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Neural Networks and Deep Learning

A Textbook

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can be obtained when one has a good idea of how a particular computational node relates to the input data. Examples of such parameter-sharing methods are as follows:

1. *Sharing weights in autoencoders:* The symmetric weights in the encoder and decoder portion of the autoencoder are often shared. Although an autoencoder will work whether or not the weights are shared, doing so improves the regularization properties of the algorithm. In a single-layer autoencoder with linear activation, weight sharing forces orthogonality among the different hidden components of the weight matrix. This provides the same reduction as singular value decomposition.

2. *Recurrent neural networks:* These networks are often used for modeling sequential data, such as time-series, biological sequences, and text. The last of these is the most commonly used application of recurrent neural networks. In recurrent neural networks, a time-layered representation of the network is created in which the neural network is replicated across layers associated with time stamps. Since each time stamp is assumed to use the same model, the parameters are shared between different layers. Recurrent neural networks are discussed in detail in Chapter 7.

3. *Convolutional neural networks:* Convolutional neural networks are used for image recognition and prediction. Correspondingly, the inputs of the network are arranged into a rectangular grid pattern, along with all the layers of the network. Furthermore, the weights across contiguous patches of the network are typically shared. The basic idea is that a rectangular patch of the image corresponds to a portion of the visual field, and it should be interpreted in the same way no matter where it is located. In other words, a carrot means the same thing whether it is at the left or the right of the image. In essence, these methods use semantic insights about the data to reduce the parameter footprint, share weights, and sparsify the connections. Convolutional neural networks are discussed in Chapter 8.

In many of these cases, it is evident that parameter sharing is enabled by the use of domain-specific insights about the training data as well as a good understanding of how the computed function at a node relates to the training data. The modifications to the backpropagation algorithm required for enabling weight sharing are discussed in Section 3.2.9 of Chapter 3.

An additional type of weight sharing is *soft weight sharing* [360]. In soft weight sharing, the parameters are not completely tied, but a penalty is associated with them being different. For example, if one expects the weights w_i and w_j to be similar, the penalty $\lambda(w_i - w_j)^2/2$ might be added to the loss function. In such a case, the quantity $\alpha\lambda(w_j - w_i)$ might be added to the update of w_i, and the quantity $\alpha\lambda(w_i - w_j)$ might be added to the update of w_j. Here, α is the learning rate. These types of changes to the updates tend to pull the weights towards each other.

4.10 Regularization in Unsupervised Applications

Although overfitting does occur in unsupervised applications, it is often less of a problem. In classification, one is trying to learn a single bit of information associated with each example, and therefore using more parameters than the number of examples can cause overfitting. This is not quite the case in unsupervised applications in which a single training example may contain many more bits of information corresponding to the different dimensions. In general, the number of bits of information will depend on the intrinsic dimensionality of the data set. Therefore, one tends to hear fewer complaints about overfitting in unsupervised applications.

Nevertheless, there are many unsupervised settings in which it is beneficial to use regularization. A common case is one in which we have an *overcomplete* autoencoder, in which the number of hidden units is greater than the number of input units. An important goal of regularization in unsupervised applications is to impose some kind of structure on the learned representations. This approach to regularization can have different application-specific benefits like creating sparse representations or in providing the ability to clean corrupted data. As in the case of supervised models, one can use semantic insights about a problem domain in order to force a solution to have specific types of desired properties. This section will show how different types of penalties and constraints on the hidden units can create hidden/reconstructed representations with useful properties.

4.10.1 Value-Based Penalization: Sparse Autoencoders

The penalizing of sparse hidden units has unsupervised applications such as *sparse autoencoders*. Sparse autoencoders contain a much larger number of hidden units in each layer as compared to the number of input units. However, the values of the hidden units are encouraged to be 0s by either explicit penalization or by constraints. As a result, most of the values in the hidden units will be 0s at convergence. One possible approach is to impose an L_1-penalty on the hidden units in order to create sparse representations. The gradient-descent approach with L_1-penalties on the hidden units is discussed in Section 4.4.4. It is also noteworthy that the use of L_1-regularization seems to be somewhat unusual in the autoencoder literature (although there is no reason not to use it). Other constraint-based methods exist, such as allowing only the top-k hidden units to be activated. In most of these cases, the constraints are chosen in such a way that the backpropagation approach can be modified in a reasonable way. For example, if only the top-k units are selected for activation, then the gradient flows are allowed to backpropagate only through these chosen units. Constraint-based techniques are simply hard variations of penalty-based methods. More details are provided on some of these learning methods in Section 2.5.5.1 of Chapter 2.

4.10.2 Noise Injection: De-noising Autoencoders

As discussed in Section 4.4.1, noise injection is a form of penalty-based regularization of the weights. The use of Gaussian noise in the input is roughly equal to L_2-regularization in single-layer networks with linear activation. The de-noising autoencoder is based on noise injection rather than penalization of the weights or hidden units. However, the goal of the de-noising autoencoder is to reconstruct good examples from corrupted training data. Therefore, the type of noise should be calibrated to the nature of the input. Several different types of noise can be added:

1. *Gaussian noise:* This type of noise is appropriate for real-valued inputs. The added noise has zero mean and variance $\lambda > 0$ for each input. Here, λ is the regularization parameter.

2. *Masking noise:* The basic idea is to set a fraction f of the inputs to zeros in order to corrupt the inputs. This type of approach is particularly useful when working with binary inputs.

3. *Salt-and-pepper noise:* In this case, a fraction f of the inputs are set to either their minimum or maximum possible values according to a fair coin flip. The approach is typically used for binary inputs, for which the minimum and maximum values are 0 and 1, respectively.

De-noising autoencoders are useful when dealing with data that is corrupted. Therefore, the main application of such autoencoders is to reconstruct corrupted data. The inputs to the autoencoder are corrupted training records, and the outputs are the uncorrupted data records. As a result, the autoencoder learns to recognize the fact that the input is corrupted, and the true representation of the input needs to be reconstructed. Therefore, even if there is corruption in the test data (as a result of application-specific reasons), the approach is able to reconstruct clean versions of the test data. Note that the noise in the training data is explicitly added, whereas that in the test data is already present as a result of various application-specific reasons. For example, as shown in the top portion of Figure 4.10, one can use the approach to removing blurring or other noise from images. The nature of the noise added to the input training data should be based on insights about the type of corruption present in the test data. Therefore, one does require uncorrupted examples of the training data for best performance. In most domains, this is not very difficult to achieve. For example, if the goal is to remove noise from images, the training data might contain high-quality images as the output and artificially blurred images as the input. It is common for the de-noising autoencoder to be overcomplete, when it is used for reconstruction from corrupted data. However, this choice also depends on the nature of the input and the amount of noise added. Aside from its use for reconstructing inputs, the addition of noise is also an excellent regularizer that tends to make the approach work better for out-of-sample inputs even when the autoencoder is undercomplete.

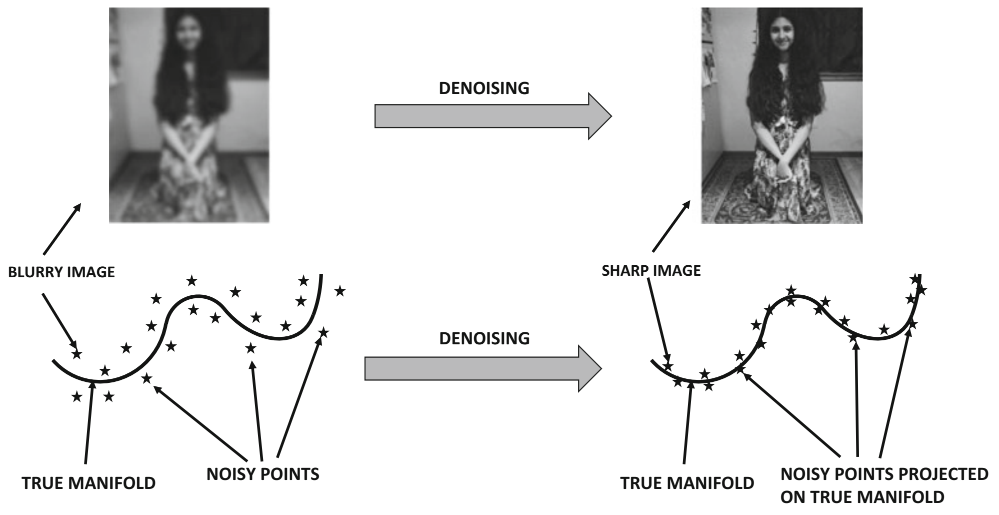


Figure 4.10: The de-noising autoencoder

The way in which the de-noising autoencoder works is that it uses the noise in the input data to learn the true manifold on which the data is embedded. Each corrupted point is projected to its "closest" matching point on the true manifold of the data distribution. The closest matching point is the expected position on the manifold from which the model predicts that the noisy point has originated. This projection is shown in the bottom portion of Figure 4.10. The true manifold is a more concise representation of the data as compared to the noisy data, and this conciseness is a result of the regularization inherent in the addition of noise to the input. All forms of regularization tend to increase the conciseness of the underlying model.

4.10.3 Gradient-Based Penalization: Contractive Autoencoders

As in the case of the de-noising autoencoder, the hidden representation of the contractive autoencoder is often overcomplete, because the number of hidden units is greater than the number of input units. A contractive autoencoder is a heavily regularized encoder in which we do not want the hidden representation to change very significantly with small changes in input values. Obviously, this will also result in an output that is less sensitive to the input. Trying to create an autoencoder in which the output is less sensitive to changes in the input seems like an odd goal at first sight. After all, an autoencoder is supposed to reconstruct the data exactly. Therefore, the goals of regularization seem to be completely at odds with those of the contractive regularization portion of the loss function.

A key point is that contractive encoders are designed to be robust only to *small* changes in the input data. Furthermore, they tend to be insensitive to those changes that are inconsistent with the manifold structure of the data. In other words, if one makes a small change to the input that does not lie on the manifold structure of the input data, the contractive autoencoder will tend to damp the change in the reconstructed representation. Here, it is important to understand that the vast majority of (randomly chosen) directions in high-dimensional input data (with a much lower-dimensional manifold) tend to be approximately orthogonal to the manifold structure, which has the effect of changing the components of the change on the manifold structure. The damping of the changes in the reconstructive representation based on the local manifold structure is also referred to as the *contractive* property of the autoencoder. As a result, contractive autoencoders tend to remove noise from the input data (like de-noising autoencoders), although the mechanism for doing this is different from that of de-noising autoencoders. As we will see later, contractive autoencoders penalize the gradients of the hidden values with respect to the inputs. When the hidden values have low gradients with respect to the inputs, it means that they are not very sensitive to small changes in the inputs (although larger changes or changes parallel to manifold structure will tend to change the gradients).

For ease in discussion, we will discuss the case where the contractive autoencoder has a single hidden layer. The generalization to multiple hidden layers is straightforward. Let $h_1 \ldots h_k$ be the values of the k hidden units for the input variables $x_1 \ldots x_d$. Let the reconstructed values in the output layer be given by $\hat{x}_1 \ldots \hat{x}_d$. Then, the objective function is given by the weighted sum of the reconstruction loss and the regularization term. The loss L for a single training instance is given by the following:

$$L = \sum_{i=1}^{d} (x_i - \hat{x}_i)^2 \tag{4.12}$$

The regularization term is constructed by using the sum of the squares of the partial derivatives of all hidden variables with respect to all input dimensions. For a problem with k hidden units denoted by $h_1 \ldots h_k$, the regularization term R can be written as follows:

$$R = \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{k} \left(\frac{\partial h_j}{\partial x_i} \right)^2 \tag{4.13}$$

In the original paper [397], the sigmoid nonlinearity is used in the hidden layer, in which case the following can be shown (cf. Section 3.2.5 of Chapter 3):

$$\frac{\partial h_j}{\partial x_i} = w_{ij} h_j (1 - h_j) \; \forall i, j \tag{4.14}$$

Here, w_{ij} is the weight of the input unit i to the hidden unit j.

The overall objective function for a single training instance is given by a weighted sum of the loss and the regularization terms.

$$\begin{aligned} J &= L + \lambda \cdot R \\ &= \sum_{i=1}^{d} (x_i - \hat{x}_i)^2 + \frac{\lambda}{2} \sum_{j=1}^{k} h_j^2 (1 - h_j)^2 \sum_{i=1}^{d} w_{ij}^2 \end{aligned}$$

This objective function contains a combination of weight and hidden unit regularization. Penalties on hidden units can be handled in the same way as discussed in Section 3.2.7 of Chapter 3. Let a_{h_j} be the pre-activation value for the node h_j. The backpropagation updates are traditionally defined in terms of the preactivation values, where the value of $\frac{\partial J}{\partial a_{h_j}}$ is propagated backwards. After $\frac{\partial J}{\partial a_{h_j}}$ is computed using the dynamic programming update of backpropagation from the output layer, one can further update it to incorporate the effect of hidden-layer regularization of h_j:

$$\begin{aligned} \frac{\partial J}{\partial a_{h_j}} &\Leftarrow \frac{\partial J}{\partial a_{h_j}} + \frac{\lambda}{2} \frac{\partial [h_j^2 (1 - h_j)^2]}{\partial a_{h_j}} \sum_{i=1}^{d} w_{ij}^2 \\ &= \frac{\partial J}{\partial a_{h_j}} + \lambda h_j (1 - h_j)(1 - 2h_j) \underbrace{\frac{\partial h_j}{\partial a_{h_j}}}_{h_j(1-h_j)} \sum_{i=1}^{d} w_{ij}^2 \\ &= \frac{\partial J}{\partial a_{h_j}} + \lambda h_j^2 (1 - h_j)^2 (1 - 2h_j) \sum_{i=1}^{d} w_{ij}^2 \end{aligned}$$

The value of $\frac{\partial h_j}{\partial a_{h_j}}$ is set to $h_j(1 - h_j)$ because the sigmoid activation is assumed, although it would be different for other activations. According to the chain rule, the value of $\frac{\partial J}{\partial a_{h_j}}$ should be multiplied with the value of $\frac{\partial a_{h_j}}{\partial w_{ij}} = x_i$ to obtain the gradient of the loss with respect to w_{ij}. However, according to the *multivariable* chain rule, we also need to directly add the derivative of the regularizer with respect to w_{ij} in order to obtain the full gradient. Therefore, the partial derivative of the hidden-layer regularizer R with respect to the weight is added as follows:

$$\begin{aligned} \frac{\partial J}{\partial w_{ij}} &\Leftarrow \frac{\partial J}{\partial a_{h_j}} \frac{\partial a_{h_j}}{\partial w_{ij}} + \lambda \frac{\partial R}{\partial w_{ij}} \\ &= x_i \frac{\partial J}{\partial a_{h_j}} + \lambda w_{ij} h_j^2 (1 - h_j)^2 \end{aligned}$$

Interestingly, if a linear hidden unit is used instead of the sigmoid, it is easy to see that the objective function will become identical to that of an L_2-regularized autoencoder. Therefore, it makes sense to use this approach only with a nonlinear hidden layer, because a linear hidden layer can be handled in a much simpler way. The weights in the encoder and decoder can be either tied or independent. If the weights are tied then the gradients over both copies of a weight need to be added. The above discussion assumes a single hidden layer, although it is easy to generalize to more hidden layers. The work in [397] showed that better compression can be achieved with the use of deeper variants of the approach.

Some interesting relationships exist between the de-noising autoencoder and the contractive autoencoder. The de-noising autoencoder achieves its goals of robustness stochastically by explicitly adding noise, whereas a contractive autoencoder achieves its goals analytically by adding a regularization term. Adding a small amount of Gaussian noise in a de-noising autoencoder achieves roughly similar goals as a contractive autoencoder, when the hidden layer uses linear activation. When the hidden layer uses linear activation, the partial derivative of the hidden unit with respect to an input is simply the connecting weight, and therefore the objective function of the contractive autoencoder becomes the following:

$$J_{linear} = \sum_{i=1}^{d} (x_i - \hat{x}_i)^2 + \frac{\lambda}{2} \sum_{i=1}^{d} \sum_{j=1}^{k} w_{ij}^2 \tag{4.15}$$

In that case, both the contractive and the de-noising autoencoders become similar to regularized singular value decomposition with L_2-regularization. The difference between the de-noising autoencoder and the contractive autoencoder is visually illustrated in Figure 4.11. In the case of the de-noising autoencoder on the left, the autoencoder learns the directions along the true manifold of uncorrupted data by using the relationship between the corrupted data in the output and the true data in the input. This goal is achieved analytically in the contractive autoencoder, because the vast majority of random perturbations are roughly orthogonal to the manifold when the dimensionality of the manifold is much smaller than the input data dimensionality. In such a case, perturbing the data point slightly does not change the hidden representation along the manifold very much. Penalizing the partial derivative of the hidden layer equally along all directions ensures that the partial derivative is significant only along the small number of directions along the true manifold, and the partial derivatives along the vast majority of orthogonal directions are close to 0. In other words, the variations that are not meaningful to the distribution of the specific training data set at hand are damped, and only the meaningful variations are kept.

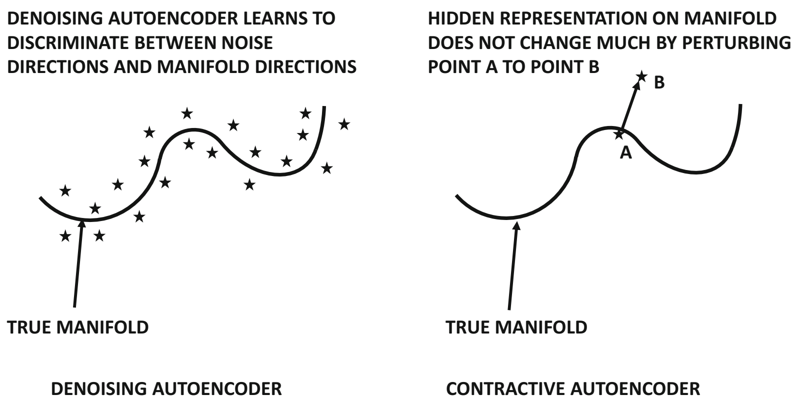

DENOISING AUTOENCODER LEARNS TO DISCRIMINATE BETWEEN NOISE DIRECTIONS AND MANIFOLD DIRECTIONS
TRUE MANIFOLD
DENOISING AUTOENCODER
HIDDEN REPRESENTATION ON MANIFOLD DOES NOT CHANGE MUCH BY PERTURBING POINT A TO POINT B
B
A
TRUE MANIFOLD
CONTRACTIVE AUTOENCODER

Figure 4.11: The difference between the de-noising and the contractive autoencoder

Another difference between the two methods is that the de-noising autoencoder shares the responsibility for regularization between the encoder and decoder, whereas the contractive autoencoder places this responsibility only on the encoder. Only the encoder portion is used in feature extraction; therefore, contractive autoencoders are more useful for feature engineering.

In a contractive autoencoder, the gradients are deterministic, and therefore it is also easier to use second-order learning methods as compared to the de-noising autoencoder. On the other hand, the de-noising autoencoder is easier to construct (with small changes to the code of an unregularized autoencoder), if first-order learning methods are used.

4.10.4 Hidden Probabilistic Structure: Variational Autoencoders

Just as sparse encoders impose a sparsity constraint on the hidden units, variational encoders impose a specific probabilistic structure on the hidden units. The simplest constraint is that the activations in the hidden units over the whole data should be drawn from the standard Gaussian distribution (i.e., zero mean and unit variance in each direction). By imposing this type of constraint, one advantage is that we can throw away the encoder after training, and simply feed samples from the standard normal distribution to the decoder in order to generate samples of the training data. However, if every object is generated from an identical distribution, then it would be impossible to either differentiate the various objects or to reconstruct them from a given input. Therefore, the *conditional* distribution of the activations in the hidden layer (with respect to a specific input object) would have a different distribution from the standard normal distribution. Even though a regularization term would try to pull even the conditional distribution towards the standard normal distribution, this goal would only be achieved over the distribution of hidden samples from the whole data rather than the hidden samples from a single object.

Imposing a constraint on the probabilistic distribution of hidden variables is more complicated than the other regularizers discussed so far. However, the key is to use a re-parametrization approach in which the encoder creates the k-dimensional mean and standard deviations vector of the conditional Gaussian distribution, and the hidden vector is sampled from this distribution as shown in Figure 4.12(a). Unfortunately, this network still has a sampling component. The weights of such a network cannot be learned by backpropagation because the stochastic portions of the computations are not differentiable, and therefore backpropagation cannot be not used. Therefore, the stochastic part of it can be addressed by the user explicitly generating k-dimensional samples in which each component is drawn from the standard normal distribution. The mean and standard deviation output by the encoder are used to scale and translate the input sample from the Gaussian distribution. This architecture is shown in Figure 4.12(b). By generating the stochastic potion explicitly as a part of the input, the resulting architecture is now fully deterministic, and its weights can be learned by backpropagation. Furthermore, the values of the generated samples from the standard normal distribution will need to be used in the backpropagation updates.

For each object $\overline{X}$, separate hidden activations for the mean and standard deviation are created by the encoder. The k-dimensional activations for the mean and standard deviation are denoted by $\overline{\mu}(\overline{X})$ and $\overline{\sigma}(\overline{X})$, respectively. In addition, a k-dimensional sample $\overline{z}$ is generated from $\mathcal{N}(0, I)$, where I is the identity matrix, and treated as an input into the hidden layer by the user. The hidden representation $\overline{h}(\overline{X})$ is created by scaling this random input vector $\overline{z}$ with the mean and standard deviation as follows:

$$\overline{h}(\overline{X}) = \overline{z} \odot \overline{\sigma}(\overline{X}) + \overline{\mu}(\overline{X}) \tag{4.16}$$

Here, $\odot$ indicates element-wise multiplication. These operations are shown in Figure 4.12(b) with the little circles containing the multiplication and addition operators. The elements of the vector $\overline{h}(\overline{X})$ for a particular object will obviously diverge from the standard normal distribution unless the vectors $\overline{\mu}(\overline{X})$ and $\overline{\sigma}(\overline{X})$ contain only 0s and 1s, respectively. This will not be the case because of the reconstruction component of the loss, which forces the conditional distributions of the hidden representations of particular points to have different means and lower standard deviations than that of the standard normal distribution (which is like a prior distribution). The distribution of the hidden representation of a particular point is a posterior distribution (conditional on the specific training data point), and therefore it will differ from the Gaussian prior. The overall loss function is expressed as a weighted sum of the reconstruction loss and the regularization loss. One can use a variety of choices for the reconstruction error, and for simplicity we will use the squared loss, which is defined as follows:

$$L = ||\overline{X} - \overline{X}'||^2 \tag{4.17}$$

Here, $\overline{X}'$ is the reconstruction of the input point $\overline{X}$ from the decoder. The regularization loss R is simply the Kullback-Leibler (KL)-divergence measure of the conditional hidden distribution with parameters $(\overline{\mu}(\overline{X})), \overline{\sigma}(\overline{X}))$ with respect to the k-dimensional Gaussian distribution with parameters $(0, I)$. This value is defined as follows:

$$R = \frac{1}{2}\left(\underbrace{||\overline{\mu}(\overline{X})||^2}_{\overline{\mu}(\overline{X})_i \Rightarrow 0} + \underbrace{||\overline{\sigma}(\overline{X})||^2 - 2\sum_{i=1}^{k} \ln(\overline{\sigma}(\overline{X})_i)}_{\overline{\sigma}(\overline{X})_i \Rightarrow 1} - k\right) \tag{4.18}$$

Below some of the terms, we have annotated the specific effects of these terms in pushing parameters in particular directions. The constant term does not really do anything but it is a part of the KL-divergence function. Including the constant term does have the cosmetically satisfying effect that the regularization portion of the objective function reduces to 0, if the parameters $(\overline{\mu}(\overline{X})), \overline{\sigma}(\overline{X}))$ are the same as those of the isotropic Gaussian distribution with zero mean and unit variance in all directions. However, this will not be the case for any specific data point because of the effect of the reconstruction portion of the objective function. Over all training data points, the distribution of the hidden representation will, however, move closer to the standardized Gaussian because of the regularization term. The overall objective function J for the data point $\overline{X}$ is defined as the weighted sum of the reconstruction loss and the regularization loss:

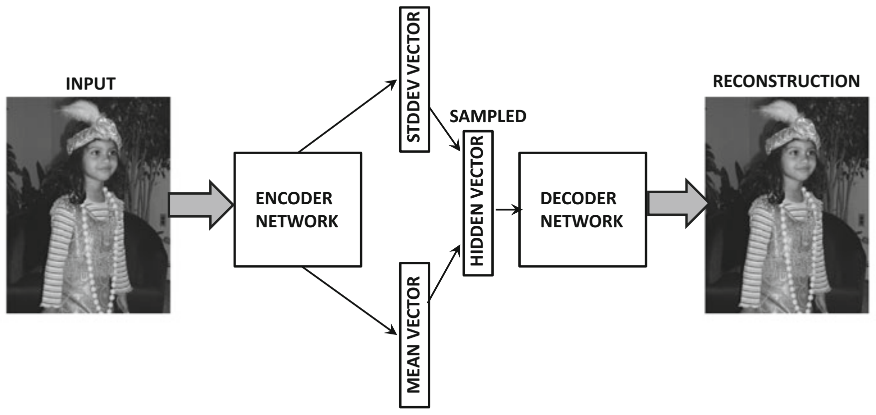
$$J = L + \lambda R \tag{4.19}$$

Here, $\lambda > 0$ is the regularization parameter. Small values of λ will favor exact reconstruction, and the approach will behave like a traditional autoencoder. The regularization term forces the hidden representations to be stochastic, so that multiple hidden representations generate almost the same point. This increases generalization power because it is easier to model a new image that is like (but not an exact likeness of) an image in the training data within the stochastic range of hidden values. However, since there will be overlaps among the distributions of the hidden representations of similar points, it has some undesirable side effects. For example, the reconstructions tend to be blurry, when using the approach to reconstruct images. This is caused by an averaging effect over somewhat similar points. In the extreme case, if the value of λ is chosen to be exceedingly large, then all points will have the same hidden distribution (which is an isotropic Gaussian distribution with zero mean and unit variance). The reconstruction might provide a gross averaging over large numbers of training points, which will not be meaningful. The blurriness of the reconstructions of the variational autoencoder is an undesirable property of this class of models in comparison with several other related models for generative modeling.

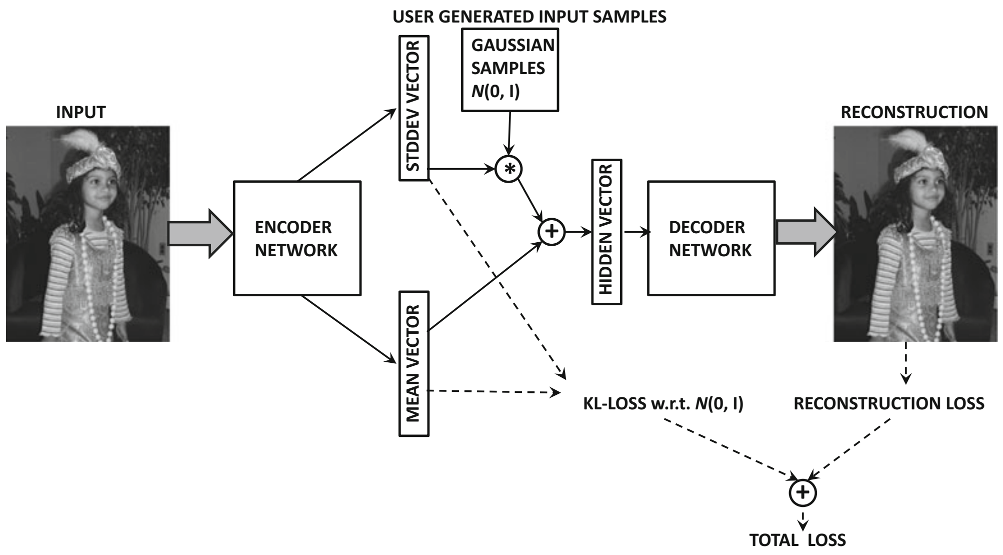
Training the Variational Autoencoder

The training of a variational autoencoder is relatively straightforward because the stochasticity has been pulled out as an additional input. One can backpropagate as in any traditional neural network. The only difference is that one needs to backpropagate across the unusual form of Equation 4.16. Furthermore, one needs to account for the penalties of the hidden layer during backpropagation.

First, one can backpropagate the loss L up to the hidden state $\overline{h}(\overline{X}) = (h_1 \dots h_k)$ using traditional methods. Let $\overline{z} = (z_1 \dots z_k)$ be the k random samples from $\mathcal{N}(0, 1)$, which are used in the current iteration. In order to backpropagate from $\overline{h}(\overline{X})$ to $\overline{\mu}(\overline{X}) = (\mu_1 \dots \mu_k)$ and $\overline{\sigma}(\overline{X}) = (\sigma_1 \dots \sigma_k)$, one can use the following relationship:



(a) Point-specific Gaussian distribution (stochastic and non-differentiable loss)



(b) Point-specific Gaussian distribution (deterministic and differentiable loss)

Figure 4.12: Re-parameterizing a variational autoencoder

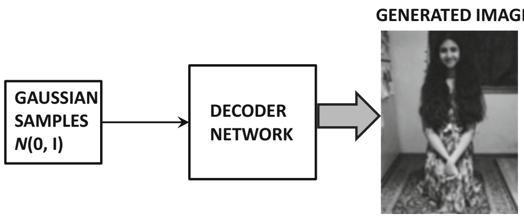


Figure 4.13: Generating samples from the variational autoencoder. The images are illustrative only.

$$J = L + \lambda R \tag{4.20}$$

$$\frac{\partial J}{\partial \mu_i} = \frac{\partial L}{\partial h_i} \underbrace{\frac{\partial h_i}{\partial \mu_i}}_{=1} + \lambda \frac{\partial R}{\partial \mu_i} \tag{4.21}$$

$$\frac{\partial J}{\partial \sigma_i} = \frac{\partial L}{\partial h_i} \underbrace{\frac{\partial h_i}{\partial \sigma_i}}_{=z_i} + \lambda \frac{\partial R}{\partial \sigma_i} \tag{4.22}$$

The values below the under-braces show the evaluations of partial derivatives of h_i with respect to μ_i and σ_i, respectively. Note that the values of $\frac{\partial h_i}{\partial \mu_i} = 1$ and $\frac{\partial h_i}{\partial \sigma_i} = z_i$ are obtained by differentiating Equation 4.16 with respect to μ_i and σ_i, respectively. The value of $\frac{\partial L}{\partial h_i}$ on the right-hand side is available from backpropagation. The values of $\frac{\partial R}{\partial \mu_i}$ and $\frac{\partial R}{\partial \sigma_i}$ are straightforward derivatives of the KL-divergence in Equation 4.18. Subsequent error propagation from the activations for $\overline{\mu}(\overline{X})$ and $\overline{\sigma}(\overline{X})$ can proceed in a similar way to the normal workings of the backpropagation algorithm.

The architecture of the variational autoencoder is considered fundamentally different from other types of autoencoders because it models the hidden variables in a stochastic way. However, there are still some interesting connections. In the de-noising autoencoder, one adds noise to the input; however, there is no constraint on the shape of the hidden distribution. In the variational autoencoder, one works with a stochastic hidden representation, although the stochasticity is pulled out by using it as an additional input during training. In other words, noise is added to the hidden representation rather than the input data. The variational approach improves generalization, because it encourages each input to map to its own stochastic region in the hidden space rather than mapping it to a single point. Small changes in the hidden representation, therefore, do not change the reconstruction too much. This assertion would also be true with a contractive autoencoder. However, constraining the shape of the hidden distribution to be Gaussian is a more fundamental difference of the variational autoencoder from other types of transformations.

4.10.4.1 Reconstruction and Generative Sampling

The approach can be used for creating the reduced representations as well as generating samples. In the case of data reduction, a Gaussian distribution with mean $\overline{\mu}(\overline{X})$ and standard deviation $\overline{\sigma}(\overline{X})$ is obtained, which represents the distribution of the hidden representation.

However, a particularly interesting application of the variational autoencoder is to generate samples from the underlying data distribution. Just as feature engineering methods

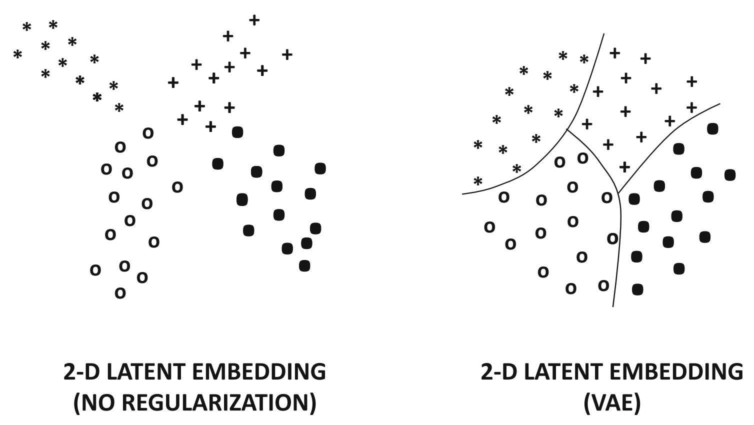


Figure 4.14: Illustrations of the embeddings created by a variational autoencoder in relation to the unregularized version. The unregularized version has large discontinuities in the latent space, which might not correspond to meaningful points. The Gaussian embedding of the points in the variational autoencoder makes sampling possible.

use only the encoder portion of the autoencoder (once training is done), variational autoencoders use only the decoder portion. The basic idea is to repeatedly draw a point from the Gaussian distribution and feed it to the hidden units in the decoder. The resulting "reconstruction" output of the decoder will be a point satisfying a similar distribution as the original data. As a result, the generated point will be a realistic sample from the original data. The architecture for sample generation is shown in Figure 4.13. The shown image is illustrative only, and does not reflect the actual output of a variational autoencoder (which is generally of somewhat lower quality). To understand why a variational autoencoder can generate images in this way, it is helpful to view the typical types of embeddings an unregularized autoencoder would create versus a method like the variational autoencoder. In the left side of Figure 4.14, we have shown an example of the 2-dimensional embeddings of the training data created by an unregularized autoencoder of a four-class distribution (e.g., four digits of MNIST). It is evident that there are large discontinuities in particular regions of the latent space, and that these sparse regions may not correspond to meaningful points. On the other hand, the regularization term in the variational autoencoder encourages the training points to be (roughly) distributed in a Gaussian distribution, and there are far fewer discontinuities in the embedding on the right-hand side of Figure 4.14. Consequently, sampling from any point in the latent space will yield meaningful reconstructions of one of the four classes (i.e., one of the digits of MNIST). Furthermore, "walking" from one point in the latent space to another along a straight line in the second case will result in a smooth transformation across classes. For example, walking from a region containing instances of '4' to a region containing instances of '7' in the latent space of the MNIST data set would result in a slow change in the style of the digit '4' until a transition point, where the handwritten digit could be interpreted either as a '4' or a '7'. This situation does occur in real settings as well because such types of confusing handwritten digits do occur in the MNIST data set. Furthermore, the placement of different digits within the embedding would be such that digit pairs with smooth transitions at confusion points (e.g., $[4, 7]$ or $[5, 6]$) are placed adjacent to one another in the latent space.

It is important to understand that the generated objects are often similar to but not exactly the same as those drawn from the training data. Because of its stochastic nature, the variational autoencoder has the ability to explore different modes of the generation process, which leads to a certain level of creativity in the face of ambiguity. This property can be put to good use by conditioning the approach on another object.

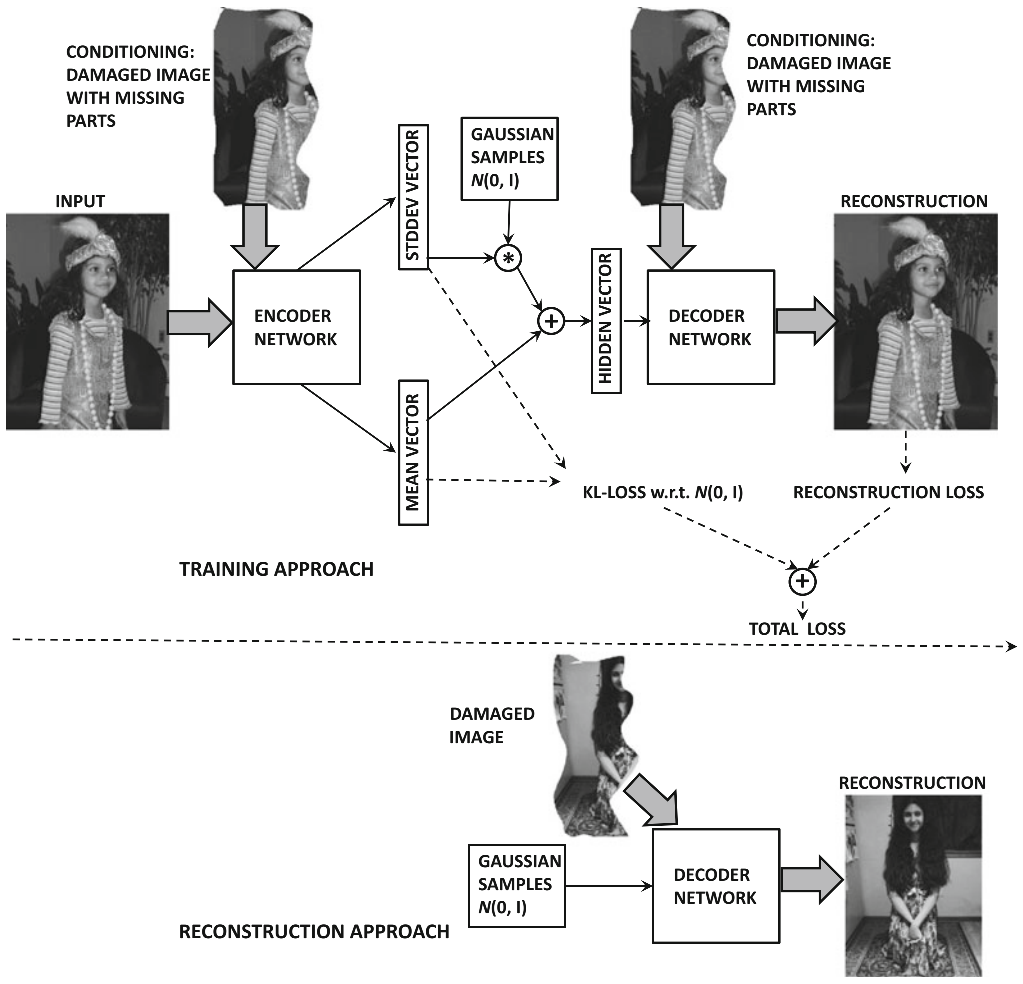


Figure 4.15: Reconstructing damaged images with the conditional variational autoencoder. The images are illustrative only.

4.10.4.2 Conditional Variational Autoencoders

One can apply conditioning to variational autoencoders in order to obtain some interesting results [510, 463]. The basic idea in conditional variational autoencoders is to add an additional conditional input, which typically provides a related context. For example, the context might be a damaged image with missing holes, and the job of the autoencoder is to reconstruct it. Predictive models will generally perform poorly in this type of setting because the level of ambiguity may be too large, and an averaged reconstruction across all images might not be useful. During the training phase, pairs of damaged and original images are needed, and therefore the encoder and decoder are able to learn how the context relates to the images being generated from the training data. The architecture of the training phase is illustrated in the upper part of Figure 4.15. The training is otherwise similar to the unconditional variational autoencoder. During the testing phase, the context is provided as an additional input, and the autoencoder reconstructs the missing portions in a reasonable way based on the model learned in the training phase. The architecture of the reconstruction phase is illustrated in the lower part of Figure 4.15. The simplicity of this architecture is particularly notable. The shown images are only illustrative; in actual executions on image data, the generated images are often blurry, especially in the missing portions. This is a type of image-to-image translation approach, which will be revisited in Chapter 10 under the context of a discussion on *generative adversarial networks*.

4.10.4.3 Relationship with Generative Adversarial Networks

Variational autoencoders are closely related to another class of models, referred to as generative adversarial networks. However, there are some key differences as well. Like variational autoencoders, generative adversarial networks can be used to create images that are similar to a base training data set. Furthermore, conditional variants of both models are useful for completing missing data, especially in cases where the ambiguity is large enough to require a certain level of creativity from the generative process. However, the results of generative adversarial networks are often more realistic because the decoders are explicitly trained to create good counterfeits. This is achieved by having a discriminator as a judge of the quality of the generated objects. Furthermore, the objects are also generated in a more creative way because the generator is never shown the original objects in the training data set, but is only given guidance to fool the discriminator. As a result, generative adversarial networks learn to create creative counterfeits. In certain domains such as image and video data, this approach can have remarkable results; unlike variational autoencoders, the quality of the images is not blurry. One can create vivid images and videos with an artistic flavor, that give the impression of dreaming. These techniques can also be used in numerous applications like text-to-image or image-to-image translation. For example, one can specify a text description, and then obtain a fantasy image that matches the description [392]. Generative adversarial networks are discussed in Section 10.4 of Chapter 10.

4.11 Summary

Neural networks often contain a large number of parameters, which causes overfitting. One solution is to restrict the size of the networks up front. However, such an approach often provides suboptimal solutions when the model is complex and sufficient data are available. A more flexible approach is to use tunable regularization, in which a large number of parameters are allowed. In such cases, the regularization restricts the size of the parameter space in a soft way. The most common form of regularization is penalty-based regularization. It is common to use penalties on the parameters, although it is also possible to use penalties on the activations of the hidden units. The latter approach leads to sparse representations in the hidden units. Ensemble learning is a common approach to reduce variance, and some ensemble methods like *Dropout* are specifically designed for neural networks. Other common regularization methods include early stopping and pretraining. Pretraining acts as a regularizer by acting as a form of semi-supervised learning, which works from the simple to the complex by initializing with a simple heuristic and using backpropagation to discover

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