centric applications. Graphs are structural entries containing *nodes* and *edges* connecting them. For example, in a social network, each person is a node, and a friendship link between two people is an edge. In this particular exposition, we consider the case of very large networks like the Web, a social network, or a communication network. The goal is to embed the nodes into feature vectors, so that the graph captures the relationships between nodes. For simplicity we consider undirected graphs, although directed graphs with weights on the edges can be easily handled with very few changes to the exposition below.

Consider an $n \times n$ adjacency matrix $B = [b_{ij}]$ for a graph with n nodes. The entry b_{ij} is 1 if an undirected edge exists between nodes i and j. Furthermore, the matrix B is symmetric, because we have $b_{ij} = b_{ji}$ for an undirected graph. In order to determine the embedding, we would like to determine two $n \times p$ factor matrices U and V, so that B can be derived as a function of UV^T. In the simplest case, one can set B to exactly UV^T, which is no different than a traditional matrix factorization method for factoring graphs [4]. However, for binary matrices, one can do better and use logistic matrix factorization instead. In other words, each entry of B is generated using the matrix of Bernoulli parameters in $f(UV^T)$, where $f(\cdot)$ is the element-wise application of the sigmoid function to each entry of the matrix in its argument:

$$f(x) = \frac{1}{1 + \exp(-x)} \tag{2.61}$$

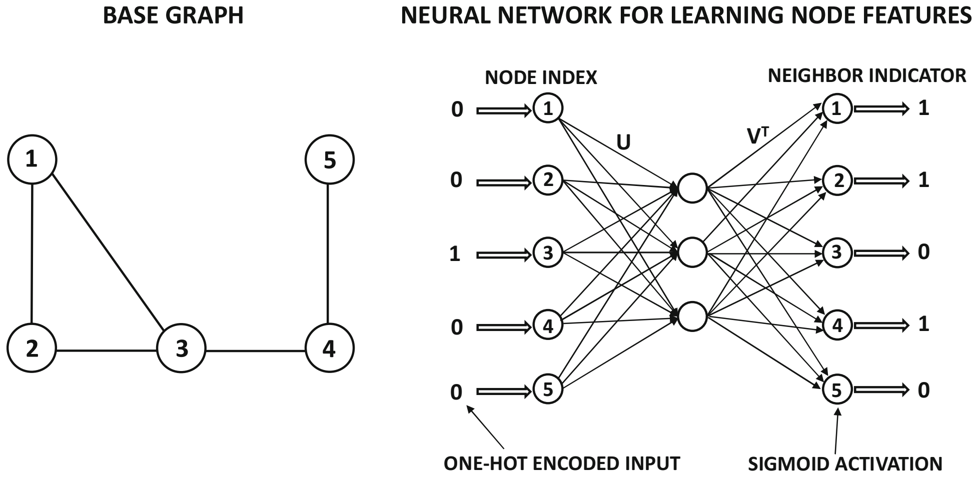


Figure 2.17: A graph of five nodes is shown together with a neural architecture for row index to neighbor indicator mapping. The shown input and output represent node 3 and its neighbors. Note the similarity to Figure 2.13. The main difference is that there are no missing values above, and the number of inputs is the same as the number of outputs for a square matrix. Both input and outputs are binary vectors. However, if negative sampling is used with sigmoid activation, most output nodes with zero values may be dropped.

Therefore, if $\overline{u}_i$ is the ith row of U and $\overline{v}_j$ is the jth row of V, we have the following:

$$b_{ij} \sim \text{Bernoulli distribution with parameter } f(\overline{u}_i \cdot \overline{v}_j) \tag{2.62}$$

This type of generative model is typically solved using a log-likelihood model. Furthermore, *the problem formulation is identical to the logistic matrix factorization equivalent of the SGNS model in word2vec.*

Note that all *word2vec* models are logistic/multinomial variants of the model in Figure 2.13 that maps row indexes to values with linear activation. In order to explain this point, we show the neural architecture in Figure 2.17 for a toy graph containing 5 nodes. The input is the one-hot encoded index of a row in B (i.e., node), and the output is the list of all 0/1 values for all nodes in the network. In this particular case, we have shown the input for node 3 and its corresponding output. Since the node 3 has three neighbors, the output vector contains three 1s. Note that this architecture is not very different from Figure 2.13 except that it uses a sigmoid activations at the output (rather than linear activations). Furthermore, since the number of 0s is usually much greater[8] than the number of 1s in the output, it is possible to drop many of the 0s with the use of negative sampling. This type of negative sampling will create a situation similar to that of Figure 2.14. With this neural architecture, the gradient-descent steps will be identical to the SGNS model of *word2vec*. The main difference is that a node appears at most once as a neighbor of another node, whereas a word might appear more than once in the context of another word. Allowing arbitrary counts on the edges takes away this distinction.

[8] This fact is not evident in the toy example of Figure 2.17. In practice, the degree of a node is a tiny fraction of the total number of nodes. For example, a person might have 100 friends in a social network of millions of nodes.

2.7.1 Handling Arbitrary Edge Counts

The aforementioned discussion assumes that the weight of each edge is binary. Consider a setting in which an arbitrary count c_{ij} is associated with the edge (i, j). In such cases, both positive and negative sampling are required. The first step is to sample an edge (i, j) from the network with probability proportional to c_{ij}. The input is, therefore, a one-hot encoded vector of the node at one end point (say, i) of this edge. The output is the one-hot encoding of node j. By default, both the input and output are n-dimensional vectors. However, if negative sampling is used, then one can reduce the output vector to a $(k + 1)$-dimensional vector. Here, $k \ll n$ is a parameter that defines the sampling rate. A total of k negative nodes are sampled with probabilities proportional to their (weighted) degrees[9] and the outputs of these nodes are 0s. One can compute the log-likelihood loss by treating each output as the outcome of a Bernoulli trial, where the parameter of the Bernoulli trial is the output of the sigmoid activation function. The gradient descent is performed with respect to this loss. This variant is an almost exact simulation of the SGNS variant of the *word2vec* model.

2.7.2 Multinomial Model

The vanilla skip-gram model of *word2vec* is a multinomial model. It is also possible to use a multinomial model to create the embedding. The only difference is that the final layer of the neural network in Figure 2.17 needs to use softmax activation (instead of the sigmoid activation function). Furthermore, negative sampling is not used in the multinomial model, and both input and output layers contain exactly n nodes. As in the SGNS model, a single edge (i, j) is sampled with probability proportional to c_{ij} to create each input-output pair. The input is the one-hot encoding of i and the output is the one-hot encoding of j. One can also use mini-batch sampling of edges to improve performance. The stochastic gradient-descent steps of this model are virtually similar to those used in the vanilla skip-gram model of *word2vec*.

2.7.3 Connections with DeepWalk and Node2vec

The recently proposed *DeepWalk* [372] and *node2vec* models [164] belong to the family of multinomial models discussed above (with specialized preprocessing steps). The main difference is that the *DeepWalk* and *node2vec* models use depth-first or breadth-first walks to (indirectly) generate c_{ij}. *DeepWalk* is itself a precursor to (and special case of) *node2vec* in terms of how the random walks are performed. In this case, c_{ij} can be interpreted as the number of times that node j appears in the neighborhood of node i because it was included in a breadth-first or depth-first walk starting at node i. One can view the value of c_{ij} in the walk-based models as providing a more robust measure of the affinity between nodes i and j, as compared to the raw weights in the original graph. Of course, there is nothing sacrosanct about using a random walk to improve the robustness of c_{ij}. The number of choices is almost unlimited in terms of how to generate this type of affinity value. All *link prediction methods* [295] generate such affinity values. For example, the *Katz measure* [295], which is closely related to the number of random walks between a pair of nodes, is a robust measure of the affinity between nodes i and j.

[9] The weighted degree of node j is $\sum_r c_{rj}$.

2.8 Summary

This chapter discusses a number of neural models supervised and unsupervised learning. One of the goals was to show that many of the traditional models used in machine learning are instantiations of relatively simple neural models. Methods for binary/multiclass classification and matrix factorization were discussed. In addition, the applications of the approach to recommender systems and word embedding were introduced. When a traditional machine learning technique like singular value decomposition is generalized to a neural representation, it is often inefficient compared to its counterpart in traditional machine learning. However, the advantage of neural models is that they can usually be generalized to more powerful nonlinear models. Furthermore, it is relatively easy to experiment with nonlinear variants of traditional machine learning models with the use of neural networks. This chapter also discusses several practical applications like recommender systems, text, and graph embeddings.

2.9 Bibliographic Notes

The perceptron algorithm was proposed by Rosenblatt [405], and a detailed discussion may be found in [405]. The Widrow-Hoff algorithm was proposed in [531] and is closely related to Tikhonov-Arsenin's work [499]. The Fisher discriminant was proposed by Ronald Fisher [120] in 1936, and is a specific case of the family of linear discriminant analysis methods [322]. Even though the Fisher discriminant uses an objective function that appears o to be different from least-squares regression, it turns out to be a special case of least-squares regression in which the binary response variable is used as the regressand [40]. A detailed discussion of generalized linear models is provided in [320]. A variety of procedures such as *generalized iterative scaling*, *iteratively reweighted least-squares*, and *gradient descent* for multinomial logistic regression are discussed in [178]. The support-vector machine is generally credited to Cortes and Vapnik [82], although the primal method for L_2-loss SVMs was proposed several years earlier by Hinton [190]! This approach repairs the loss function in least-squares classification by keeping only one-half of the quadratic loss curve and setting the remaining to zero, so that it looks like a smooth version of hinge loss (try this on Figure 2.4). The specific significance of this contribution was lost within the broader literature on neural networks. Hinton's work also does not focus on the importance of regularization in SVMs, although the general notion of adding shrinkage to gradient-descent steps in neural networks was well known. The hinge-loss SVM [82] is heavily presented from the perspective of duality and the maximum-margin interpretation, making its relationship to regularized least-squares classification somewhat opaque. The relationship of SVMs to least-squares classification is more evident from other related works [400, 442], where it becomes evident that quadratic and hinge-loss SVMs are natural variations of regularized L_2-loss (i.e., Fisher discriminant) and L_1-loss classification that use the binary class variables as the regression responses [139]. The Weston-Watkins multiclass SVM was introduced in [529]. It was shown in [401] that the one-against-all approach to generalizing multiple classes seems to be as effective as the tightly integrated multiclass variants. Many hierarchical softmax methods are discussed in [325, 327, 332, 344].

An excellent overview paper on methods for reducing the dimensionality of data with neural networks is available in [198], although this work focuses on the use of a related model known as the Restricted Boltzmann Machine (RBM). The earliest introduction of the autoencoder (in a more general form) is given in the backpropagation paper [408]. This work discusses the problem of recoding between input and output patterns. Both classification and autoencoders can be considered special cases of this architecture by using an appropriate choice of input and output patterns. The paper on backpropagation [408] also discusses the special case in which the recoding of the input is the identity mapping, which is exactly the scenario of the autoencoder. More detailed discussions of the autoencoder during its early years were provided in [48, 275]. A discussion of single-layer unsupervised learning may be found in [77]. The standard method for regularizing an autoencoder is to use weight decay, which corresponds to L_2-regularization. Sparse autoencoders are discussed in [67, 273, 274, 284, 354]. Another way of regularizing the autoencoder is to penalize the derivatives during gradient descent. This ensures that the learned function does not change too much with change in input. This method is referred to as the *contractive autoencoder* [397]. Variational autoencoders can encode complex probabilistic distributions, and are discussed in [106, 242, 399]. The de-noising autoencoder is discussed in [506]. Many of these methods are discussed in detail in Chapter 4. The use of autoencoders for outlier detection is explored in [64, 181, 564], and a survey on the use in clustering is provided in [8].

The application of dimensionality reduction for recommender systems may be found in [414], although this approach uses a restricted Boltzmann machine, which is different from the matrix factorization method discussed in this chapter. An item-based autoencoder is discussed in [436], and this approach is a neural generalization of item-based neighborhood regression [253]. The main difference is that the regression weights are regularized with a constricted hidden layer. Similar works with different types of item-to-item models with the use of de-noising autoencoders are discussed in [472, 535]. A more direct generalization of matrix factorization methods may be found in [186], although the approach in [186] is slightly different from the simpler approach presented in this chapter. The incorporation of content in building recommender systems for deep learning is discussed in [513]. A multiview deep learning approach, which has also been extended to temporal recommender systems in a later work [465], is proposed in [110]. A survey of deep learning methods for recommenders may be found in [560].

The *word2vec* model is proposed in [325, 327], and a detailed exposition may be found in [404]. The basic idea has been extended to sentence- and paragraph-level embeddings, with a model, which is referred to as *doc2vec* [272]. An alternative of *word2vec* that uses a different type of matrix factorization is GloVe [371]. Multi-lingual word embeddings are presented in [9]. The extension of *word2vec* to graphs with node-level embeddings is provided in the *DeepWalk* [372] and *node2vec* [164] models. Various types of network embeddings are discussed in [62, 512, 547, 548].

2.9.1 Software Resources

Machine learning models like linear regression, SVMs, and logistic regression are available from *scikit-learn* [587]. The DISSECT (Distributional Semantics Composition Toolkit) [588] is a toolkit that uses word co-occurrence counts in order to create embeddings. The GloVe method is available from Stanford NLP [589] and the **gensim** library [394]. The *word2vec* tool is available under the Apache license [591], and as a **TensorFlow** version [592]. The **gensim** library has Python implementations of *word2vec* and *doc2vec* [394]. Java versions of *doc2vec*, *word2vec*, and GloVe may be found in the **DeepLearning4j** repository [590]. In several cases, one can simply download pre-trained versions of the representations (on a large corpus that is considered generally representative of text) and use them directly, as a convenient alternative to training for the specific corpus at hand. The *node2vec* software is available from the original author at [593].

2.10 Exercises

1. Consider the following loss function for training pair $(\overline{X}, y)$:

$$L = \max\{0, a - y(\overline{W} \cdot \overline{X})\}$$

The test instances are predicted as $\hat{y} = \text{sign}\{\overline{W} \cdot \overline{X}\}$. A value of $a = 0$ corresponds to the perceptron criterion and a value of $a = 1$ corresponds to the SVM. Show that any value of $a > 0$ leads to the SVM with an unchanged optimal solution when no regularization is used. What happens when regularization is used?

2. Based on Exercise 1, formulate a generalized objective for the Weston-Watkins SVM.

3. Consider the unregularized perceptron update for binary classes with learning rate α. Show that using any value of α is inconsequential in the sense that it only scales up the weight vector by a factor of α. Show that these results also hold true for the multiclass case. Do the results hold true when regularization is used?

4. Show that if the Weston-Watkins SVM is applied to a data set with $k = 2$ classes, the resulting updates are equivalent to the binary SVM updates discussed in this chapter.

5. Show that if multinomial logistic regression is applied to a data set with $k = 2$ classes, the resulting updates are equivalent to logistic regression updates.

6. Implement the softmax classifier using a deep-learning library of your choice.

7. In linear-regression-based neighborhood models, the rating of an item is predicted as a weighted combination of the ratings of other items of the same user, where the item-specific weights are learned with linear regression. Show how you can construct an autoencoder architecture to create this type of model. Discuss the relationship of this architecture with the matrix factorization architecture.

8. **Logistic matrix factorization:** Consider an autoencoder which has an input layer, a single hidden layer containing the reduced representation, and an output layer with sigmoid units. The hidden layer has linear activation:

   (a) Set up a negative log-likelihood loss function for the case when the input data matrix is known to contain binary values from $\{0, 1\}$.

   (b) Set up a negative log-likelihood loss function for the case when the input data matrix contains real values from $[0, 1]$.

9. **Non-negative matrix factorization with autoencoders:** Let D be an $n \times d$ data matrix with non-negative entries. Show how you can approximately factorize $D \approx UV^T$ into two non-negative matrices U and V, respectively, by using an autoencoder architecture with d inputs and outputs. [Hint: Choose an appropriate activation function in the hidden layer, and modify the gradient-descent updates.]

10. **Probabilistic latent semantic analysis:** Refer to [99, 206] for a definition of probabilistic latent semantic analysis. Propose a modification of the approach in Exercise 9 for probabilistic latent semantic analysis. [Hint: What is the relationship between non-negative matrix factorization and probabilistic latent semantic analysis?]

11. Simulating a model combination ensemble: In machine learning, a model combination ensemble averages the scores of multiple models in order to create a more robust classification score. Discuss how you can approximate the averaging of an Adaline and logistic regression with a two-layer neural network. Discuss the similarities and differences of this architecture with an actual model combination ensemble when backpropagation is used to train it. Show how to modify the training process so that the final result is a fine-tuning of the model combination ensemble.

12. Simulating a stacking ensemble: In machine learning, a stacking ensemble creates a higher-level classification model on top of features learned from first-level classifiers. Discuss how you can modify the architecture of Exercise 11, so that the first level of classifiers correspond to an Adaline and a logistic regression classifier and the higher-level classifier corresponds to a support vector machine. Discuss the similarities and differences of this architecture with an actual stacking ensemble when backpropagation is used to train it. Show how you can modify the training process of the neural network so that the final result is a fine-tuning of the stacking ensemble.

13. Show that the stochastic gradient-descent updates of the perceptron, Widrow-Hoff learning, SVM, and logistic regression are all of the form $\overline{W} \Leftarrow \overline{W}(1 - \alpha\lambda) + \alpha y[\delta(\overline{X}, y)]\overline{X}$. Here, the mistake function $\delta(\overline{X}, y)$ is $1 - y(\overline{W} \cdot \overline{X})$ for least-squares classification, an indicator variable for perceptron/SVMs, and a probability value for logistic regression. Assume that α is the learning rate, and $y \in \{-1, +1\}$. Write the specific forms of $\delta(\overline{X}, y)$ in each case.

14. The linear autoencoder discussed in the chapter is applied to each d-dimensional row of the $n \times d$ data set D to create a k-dimensional representation. The encoder weights contain the $k \times d$ weight matrix W and the decoder weights contain the $d \times k$ weight matrix V. Therefore, the reconstructed representation is DW^TV^T, and the aggregate loss value $||DW^TV^T - D||^2$ is minimized over the entire training data set.

(a) For a fixed value of V, show that the optimal matrix W must satisfy $D^TD(W^TV^TV - V) = 0$.

(b) Use (a) to show that if the $n \times d$ matrix D has rank d, we have $W^TV^TV = V$.

(c) Use (b) to show that $W = (V^TV)^{-1}V^T$. Assume that V^TV is invertible.

(d) Repeat exercise parts (a), (b), and (c), when the encoder-decoder weights are tied as $W = V^T$. Show that the columns of V must be orthonormal.