

MASTER THESIS

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Neural Networks and Knowledge Distillation

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Mathematics

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Dedication.

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Introduction

In the recent years we have experienced a remarkable surge in artificial intelligence (AI). This rise has been fueled by an increase in computational power, making the creation of more powerful and complex models feasible. However, when deploying a model to a large number of users, we are usually more stringent regarding latency, as well as computational and storage capacity. Yet, simply using a smaller model does not take full advantage of the training capacity we usually possess.

A proposed solution to these seemingly opposing constrains is knowledge distillation. This approach involves training a large model, known as the teacher, and transferring its knowledge to a smaller model, called student, we want to deploy. We believe that the teacher is able to better extract the structure from the data. It learns to differentiate between large number of classes and then correctly predict the label when exposed to new data. Additionally, the trained model also assigns weights to all of the possible classes, which are then converted into probabilities using a softmax function. Even though these are often very small for the incorrect answers, they can still provide valuable information about how the larger model generalizes.

For example, an image of a horse will be correctly labeled by the teacher model with high probability close to 1. However, the model might also assign a small but nonzero probability that the image is a zebra. We argue that this probability will still be many times higher than the probability assigned to an unrelated class, such as a car.

Transferring this knowledge from the teacher to the student is done through distillation, where the student model is trained using the class probabilities produced by the teacher as soft targets. In the original paper, the distillation process is formulated as the minimization of the Kullback–Leibler (KL) divergence.

In this work, we propose enhancing the distillation process by replacing the KL divergence with Rényi divergence, which serves as its generalization, and introduces an additional hyperparameter α . We aim to formally define this new distillation framework, analyze the theoretical properties of Rényi-based distillation, and conduct experiments to evaluate the appropriateness of this approach.

1. Rényi Divergence and Knowledge Distillation

In this chapter, we begin by examining the concepts of entropy, cross-entropy, and divergence. In particular, we define Rényi divergence, establish its connection to KL divergence, and inspect some of the theoretical properties stated in van Erven and Harremoës [2012]. In the second part, we formally define the notion of knowledge distillation, as proposed in Hinton et al. [2015], and inspect some of the theoretical results presented therein. Furthermore, we analyze how these results change when incorporating Rényi divergence into the distillation process.

1.1 KL Divergence and Rényi Divergence

The concept of entropy, as the amount of uncertainty regarding the outcome of an experiment, was introduced by Shannon [1948].

Definition 1. The entropy of a probability distribution $P = (p_1, \ldots, p_n)$ is given by

$$H(P) = -\sum_{i=1}^{n} p_i \log p_i,$$

where we adopt the convention that $0 \log 0 = 0$.

Example. Let P be the probability distribution of a fair coin toss, i.e., $P = (\frac{1}{2}, \frac{1}{2})$. The entropy H(P) is approximately 0.693. Next, let Q represent the probability distribution of an unfair coin toss, i.e., $Q = (\frac{4}{10}, \frac{6}{10})$. Here, the entropy H(Q) is smaller than H(P), approximately 0.673. In other words, we are less uncertain about the outcome of the unfair coin toss than about the fair coin toss.

To determine the similarity between two probability distributions, we cannot simply subtract their entropies. For example, the entropy of $P_1 = (\frac{4}{10}, \frac{6}{10})$ is the same as the entropy of $P_2 = (\frac{6}{10}, \frac{4}{10})$, yet they represent different distributions. Therefore, we use the concept of divergence, as proposed by Kullback and Leibler [1951]. First, we define a related notion of cross-entropy.

Definition 2. The cross-entropy of a probability distribution $P = (p_1, \ldots, p_n)$ relative to another distribution $Q = (q_1, \ldots, q_n)$ is given by

$$H(P,Q) = -\sum_{i=1}^{n} p_i \log q_i,$$

where we adopt the convention that $0 \log 0 = 0$.

Example. Let P and Q be the probability distributions as described in the example above, i.e., $P=(\frac{1}{2},\frac{1}{2})$ and $Q=(\frac{4}{10},\frac{6}{10})$. The cross-entropy of P relative to Q is $H(P,Q)\approx 0.714$. On the other hand $H(Q,P)\approx 0.693$ and we observe that cross-entropy is not symmetric in its arguments.

Definition 3. The Kullback-Leibler divergence (KL divergence) of a probability distribution $P = (p_1, \ldots, p_n)$ relative to another distribution $Q = (q_1, \ldots, q_n)$ is given by

$$D_{KL}(P||Q) = \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i},$$

where we adopt the convention that $\frac{0}{0} = 0$ and $\frac{x}{0} = \infty$ for x > 0.

We can decompose the KL divergence into two terms, as

$$D_{KL}(P||Q) = \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i}$$

$$= \sum_{i=1}^{n} p_i \log p_i + \left(-\sum_{i=1}^{n} p_i \log q_i\right),$$

$$= -H(P) + H(P, Q)$$
(1.1)

and we observe that cross-entropy can be decomposed into entropy and KL divergence.

Example. Let P and Q be probability distributions, given as $P=(\frac{1}{2},\frac{1}{2})$ and $Q=(\frac{4}{10},\frac{6}{10})$. From the previous examples, we know that $H(P)\approx 0.693$ and $H(P,Q)\approx 0.714$. Using Equation 1.1, we can calculate the KL divergence of P relative to Q as $D_{\mathrm{KL}}(P\|Q)=-H(P)+H(P,Q)\approx 0.021$.

Kullback–Leibler divergence was later generalized by Rényi [1961]. We begin with the definition.

Definition 4. The Rényi divergence of order α of a probability distribution $P = (p_1, \ldots, p_n)$ relative to another distribution $Q = (q_1, \ldots, q_n)$ is given by

$$D_{\alpha}(P||Q) = \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_i^{\alpha} q_i^{1-\alpha},$$

where α is positive number distinct from 1, and we adopt the convention that $\frac{0}{0} = 0$ and $\frac{x}{0} = \infty$ for x > 0.

This definition of Rényi divergence assumes that probability distributions P and Q are discrete. For continuous spaces we can substitute the sum by Lebesgue integral (see van Erven and Harremoës [2012]). Now, we present an example that motivated the introduction of the normalization term $\frac{1}{\alpha-1}$ in the definition.

Example. Let Q be a probability distribution and A be a set, such that Q(A) > 0. Define P as the conditional distribution of Q given A, i.e. $P(x) = Q(x|A) = \frac{Q(x)}{Q(A)}$, for $x \in A$. Now compute the Rényi divergence of P relative to Q

$$D_{\alpha}(P||Q) = \frac{1}{\alpha - 1} \log \sum_{x \in A} P(x)^{\alpha} Q(x)^{1 - \alpha},$$

$$= \frac{1}{\alpha - 1} \log \sum_{x \in A} \left(\frac{Q(x)}{Q(A)}\right)^{\alpha} Q(x)^{1 - \alpha},$$

$$= \frac{1}{\alpha - 1} \log \sum_{x \in A} \frac{Q(x)}{Q(A)^{\alpha}},$$

$$= \frac{1}{\alpha - 1} \log \left(Q(A)^{-\alpha} \sum_{x \in A} Q(x)\right),$$

$$= \frac{1}{\alpha - 1} \log Q(A)^{1 - \alpha},$$

$$= -\log Q(A).$$

In this particular example we observe that the factor $\frac{1}{\alpha-1}$ in the definition Rényi divergence has the effect that $D_{\alpha}(P||Q)$ does not depend on α in this example. This factor is moreover crucial in the following consideration.

Definition 4 was formulated for orders $\alpha \in (0,1) \cup (1,\infty)$. We now show that the limits on the borders of the domain for α exist and therefore Rényi divergence can be naturally extended to the cases $\alpha = 0, 1, \infty$. That is, we inspect the limits

$$D_0(P||Q) = \lim_{\alpha \to 0+} D_{\alpha}(P||Q),$$

$$D_1(P||Q) = \lim_{\alpha \to 1} D_{\alpha}(P||Q),$$

$$D_{\infty}(P||Q) = \lim_{\alpha \to \infty} D_{\alpha}(P||Q).$$

where P and Q are discrete distributions on $\{1, \dots, n\}$. For $\alpha = 0$, we have

$$\lim_{\alpha \to 0+} D_{\alpha}(P \| Q) = \lim_{\alpha \to 0+} \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_{i}^{\alpha} q_{i}^{1-\alpha},$$

$$= -\log \sum_{i=1}^{n} \lim_{\alpha \to 0+} p_{i}^{\alpha} q_{i}^{1-\alpha},$$

$$= -\log \sum_{i=1}^{n} q_{i} \lim_{\alpha \to 0+} p_{i}^{\alpha}$$

$$= -\log \sum_{i=1}^{n} q_{i} \mathbb{1}\{p_{i} > 0\},$$
(1.2)

where $\mathbb{1}$ is the indicator function. For $\alpha = 1$, the limit

$$\lim_{\alpha \to 1} \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_i^{\alpha} q_i^{1 - \alpha}$$

is of an indeterminate form $\frac{0}{0}$, allowing us to apply L'Hopital's Rule and we obtain

$$\lim_{\alpha \to 1} \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_i^{\alpha} q_i^{1-\alpha} = \lim_{\alpha \to 1} \frac{\sum_{i=1}^{n} p_i^{\alpha} q_i^{1-\alpha} \log p_i - p_i^{\alpha} q_i^{1-\alpha} \log q_i}{\sum_{i=1}^{n} p_i^{\alpha} q_i^{1-\alpha}},$$

$$= \frac{\sum_{i=1}^{n} p_i \log p_i - p_i \log q_i}{\sum_{i=1}^{n} p_i},$$

$$= \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i}.$$
(1.3)

Lastly, for $\alpha = \infty$, we denote $Z(\alpha) = \sum_{i=1}^n p_i^{\alpha} q_i^{1-\alpha}$, and $M = \max_i \frac{p_i}{q_i}$ and let $j \in \{1, \dots, n\}$ be the first index at which this maximum is attained. We have

$$M^{\alpha} q_j \le Z(\alpha) \le M^{\alpha} \sum_{i=1}^n q_i. \tag{1.4}$$

Taking the logarithm and dividing by $\alpha - 1$ preserves the inequalities, as the logarithm is a monotonic function and $\alpha > 1$. From (1.4), we obtain that

$$\frac{\alpha log M + \log q_j}{\alpha - 1} \le \frac{1}{\alpha - 1} \log Z(\alpha) \le \frac{\alpha log M + \log 1}{\alpha - 1}.$$

Taking the limit $\alpha \to \infty$

$$\log M = \lim_{\alpha \to \infty} \frac{\alpha log M + \log q_j}{\alpha - 1} \le \lim_{\alpha \to \infty} \frac{1}{\alpha - 1} \log Z(\alpha) \le \lim_{\alpha \to \infty} \frac{\alpha log M + \log 1}{\alpha - 1} = \log M.$$

Thus,

$$\lim_{\alpha \to \infty} \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_i^{\alpha} q_i^{1-\alpha} = \lim_{\alpha \to \infty} \frac{1}{\alpha - 1} \log Z(\alpha) = \log M,$$

$$= \max_{i} \log \frac{p_i}{q_i}.$$
(1.5)

The limits (1.2), (1.3), (1.5) allow us to define the Rényi divergences

$$D_0(P||Q) = -\log \sum_{i=1}^n q_i \, \mathbb{1}\{p_i > 0\},$$

$$D_1(P||Q) = \sum_{i=1}^n p_i \log \frac{p_i}{q_i},$$

$$D_{\infty}(P||Q) = \max_i \log \frac{p_i}{q_i}.$$

Comparing to Definition 3, we see that

$$D_1(P||Q) = D_{KL}(P||Q),$$

and Rényi divergence indeed generalizes KL divergence.

Another important case of Rényi divergence is for $\alpha = \frac{1}{2}$. For only this value the Rényi divergence is symmetric, i.e., $D_{1/2}(P||Q) = D_{1/2}(Q||P)$. Even with this additional property, it still does not satisfy the definition of a metric, as the triangle inequality does not hold. However, Rényi divergence of order $\frac{1}{2}$ can be

rewritten as a function of the squared Hellinger distance, which, as defined in Cheng et al. [2024], for discrete probability distributions P and Q is given by

$$H^{2}(P||Q) = \frac{1}{2} \sum_{i=1}^{n} (p_{i}^{\frac{1}{2}} - q_{i}^{\frac{1}{2}})^{2}.$$

We also get a relation

$$\frac{1}{2} \sum_{i=1}^{n} (p_i^{\frac{1}{2}} - q_i^{\frac{1}{2}})^2 = \frac{1}{2} \left(\sum_{i=1}^{n} p_i + \sum_{i=1}^{n} q_i - 2 \sum_{i=1}^{n} p_i^{\frac{1}{2}} q_i^{\frac{1}{2}} \right) = 1 - \sum_{i=1}^{n} p_i^{\frac{1}{2}} q_i^{\frac{1}{2}},$$

which we can use in the definition of Rényi divergence of order $\frac{1}{2}$ to express it in terms of the Hellinger distance

$$D_{1/2}(P||Q) = \frac{1}{\frac{1}{2} - 1} \log \sum_{i=1}^{n} p_i^{\frac{1}{2}} q_i^{1 - \frac{1}{2}} = -2 \log(1 - H^2(P||Q)).$$

We can also establish a connection between Rényi divergence of order α and $1-\alpha$ for $0<\alpha<1$.

$$D_{1-\alpha}(P||Q) = \frac{1}{-\alpha} \log \sum_{i=1}^{n} p_i^{1-\alpha} q_i^{\alpha},$$

$$= \frac{1-\alpha}{\alpha} \left(\frac{\alpha}{1-\alpha} \frac{1}{-\alpha} \log \sum_{i=1}^{n} q_i^{\alpha} p_i^{1-\alpha} \right),$$

$$= \frac{1-\alpha}{\alpha} D_{\alpha}(Q||P).$$

Example. Let us have a probability distributions $Q = (\frac{4}{10}, \frac{6}{10})$ and P = (p, 1-p) for some $p \in [0, 1]$. On the left side of Figure 1.1, we plot $D_{\alpha}(P||Q)$ as a function of p, for different values of α . Clearly when $p = \frac{4}{10}$, the divergence is zero for any α since both distributions are identical. Additionally, the divergence remains the same for any α , when p = 0 or p = 1. This follows from the fact that $D_{\alpha}(P||Q) = \frac{1}{\alpha-1}\log q_1^{1-\alpha} = -\log q_1$ when p = 1 and $D_{\alpha}(P||Q) = -\log q_2$ when p = 0.

On the right side of Figure 1.1, we plot $D_{\alpha}(P||Q)$ as a function of q, where we now set $P = (\frac{4}{10}, \frac{6}{10})$ and Q = (q, 1-q). Again, the divergence is always equal to zero, when the distributions are identical, e.g. when $q = \frac{4}{10}$. However, for q = 0 or q = 1, we obtain the expression $\frac{x}{0}$ for x > 0, which as defined in Definition 4, is set to ∞ for $\alpha \in (0,1) \cap (1,\infty)$. Thus, the divergence is also ∞ . For $\alpha = 1$, the divergence is also infinite,, as follows from Definition 3. Interestingly, for $\alpha = 0$, from (1.2) we derive that the divergence is 0, which it is for any q.

For other values of α , the divergence varies, but a clear ordering emerges. That is, in the first example, the value of $D_{\alpha}(P||Q)$ for $\alpha > \beta$ is greater than or equal to $D_{\beta}(P||Q)$ for any $p \in [0,1]$, this is also true for the second example for any $p \in [0,1]$. Moreover, as shown by van Erven and Harremoës [2012], this holds in general, as Rényi divergence is non-decreasing in α .

Additionally, in the first example, we observe that for larger values of α the derivative is greater when p is close to $\frac{4}{10}$, whereas it is smaller when p is near 0 or 1. The opposite holds for smaller values of α . Conversely, for the second example, the derivative is high as we get near 0 or 1, actually it converges to

infinity for $\alpha > 0$. As shown in the figure, the rate of this convergence is slower for small values of α .

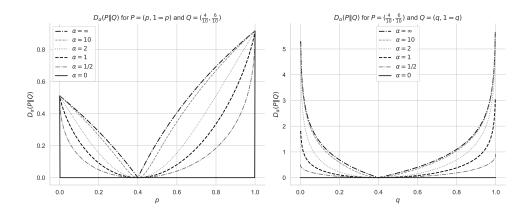


Figure 1.1: Example of Rényi divergence for a fixed distribution and another varying along the x-axis.

The final property we focus on is the lower semi-continuity.

Theorem 1. Suppose we have a discrete sample space $\mathcal{Z} = \{z_1, z_2, z_3, \dots\}$ and sigma-algebra \mathcal{A} is the power set of \mathcal{Z} . Then, for any order $\alpha \in (0, \infty]$, the Rényi divergence is a lower semi-continuous function of the pair (P, Q) in the weak topology.

Proof. Let P_1, P_2, \cdots and Q_1, Q_2, \cdots be sequences of discrete distributions that weakly converge to P and Q, respectively. We need to show

$$\liminf_{n\to\infty} D_{\alpha}(P_n||Q_n) \ge D_{\alpha}(P||Q).$$

Firstly, the weak convergence of discrete distribution P means that for every bounded continuous function h

$$\int hdP_n \to \int hdP.$$

As the sample set is discrete, we may set $h = \mathbb{1}\{z_i\}$ for any $i \in \mathbb{N}$, which is a bounded continuous function, and we obtain

$$P_n(z_i) = \int \mathbb{1}\{z_i\} dP_n \to \int \mathbb{1}\{z_i\} dP = P(z_i).$$

Now, any measurable set $A \in \mathcal{A}$ is just union of the individual elementary outcomes z_i and thus the probability on any set A is just the sum of the probabilities of the elementary outcomes. Using the convergence above we get

$$P_n(A) = \sum_{z_i \in A} P_n(z_i) \to \sum_{z_i \in A} P(z_i) = P(A),$$

and we proved that sequences P_1, P_2, \cdots and Q_1, Q_2, \cdots also converge pointwise to P and Q, respectively. Thus, also the sequence of the pairs (P_n, Q_n) converges pointwise to (P, Q).

Now, we can apply Fatou's lemma term-by-term on the sum

$$\liminf_{n\to\infty} \sum_{i} P_n(z_i)^{\alpha} Q_n(z_i)^{1-\alpha} \ge \sum_{i} \liminf_{n\to\infty} P_n(z_i)^{\alpha} Q_n(z_i)^{1-\alpha} \ge \sum_{i} P(z_i)^{\alpha} Q(z_i)^{1-\alpha}.$$

Taking the logarithm and scaling the by $\frac{1}{\alpha-1}$ preserves this inequality, thus yielding the lower semi-continuity of $D_{\alpha}(P||Q)$.

1.2 Knowledge Distillation

Let us define a machine learning model as a function that maps input data to output predictions

$$f_{\theta}: \mathcal{X} \to \mathcal{Y},$$

where \mathcal{X} is the input space, \mathcal{Y} is the output space and θ represents the set of parameters of the model. In our case, as input, the model receives images from \mathcal{X} , where each image is represented as a tensor in $\mathbb{R}^{h \times w \times c}$, where h and w denote the height and width in pixels, respectively, and c represents the number of channels, where for RGB images c = 3. We assume a classification task with n classes, i.e., $\mathcal{Y} = \mathbb{R}^n$, so the model outputs a vector of n real-valued scores, referred to as logits, given by

$$z = f_{\theta}(x), \tag{1.6}$$

for $x \in \mathcal{X}$. To convert these logits into probabilities, we use the softmax function, which is defined as

$$\sigma(s)_c = \frac{e^s}{\sum_{k=1}^n e^s}, \qquad c = 1, 2, \dots, n,$$
 (1.7)

where $s \in \mathcal{Y}$. Now let

$$q_c = \sigma(z)_c, \qquad c = 1, 2, \cdots, n,$$

which represents the probability that x belongs to class c. We denote the probability distribution produced by the model f_{θ} as $Q = (q_1, q_2, \dots, q_n)$.

Additionally, a hyperparameter T, called temperature, is introduced to control the entropy of the output distribution. That is we set for T > 0

$$q_c^T = \sigma \left(\frac{z}{T}\right)_c, \qquad c = 1, 2, \cdots, n.$$

The produced probability distribution is $Q^T = (q_1^T, q_2^T, \dots, q_n^T)$. The process in called temperature scaling and popular choices for T according to Cho and Hariharan [2019] are 3, 4 and 5. Clearly, $Q^1 = Q$.

Example. Following the example from the introduction, suppose a model f_{θ} that for given input yields logits for the classes "horse", "zebra", and "car", equal to 5.4, 0.2, and -1.3 respectively. In Figure 1.2, we see the logit values in a bar chart, along with the computed probabilities using the softmax function, both without and with temperature scaling, the latter corresponding to T=4.

Without temperature scaling, the model is highly confident that the input belongs to the class horse (> 0.99), while the probabilities for the remaining classes are essentially zero. We observe that the effect of the temperature scaling is that the model is less confident about the true label while the order of the class probabilities in maintained.

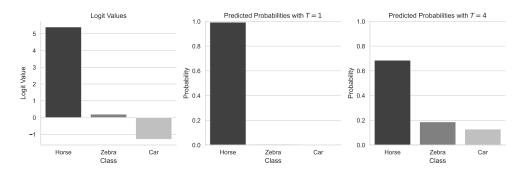


Figure 1.2: Example of temperature scaling.

Let $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ be a dataset, containing a total of N samples, where $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ for all $i \in \{1, 2, \dots, N\}$.

The training of the model f_{θ} involves minimizing the loss function

$$\mathcal{L}_{CE}(\theta) = \sum_{i=1}^{N} H(y_i || Q) = -\sum_{i=1}^{N} \sum_{j=1}^{n} y_{i,j} \log q_j,$$
 (1.8)

with respect to the parameters θ , where Q is the probability distribution obtained by applying the softmax function to the model's output, and y_i is the one-hot ground-truth label.

Remark. Our notation for the loss function in this chapter is a simplification. In general, a loss function is a deterministic function $\mathcal{L}: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$. Thus, we simplify $\mathcal{L}_{CE}(\theta) = \mathcal{L}_{CE}(y, f_{\theta}(x))$, where $(x, y) \in \mathcal{X} \times \mathcal{Y}$.

Although KL divergence provides a more intuitive measure of the difference between two distributions, being zero when the distributions are equal, unlike cross-entropy, we did not use it in Equation 1.8. As shown in Equation 1.1, H(P) does not depend on Q. Thus, the derivative of $D_{KL}(P||Q)$ with respect to Q is equal to the derivative of H(P||Q). Moreover, since cross-entropy is computationally simpler, especially when P represents one-hot labels, it is often preferred over KL divergence in machine learning applications.

Remark. In the context of knowledge distillation, the training process defined in Equation 1.8 is referred to as vanilla training. This serves as a benchmark against which we compare the results of knowledge distillation.

Definition 5. Knowledge distillation is a model compression technique where a smaller student model f_{θ} is trained to mimic a larger teacher model f_{t} , which has been already pre-trained. The student model outputs logits z, which are converted into probability distribution $Q^{T} = (q_{1}^{T}, \dots, q_{n}^{T})$ using softmax function introduced in Equation 1.7,

$$q_c^T = \sigma \left(\frac{z}{T}\right)_c = \frac{e^{\frac{z_c}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}}, \qquad c = 1, 2, \dots, n.$$

Similarly, the teacher model outputs logits v, which are converted into probability distribution $P^T = (p_1^T, \dots, p_n^T)$ using softmax function,

$$p_c^T = \sigma \left(\frac{v}{T}\right)_c = \frac{e^{\frac{v_c}{T}}}{\sum_{k=1}^n e^{\frac{v_k}{T}}}, \qquad c = 1, 2, \dots, n.$$

The training process utilizes a transfer dataset \mathcal{D} and optimizes the loss function of the form

$$\mathcal{L}(\theta) = (1 - \beta)\mathcal{L}_{CE}(\theta) + \beta\mathcal{L}_{KL}(\theta), \tag{1.9}$$

where $\mathcal{L}_{CE}(\theta)$ is the standard cross-entropy loss with ground truth labels

$$\mathcal{L}_{CE}(\theta) = \sum_{i=1}^{N} H(y_i || Q),$$

$$= -\sum_{i=1}^{N} \sum_{j=1}^{n} y_{i,j} \log q_j,$$
(1.10)

and $\mathcal{L}_{KL}(\theta)$ is the Kullback-Leibler divergence loss with teacher's predictions

$$\mathcal{L}_{KL}(\theta) = T^2 \sum_{i=1}^{N} D_{KL}(P^T || Q^T),$$

$$= T^2 \sum_{i=1}^{N} \sum_{j=1}^{n} p_j^T \log \frac{p_j^T}{q_j^T},$$
(1.11)

 y_i is the one-hot ground-truth label, and T and β are hyperparameters.

The hyperparameter T in Definition 5 denotes temperature. During training, we apply temperature scaling to both the teacher and the student in Equation 1.11. By increasing T, we soften the probabilities, thus retaining inter-class similarities by driving the predictions away from 0 and 1. The second hyperparameter, β , controls the balance between training on the true labels and training on the so-called soft targets provided by the teacher model. A common choice for β is 0.9 (see Cho and Hariharan [2019]).

Remark. In many cases, the teacher model f_t from Definition 5, has been pretrained on the same dataset \mathcal{D} . However, this is not always the case, for example, the teacher model may be trained on a much broader dataset or one that contains many more classes.

We observe that, unlike in Equation 1.10, which is simply the sum of the cross-entropies, in Equation 1.11, the total loss also includes the term T^2 . To understand the origin of this term we first calculate the derivatives of KL divergence $D_{\mathrm{KL}}(P^T || Q^T)$ with respect to the logits of Q^T . We compute the following

$$\begin{split} \frac{\partial D_{\mathrm{KL}}(P^T \| Q^T)}{\partial z_j} &= \frac{\partial H(P^T \| Q^T)}{\partial z_j} = -\frac{\partial}{\partial z_j} \sum_{i=1}^n p_i^T \log \frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}}, \\ &= \left(\sum_{i=1}^n p_i^T\right) \frac{\partial}{\partial z_j} \log \sum_{k=1}^n e^{\frac{z_k}{T}} - \frac{\partial}{\partial z_j} \sum_{i=1}^n p_i^T \frac{z_i}{T}, \\ &= \frac{1}{T} \frac{e^{z_j}}{\sum_{k=1}^n e^{z_k}} - \frac{p_j^T}{T}, \\ &= \frac{1}{T} (q_j^T - p_j^T). \end{split}$$

Thus, the derivative of both KL divergence and cross-entropy is given by

$$\frac{\partial D_{\mathrm{KL}}(P^T \| Q^T)}{\partial z_j} = \frac{\partial H(P^T \| Q^T)}{\partial z_j} = \frac{1}{T} (q_j^T - p_j^T). \tag{1.12}$$

Now, similarly to Hinton et al. [2015], we assume centered logits $\sum_{k=1}^{n} z_k = \sum_{k=1}^{n} v_k = 0$. Then we have

$$\frac{\partial H(P^T || Q^T)}{\partial z_j} = \frac{1}{T} (q_j^T - p_j^T) = \frac{1}{T} \left(\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}} - \frac{e^{\frac{v_j}{T}}}{\sum_{k=1}^n e^{\frac{v_k}{T}}} \right). \tag{1.13}$$

Now, we approximate the exponential function using a Taylor polynomial of degree one and we obtain

$$\frac{\partial H(P^T \| Q^T)}{\partial z_j} \approx \frac{1}{T} \left(\frac{1 + \frac{z_j}{T}}{n + \sum_{k=1}^n \frac{z_k}{T}} - \frac{1 + \frac{v_j}{T}}{n + \sum_{k=1}^n \frac{v_k}{T}} \right) = \frac{1}{nT^2} (z_j - v_j). \tag{1.14}$$

Thus, the loss gradient decreases proportionally to $\frac{1}{T^2}$ as the temperature T increases. By incorporating the term T^2 into Equation 1.11, we ensure that the relative contribution of $\mathcal{L}_{\text{CE}}(\theta)$ and $\mathcal{L}_{\text{KL}}(\theta)$ remains approximately the same.

For lower temperature, where the approximation by the Taylor polynomial is very inaccurate, Hinton et al. [2015] states that the distillation pays less attention to matching logits much more negative than average. This is advantageous, as they may be significantly noisier, given that the student model is not penalized for them during training. On the other hand, they might convey useful information about the knowledge acquired by the teacher. Based on empirical evidence, the authors claim that ignoring large negative logits has a positive effect, as intermediate temperatures yield the best results.

Now, we replace the KL divergence loss in (1.11) by a general Rényi divergence of order α . Thus, the loss function (1.9) is replaced by

$$\mathcal{L}(\theta) = (1 - \beta)\mathcal{L}_{CE}(\theta) + \beta\mathcal{L}_{\alpha}(\theta), \tag{1.15}$$

where

$$\mathcal{L}_{\alpha}(\theta) = \frac{T^{2}}{\alpha} \sum_{i=1}^{N} D_{\alpha}(P^{T} \| Q^{T}),$$

$$= \frac{T^{2}}{\alpha} \sum_{i=1}^{N} \sum_{j=1}^{n} \frac{1}{\alpha - 1} \log(p_{j}^{T})^{\alpha} (q_{j}^{T})^{1 - \alpha}.$$
(1.16)

Similarly to above for (1.11) we elaborate on the normalizing factor in Equation 1.16 which is now equal to $\frac{T^2}{\alpha}$. Firstly, we compute the derivatives of $D_{\alpha}(P^T || Q^T)$ with respect to the logits of Q^T . For simplicity, we omit T in P^T, Q^T, p^T and q^T . We have

$$\frac{\partial D_{\alpha}(P||Q)}{\partial z_{j}} = \frac{\partial}{\partial z_{j}} \frac{1}{\alpha - 1} \log \sum_{i=1}^{n} p_{i}^{\alpha} \left(\frac{e^{\frac{z_{i}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}} \right)^{1 - \alpha}.$$

Now denote $Z = \sum_{i=1}^n p_i^{\alpha} \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}} \right)^{1-\alpha}$. By the chain rule we have

$$\frac{\partial D_{\alpha}(P||Q)}{\partial z_{i}} = \frac{\partial}{\partial z_{i}} \frac{1}{\alpha - 1} \log Z = \frac{1}{\alpha - 1} \frac{1}{Z} \frac{\partial Z}{\partial z_{i}}.$$

Now we need to calculate $\frac{\partial Z}{\partial z_j}$.

$$\begin{split} \frac{\partial Z}{\partial z_{j}} &= \frac{\partial}{\partial z_{j}} \sum_{i=1}^{n} p_{i}^{\alpha} \left(\frac{e^{\frac{z_{i}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{1-\alpha}, \\ &= \frac{\partial}{\partial z_{j}} p_{j}^{\alpha} \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{1-\alpha} + \frac{\partial}{\partial z_{j}} \sum_{i \neq j}^{n} p_{i}^{\alpha} \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{1-\alpha}, \\ &= p_{j}^{\alpha} (1-\alpha) \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{-\alpha} \frac{\frac{1}{T} \sum_{k=1}^{n} e^{\frac{z_{k}}{T}} e^{\frac{z_{j}}{T}} - \frac{1}{T} e^{\frac{z_{j}}{T}} e^{\frac{z_{j}}{T}}}{\left(\sum_{k=1}^{n} e^{\frac{z_{j}}{T}}\right)^{2}} \\ &- \sum_{i \neq j}^{n} p_{i}^{\alpha} \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{-\alpha} (1-\alpha) \frac{e^{\frac{z_{j}}{T}}}{\left(\sum_{k=1}^{n} e^{\frac{z_{j}}{T}}\right)^{2}} e^{\frac{z_{j}}{T}} \frac{1}{T}, \\ &= \frac{1-\alpha}{T} \left[p_{j}^{\alpha} \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}}\right)^{1-\alpha} \frac{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}} - e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}} \right], \\ &= \frac{1-\alpha}{T} \left[p_{j}^{\alpha} q_{j}^{1-\alpha} (1-q_{j}) - \sum_{i \neq j}^{n} p_{i}^{\alpha} q_{i}^{1-\alpha} q_{j} \right], \\ &= \frac{1-\alpha}{T} \left[p_{j}^{\alpha} q_{j}^{1-\alpha} - q_{j} \sum_{i=1}^{n} p_{i}^{\alpha} q_{i}^{1-\alpha} \right], \\ &= \frac{1-\alpha}{T} (p_{j}^{\alpha} q_{j}^{1-\alpha} - q_{j} \sum_{i=1}^{n} p_{i}^{\alpha} q_{i}^{1-\alpha} \right], \end{split}$$

Now, inserting $\frac{\partial Z}{\partial z_j}$ into the original equation, we obtain

$$\frac{\partial D_{\alpha}(P||Q)}{\partial z_j} = \frac{1}{\alpha - 1} \frac{\frac{1 - \alpha}{T} (p_j^{\alpha} q_j^{1 - \alpha} - q_j Z)}{Z} = \frac{q_j Z - p_j^{\alpha} q_j^{1 - \alpha}}{TZ}.$$

We can also substitute the original expression for Z and simplify the result to derive

$$\frac{\partial D_{\alpha}(P||Q)}{\partial z_j} = \frac{1}{T} \left(q_j - \frac{p_j^{\alpha} q_j^{1-\alpha}}{\sum_{i=1}^n p_i^{\alpha} q_i^{1-\alpha}} \right), \tag{1.17}$$

where for $\alpha = 1$, we arrive at the same result as for KL divergence.

If the distribution P represents one-hot labels, the derivative simplifies to the same form as in Equation 1.13. This holds for any choice of α , which is why we do not modify the \mathcal{L}_{CE} term in knowledge distillation or vanilla training.

From the result in Equation 1.17, we derive an analogous expression to Equation 1.14, using previously established notation and assumption of centered logits. Moreover, we approximate the exponential function using a Taylor polynomial of degree one. We derive

$$\begin{split} \frac{\partial D_{\alpha}(P\|Q)}{\partial z_{j}} &= \frac{1}{T} \left[\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}} - \left(\frac{e^{\frac{v_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{v_{k}}{T}}} \right)^{\alpha} \left(\frac{e^{\frac{z_{j}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}} \right)^{1-\alpha} \right. \\ & \left. \left(\sum_{i=1}^{n} \left(\frac{e^{\frac{v_{i}}{T}}}{\sum_{k=1}^{n} e^{\frac{v_{k}}{T}}} \right)^{\alpha} \left(\frac{e^{\frac{z_{i}}{T}}}{\sum_{k=1}^{n} e^{\frac{z_{k}}{T}}} \right)^{1-\alpha} \right] \right], \\ & \approx \frac{1}{T} \left[\frac{1 + \frac{z_{j}}{T}}{n + \sum_{k=1}^{n} \frac{z_{k}}{T}} - \frac{1 + \frac{\alpha v_{j}}{T}}{\left(n + \sum_{k=1}^{n} \frac{v_{k}}{T} \right)^{\alpha}} \frac{1 + \frac{(1-\alpha)z_{j}}{T}}{\left(n + \sum_{k=1}^{n} \frac{z_{k}}{T} \right)^{1-\alpha}} \right. \\ & \left. \left(\sum_{i=1}^{n} \frac{1 + \frac{\alpha v_{i}}{T}}{\left(n + \sum_{k=1}^{n} \frac{v_{k}}{T} \right)^{\alpha}} \frac{1 + \frac{(1-\alpha)z_{i}}{T}}{\left(n + \sum_{k=1}^{n} \frac{z_{k}}{T} \right)^{1-\alpha}} \right)^{-1} \right], \\ & = \frac{1}{T} \left[\frac{1 + \frac{z_{j}}{T}}{n} - \frac{1 + \frac{\alpha v_{j}}{T} + \frac{(1-\alpha)z_{j}}{T} + \frac{\alpha (1-\alpha)v_{j}z_{j}}{T^{2}}}{n} \right. \\ & \left. \left(\frac{1}{n} \sum_{i=1}^{n} 1 + \frac{\alpha v_{i}}{T} + \frac{(1-\alpha)z_{i}}{T} + \frac{\alpha (1-\alpha)v_{i}z_{i}}{T^{2}} \right)^{-1} \right]. \end{split}$$

When using the approximation of the exponential function by the first Taylor polynomial, we assume that the higher-order terms are negligible. Particularly, this means that $\alpha^2 v_j^2 = o(T^2)$ and $(1-\alpha)^2 z_j^2 = o(T^2)$. From this we get αv_j and $(1-\alpha)z_j$ are o(T). Thus, their product is $o(T^2)$, which means that $\frac{\alpha(1-\alpha)v_jz_j}{T^2} \approx 0$.

This, together with the previously mentioned assumption of zero-meaned logits, allows us to further simplify the formula.

$$\frac{\partial D_{\alpha}(P||Q)}{\partial z_j} \approx \frac{1}{T} \left[\frac{1 + \frac{z_j}{T}}{n} - \frac{1 + \frac{\alpha v_j}{T} + \frac{(1 - \alpha)z_j}{T}}{n} \left(\frac{n}{n} \right)^{-1} \right] = \frac{\alpha}{nT^2} (z_j - v_j).$$

This formula is similar to that of KL divergence (1.14), except that it is multiplied by α .

2. Stochastic Gradient Descent and Residual Neural Network

In the previous section, we defined the loss function for knowledge distillation incorporating Rényi divergence. In this chapter, we discuss how to minimize this function during training using the stochastic gradient descent algorithm. Additionally, we introduce the model chosen for f_{θ} , which is a Residual Neural Network. Both of these components will be utilized in the practical part of the thesis.

2.1 Stochastic Gradient Descent

Let f_{θ} be a model as defined in (1.6), with with set parameters θ . During training the goal is to minimize the loss function with respect to the parameters θ . Our loss function as defined in Equation 1.15 is given by

$$\mathcal{L}(y, f_{\theta}(x)) = (1 - \beta)\mathcal{L}_{CE}(y, f_{\theta}(x)) + \beta\mathcal{L}_{\alpha}(y, f_{\theta}(x)), \tag{2.1}$$

where $(x, y) \in \mathcal{X} \times \mathcal{Y}$.

We define expected risk of a model f_{θ} given a loss function \mathcal{L} as

$$E(f_{\theta}) = \mathsf{E} \left[\mathcal{L}(y, f_{\theta}(x)) \right], \tag{2.2}$$

where $(x,y) \in \mathcal{X} \times \mathcal{Y}$, which measures the generalization performance of the model f_{θ} . Unfortunately, the distribution of (x,y) is unknown, thus we have to settle for empirical risk which is given by

$$E_N(f_{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(y_i, f_{\theta}(x_i)),$$

where $(x_i, y_i) \in \mathcal{D}$.

The gradient descent (GD) algorithm, proposed by Rumelhart et al. [1986], aims to minimize the empirical risk $E_N(f_\theta)$. In each iteration, the parameters θ are updated using the gradient of the loss function as follows

$$\theta_{t+1} = \theta_t - \gamma \frac{1}{N} \sum_{i=1}^{N} \nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)),$$

where θ_t are the parameters of the model after t iterations of the gradient descent algorithm, γ is the learning rate and $(x_i, y_i) \in \mathcal{D}$. The total number of iterations and learning rate γ are hyperparameters. This algorithm is sometimes called the total gradient algorithm.

A drastic simplification of the previous algorithm is the stochastic gradient descent (SGD) algorithm. In each iteration, the parameters θ are updated as follows

$$\theta_{t+1} = \theta_t - \gamma \nabla_{\theta} \mathcal{L}(y_j, f_{\theta}(x_j)),$$

where $(x_j, y_j) \in \mathcal{D}$ is a single randomly picked datapoint from the dataset.

As noted by Bottou [2010], SGD directly optimizes the expected risk (2.2) since the datapoints are randomly drawn from the ground truth distribution.

According to Bottou [1991], there are three main advantages of using SGD over GD. First, in datasets with redundancy, only a small subset of datapoints is needed to obtain a good estimate of the gradient, making SGD more efficient. Second, while gradient descent may converge to a local minimum from which it cannot escape, the randomness in SGD often allows it to overcome such traps. Finally, SGD enables the assignment of weights to individual datapoints during random selection, helping to correct for underrepresentation or overrepresentation in the dataset relative to the real population.

The main drawback of stochastic gradient descent is the high variance of the estimator of the expected risk, as it relies on only a single sample. To retain the advantages while reducing variance, the mini-batch stochastic gradient descent algorithm was introduced, defined as follows

$$\theta_{t+1} = \theta_t - \gamma \frac{1}{B} \sum_{i=1}^{B} \nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)),$$

where $(x_j, y_j) \in \mathcal{D}$ and B < N is the batch size, which is typically a power of 2. Additionally, we introduce weight decay λ regularization term to discourage large values of θ , along with Nesterov momentum μ based on the formula from Sutskever et al. [2013]. Both λ and μ are hyperparameters. The resulting algorithm is as follows

$$b_{t+1} = \mu b_t + \left(\frac{1}{B} \sum_{i=1}^{B} \nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)) + \lambda \theta_t\right),$$

$$\theta_{t+1} = \theta_t - \gamma \left(\frac{1}{B} \sum_{i=1}^{B} \nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)) + \lambda \theta_t + \mu b_{t+1}\right).$$

The gradient of the loss function is calculated using backpropagation, that is

$$\nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)) = \frac{\partial \mathcal{L}(y_i, f_{\theta}(x_i))}{\partial \theta} = \frac{\partial \mathcal{L}(y_i, f_{\theta}(x_i))}{\partial z} \frac{\partial z}{\partial \theta},$$

where z is the vector of the logits that the model outputs. From Equations 1.12, 1.16, 1.17 and 2.1 we get

$$\frac{\partial \mathcal{L}(y_i, f_{\theta}(x_i))}{\partial z} = (1 - \beta) \frac{\partial \mathcal{L}_{CE}(y_i, f_{\theta}(x_i))}{\partial z} + \beta \frac{\partial \mathcal{L}_{\alpha}(y_i, f_{\theta}(x_i))}{\partial z},
= (1 - \beta)(Q - y_i) + \beta \frac{T}{\alpha} \left(Q^T - \frac{(P^T)^{\alpha} \odot (Q^T)^{1 - \alpha}}{\langle (P^T)^{\alpha}, (Q^T)^{1 - \alpha} \rangle} \right),$$

where P^T and Q^T as in Definition 5, \odot denotes the element-wise product, and $\langle \cdot, \cdot \rangle$ represents the scalar product. Thus, the gradient is given by

$$\nabla_{\theta} \mathcal{L}(y_i, f_{\theta}(x_i)) = \left[(1 - \beta)(Q - y_i) + \beta \frac{T}{\alpha} \left(Q^T - \frac{(P^T)^{\alpha} \odot (Q^T)^{1 - \alpha}}{\langle (P^T)^{\alpha}, (Q^T)^{1 - \alpha} \rangle} \right) \right] \frac{\partial z}{\partial \theta}.$$

What remains to be calculated is $\frac{\partial z}{\partial \theta}$, which depends on the architecture of the student model.

2.2 Residual Neural Network

When using knowledge distillation, we need to define the architectures of both the teacher and student models. In this thesis, we chose to use a residual neural network (ResNet). To fully understand its architecture, we first need to define a neuron. The output of a single neuron is given by the following equation

$$z_j = h(\sum_{i=1}^k w_{ij} x_i + b_j), \qquad j = 1, \dots, l,$$

where, $x \in \mathbb{R}^k$ is the input vector, z_j is the output of j-th neuron, w_{ij} represents the weights between the i-th input and the j-th neuron, b_j is the bias for the j-th neuron, and h is the activation function. Commonly used activation functions include the identity function, sigmoid, hyperbolic tangent, and rectified linear unit (ReLU), which is defined as

$$ReLU(x) = max(0, x),$$

which is the activation function used in ResNet.

A layer in a neural network consists of multiple neurons operating in parallel, each computing an output z_j based on its own weights and biases. The output of a layer is a vector of all individual neuron outputs, i.e. $z = (z_1, \dots, z_l)$, where l represents the number of neurons in a layer.

To create a multi-layer neural network, we feed the output of one layer as the input to the next. This type of layer is called a dense (fully connected) layer. The size of each layer may vary, and we denote the total number of layers by L.

This type of layer is not the most common in the ResNet architecture; instead, the convolutional layer is more widely used. Here, the input to the layer is $x \in \mathbb{R}^{h \times w \times c}$, representing an image. For fixed channel k, the output is also an image y given by

$$y_{i,j,k} = \sum_{m=-H}^{H} \sum_{n=-W}^{W} x_{i+m,j+n,k} \cdot K_{m,n}, \qquad (2.3)$$

where $i=1+H, \dots, h-H$, $j=1+W, \dots, w-W$, $K \in \mathbb{R}^{k_h \times k_q}$ is a kernel, $k_h=2H+1$ and $k_w=2W+1$. The values of K are also learned during training. We mostly consider only square kernels, i.e. $k_h=k_w$.

As we see, the output has a different dimension $y \in \mathbb{R}^{(h-2H)\times(w-2W)\times c}$, compared to the input x. This is often undesirable, so we use a method called padding. Using this technique, y is computed as in 2.3 for all $i=1,\dots,h$ and $j=1,\dots,w$, while defining $x_{u,v,k}=0$ for any u<1, u>h, v<1 or v>w.

It is common that there are multiple different kernels in one convolutional layer, each for a different channel, or even more. Thus, the output of a convolutional layer is a collection of images.

The advantage of convolution is that it focuses on local regions of an image, allowing it to detect patterns such as object edges. Additionally, convolution can recognize the same pattern regardless of its location in the image.

We also introduce stride, the output of a layer is computed as

$$y_{i,j,k} = \sum_{m=-H}^{H} \sum_{n=-W}^{W} x_{s \cdot i + m, s \cdot j + n, k} \cdot K_{m,n},$$

where $s \in \mathbb{N}$ is a stride. If s = 2, the output is half the height and width of the input. Thus, $y \in \mathbb{R}^{\frac{h}{2} \times \frac{w}{2} \times c}$.

Another type of layer is the pooling layer, which is similar to a convolutional layer with stride, typically set to 2. However, instead of applying a kernel, it applies a function to the local region. If the function returns the maximum value, it is called max pooling (MaxPool), if it returns the mean, it is called average pooling (AvgPool). There is also a specific type called global max pooling (GMP), where we take the maximum value over the entire image for each channel. As a result, the output is a vector \mathbb{R}^c .

Now, we can define the plain network as described in He et al. [2016], which serves as the backbone of ResNet. The convolutional layers primarily use 3×3 kernels and follow two design rules. When performing convolution with a stride of 1, the number of kernels matches the number of input channels. However, when using a stride of 2, the number of kernels doubles to preserve the complexity. The network ends with a global average pooling layer and a fully-connected layer.

To transform this plain network into ResNet, we introduce the fundamental building block of residual learning—the residual block. This residual block is composed of a function \mathcal{F} and so-called shortcut, represented by an identity function. The function \mathcal{F} represents multiple layers of the neural network and it the part of residual mapping to be learned. The output of this building block y then follows

$$y = \text{ReLU}(\mathcal{F}(x) + x),$$
 (2.4)

where x is the input. This process is depicted in Figure 2.1. If y and x are of a different dimension, we perform linear projection on x, thus, we get

$$y = \text{ReLU}(\mathcal{F}(x) + Wx), \tag{2.5}$$

where W is a matrix of appropriate dimension.

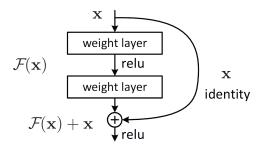


Figure 2.1: Residual block (He et al. [2016]).

The number of layers in \mathcal{F} may vary, but the authors used two layers. Thus, we construct ResNet from the plain network by introducing shortcuts, as shown in Figure 2.2, where solid lines represent the use of Equation 2.4, and dotted lines represent the use of Equation 2.5.

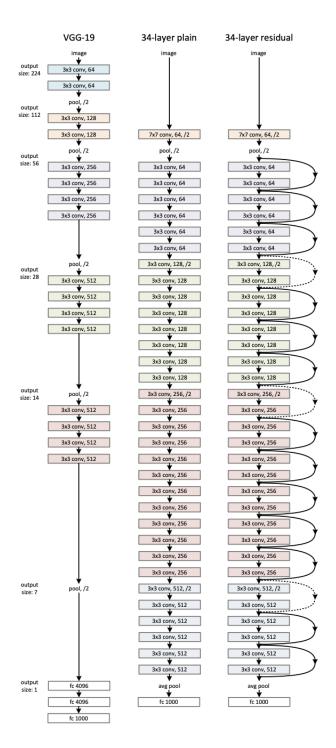


Figure 2.2: Example of network architecture (He et al. [2016]). Left: VGG-19 model as a reference. Middle: a plain network with 34 layers. Right: residual network with 34 layers (ResNet34).

Conclusion

Bibliography

- Léon Bottou. Stochastic gradient learning in neural networks. 1991. URL http://leon.bottou.org/papers/bottou-91c.
- Léon Bottou. Large-scale machine learning with stochastic gradient descent. *Proc.* of COMPSTAT, 09 2010. doi: 10.1007/978-3-7908-2604-3_16.
- JH Cheng, C Zheng, R Yamada, and D Okada. Visualization of the landscape of the read alignment shape of atac-seq data using hellinger distance metric. *Genes & Cells*, 29(1):5–16, January 2024. doi: 10.1111/gtc.13082. Epub 2023 Nov 21.
- Jang Hyun Cho and Bharath Hariharan. On the efficacy of knowledge distillation. CoRR, abs/1910.01348, 2019. URL http://arxiv.org/abs/1910.01348.
- Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. pages 770–778, 2016. doi: 10.1109/CVPR.2016.90.
- Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. Distilling the knowledge in a neural network. arXiv preprint arXiv:1503.02531, 2015.
- S. Kullback and R. A. Leibler. On information and sufficiency. *Ann. Math. Statist.*, 22(1):79–86, 1951.
- Alfréd Rényi. On measures of entropy and information. 1961. URL https://api.semanticscholar.org/CorpusID:123056571.
- David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning representations by back-propagating errors. *nature*, 323(6088):533–536, 1986.
- Claude Elwood Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27:379–423, 1948. URL http://plan9.bell-labs.com/cm/ms/what/shannonday/shannon1948.pdf.
- Ilya Sutskever, James Martens, George Dahl, and Geoffrey Hinton. On the importance of initialization and momentum in deep learning. page III–1139–III–1147, 2013.
- Tim van Erven and Peter Harremoës. Rényi divergence and kullback-leibler divergence. CoRR, abs/1206.2459, 2012. URL http://arxiv.org/abs/1206.2459.

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List of Abbreviations

A. Attachments

A.1 First Attachment