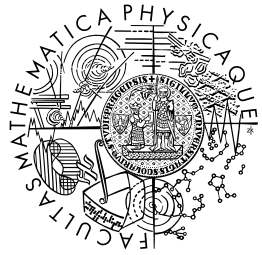

FACULTY
OF MATHEMATICS
AND PHYSICS
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MASTER THESIS

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Neural Networks and Knowledge Distillation

Department of Probability and Mathematical Statistics

Supervisor of the bachelor thesis: Mgr. Ondřej Týbl, Ph.D.

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Dedication.

Title: Neural Networks and Knowledge Distillation

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Klíčová slova: neuronové sítě, strojové učení, destilace znalostí, KL divergence

Contents

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 $P = (p_1, \dots, p_n)$ is given by*

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

where we define $0 \log 0$ as 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 $P = (p_1, \dots, p_n)$ relative to another distribution $Q = (q_1, \dots, q_n)$ 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 define $0 \log \frac{0}{0}$ as 0 and $x \log \frac{x}{0}$ as ∞ for $x > 0$.

We can decompose the KL divergence into two terms, as

$$\begin{aligned} D_{\mathrm{KL}}(P\|Q) &= \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i} \\ &= \sum_{i=1}^{n} p_i \log p_i + \left(- \sum_{i=1}^{n} p_i \log q_i \right), \\ &= - H(P) + H(P, Q) \end{aligned} \tag{1.1}$$

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

Example. Let P and Q be probability distributions, such 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 take the Rényi divergence of P relative to Q

$$
\begin{aligned}
D_\alpha(P\|Q) &= \frac{1}{\alpha-1}\log\sum_{x\in A} P(x)^\alpha Q(x)^{1-\alpha},\\
&= \frac{1}{\alpha-1}\log\sum_{x\in A}\left(\frac{Q(x)}{Q(A)}\right)^\alpha Q(x)^{1-\alpha},\\
&= \frac{1}{\alpha-1}\log\sum_{x\in A}\frac{Q(x)}{Q(A)^\alpha},\\
&= \frac{1}{\alpha-1}\log\left(Q(A)^{-\alpha}\sum_{x\in A}Q(x)\right),\\
&= \frac{1}{\alpha-1}\log Q(A)^{1-\alpha},\\
&= -\log Q(A).
\end{aligned}
$$

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

$$
\begin{aligned}
D_0(P\|Q) &= \lim_{\alpha\to 0} D_\alpha(P\|Q),\\
D_1(P\|Q) &= \lim_{\alpha\to 1} D_\alpha(P\|Q),\\
D_\infty(P\|Q) &= \lim_{\alpha\to\infty} D_\alpha(P\|Q).
\end{aligned}
$$

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

$$
\begin{aligned}
\lim_{\alpha\to 0+} D_\alpha(P\|Q) &= \lim_{\alpha\to 0+}\frac{1}{\alpha-1}\log\sum_{i=1}^n p_i^\alpha q_i^{1-\alpha},\\
&= -\log\sum_{i=1}^n \lim_{\alpha\to 0+} p_i^\alpha q_i^{1-\alpha},\\
&= -\log\sum_{i=1}^n q_i \lim_{\alpha\to 0+} p_i^\alpha\\
&= -\log\sum_{i=1}^n q_i\,\mathbb{1}\{p_i>0\},
\end{aligned}
\tag{1.2}
$$

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 $\dfrac{0}{0}$, allowing us to apply L'Hopital's Rule.

$$\begin{aligned}\lim_{\alpha\to 1}\frac{1}{\alpha-1}\log\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha} &= \lim_{\alpha\to,}\frac{\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha}\log p_i - p_i^{\alpha}q_i^{1-\alpha}\log q_i}{\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha}},\\ &= \frac{\sum_{i=1}^{n}p_i\log p_i - p_i\log q_i}{\sum_{i=1}^{n}p_i},\\ &= \sum_{i=1}^{n}p_i\log\frac{p_i}{q_i}.\end{aligned} \tag{1.3}$$

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 $j\in\{1,\cdots,n\}$ be the index at which this maximum is attained. We have

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

Taking the logarithm and dividing by $\alpha-1$ preserves the inequalities, as the logarithm is a monotonic function and $\alpha\ge 0$. We obtain

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

Taking the limit for $\alpha\to\infty$

$$\begin{aligned}\lim_{\alpha\to\infty}\frac{\alpha log M+\log q_j}{\alpha-1} \le \lim_{\alpha\to\infty}\frac{1}{\alpha-1}\log\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha} \le \lim_{\alpha\to\infty}\frac{\alpha log M+\log 1}{\alpha-1},\\ \log M \le \lim_{\alpha\to\infty}\frac{1}{\alpha-1}\log\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha} \le \log M.\end{aligned}$$

Thus,

$$\begin{aligned}\lim_{\alpha\to\infty}\frac{1}{\alpha-1}\log\sum_{i=1}^{n}p_i^{\alpha}q_i^{1-\alpha} &= \log M,\\ &= \max_i\log\frac{p_i}{q_i}.\end{aligned} \tag{1.4}$$

The limits 1.2, 1.3 , 1.4 allow us to define the Rényi divergences

$$\begin{aligned}D_0(P\|Q) &= -\log\sum_{i=1}^{n}q_i\,\mathbb{1}\{p_i>0\},\\ D_1(P\|Q) &= \sum_{i=1}^{n}p_i\log\frac{p_i}{q_i},\\ D_\infty(P\|Q) &= \max_i\log\frac{p_i}{q_i}.\end{aligned}$$

Comparing to Definition 3, we see that

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

and Rényi divergence indeed generalizes KL divergence.

In van Erven and Harremoës [2012] we can find the corresponding theorems and proves for continuous probability distributions.

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 a property of 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 $0 < \alpha < 1$.

$$\begin{aligned} D_{1-\alpha}(P\|Q) &= \frac{1}{-\alpha}\log\sum_{i=1}^{n}p_i^{1-\alpha}q_i^{\alpha}, \\ &= \frac{1-\alpha}{\alpha}\left(\frac{\alpha}{1-\alpha}\frac{1}{-\alpha}\log\sum_{i=1}^{n}q_i^{\alpha}p_i^{1-\alpha}\right), \\ &= \frac{1-\alpha}{\alpha}D_{\alpha}(Q\|P). \end{aligned}$$

Example. Let us have a probability distributions $Q = (\frac{4}{10}, \frac{6}{10})$ and $P = (p, 1-p)$ for some $p \in [0,1]$. In Figure 1.1, we plot the value of $D_\alpha(P\|Q)$ as a function of p, for different values of α. Clearly when $p = \frac{4}{10}$, the value of the divergence for any α is 0, since both probability distributions are the same. Additionally, the value of the divergence remains the same for any α, when $p = 1$ or $p = 0$. 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 $p = 0$.

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

Additionally, 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. Conversely, the opposite holds for smaller values of α.

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

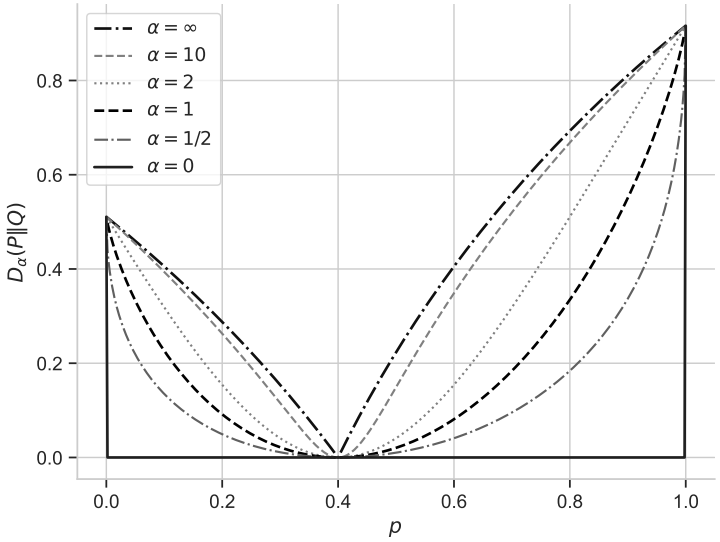

Figure 1.1: Example of temperature scaling.

Theorem 1. *Suppose we have a discrete sample space $\mathcal{Z} = \{z_1, z_2, z_3, \cdots\}$ 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

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

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

$$\int h dP_n \to \int h dP.$$

We set $h = \mathbb{1}\{z_i\}$ for any $i \in \mathbb{N}$, which is a bounded function, thus

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

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

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

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

$$z = f_\theta(x),$$

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

$$\sigma(y)_c = \frac{e^{y_c}}{\sum_{k=1}^n e^{y_k}}, \qquad c = 1, 2, \cdots, n, \tag{1.5}$$

where $y \in \mathcal{Y}$. 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 $Q = (q_1, q_2, \cdots, q_n)$.

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 $Q^T = \left(q_1^T, q_2^T, \cdots, q_n^T\right)$. 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.

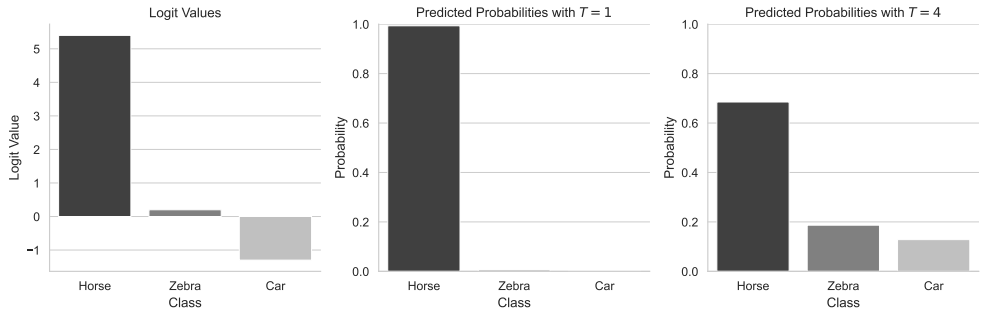

Figure 1.2: Example of temperature scaling.

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 $i \in \{1, 2, \cdots, N\}$.

Definition 5. *The training of the model f_θ involves minimizing the loss function*

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

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.

In the definition above, we use cross-entropy instead of KL divergence since, as shown in Equation 1.1, $H(P)$ does not depend on Q. Thus, the derivative of $D_{\mathrm{KL}}(P\|Q)$ with respect to Q is equivalent to the derivative of $H(P\|Q)$. This, together with the fact that cross-entropy is easier to compute, especially when P represents one-hot labels, often leads to KL divergence being replaced by cross-entropy in machine learning applications.

Remark. In the context of knowledge distillation, the training process defined in Definition 5 is referred to as vanilla training. This serves as a benchmark against which we compare the results of knowledge distillation.

Let $\mathcal{D}_t = \{(x_i, y_i)\}_{i=1}^{N_t}$ be a training dataset, containing a total of N_t samples, where $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ for all $i \in \{1, 2, \cdots, N_t\}$. In many cases, we have $\mathcal{D}_t = \mathcal{D}$.

Definition 6. *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 pre-trained on a dataset $\mathcal{D}_t$. The student model outputs logits z, which are converted into probability distribution $Q^T = (q_1^T, \cdots, q_n^T)$ using softmax function introduced in Equation 1.5,*

$$q_c^T = \frac{e^{\frac{z_c}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}}, \qquad c = 1, 2, \cdots, n.$$

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

$$p_c^T = \frac{e^{\frac{v_c}{T}}}{\sum_{k=1}^{n} e^{\frac{v_k}{T}}}, \qquad c = 1, 2, \cdots, n.$$

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

$$\mathcal{L}(\theta) = (1-\beta)\mathcal{L}_{CE}(\theta) + \beta\mathcal{L}_{KL}(\theta), \tag{1.6}$$

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

$$\begin{aligned} \mathcal{L}_{CE}(\theta) &= \sum_{i=1}^{N} H(y_i \| \tilde{P}(x_i, \theta_s)), \\ &= -\sum_{i=1}^{N}\sum_{j=1}^{n} y_{i,j} \log \tilde{p}_j(x_i, \theta_s), \end{aligned} \tag{1.7}$$

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

$$\begin{aligned} \mathcal{L}_{KL}(\theta) &= T^2 \sum_{i=1}^{N} D_{KL}(P(x_i, \theta_t) \| P(x_i, \theta_s)), \\ &= T^2 \sum_{i=1}^{N}\sum_{j=1}^{n} p_j(x_i, \theta_t) \log \frac{p_j(x_i, \theta_t)}{p_j(x_i, \theta_s)}, \end{aligned} \tag{1.8}$$

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

The hyperparameter T in Definition 6 denotes temperature. During training, we apply temperature scaling to both the teacher and the student in Equation 1.8. 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 truth labels and training on the soft targets provided by the teacher model. A common choice for β is 0.9 (see Cho and Hariharan [2019]).

We observe that, unlike in Equation 1.7, which is simply the sum of the cross-entropies, in Equation 1.8, the total loss also includes the term T^2. To understand the origin of this term we first calculate the derivatives of KL divergence $D_{\mathrm{KL}}(P\|Q)$ with respect to the logits of Q. Now, assume that P and Q are given as in Definition 6, where for simplicity of notation, we omit the term T. Now, we compute the following

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

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

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

Now, we approximate the exponential function using a Taylor polynomial for a temperature T that is high compared to the magnitude of the logits. We get

$$\frac{\partial H(P\|Q)}{\partial z_j} \approx \frac{1}{T}\left(\frac{1 + \frac{z_j}{T}}{n + \sum_{k=1}^{n} \frac{z_k}{T}} - \frac{1 + \frac{v_j}{T}}{n + \sum_{k=1}^{n} \frac{v_k}{T}}\right) = \frac{1}{nT^2}(z_j - v_j). \tag{1.9}$$

Thus, the gradient decreases proportionally to $\frac{1}{T^2}$ as the temperature T increases. By incorporating the term T^2 into Equation 1.8, we ensure that the relative contribution of $\mathcal{L}_{\mathrm{CE}}(\theta)$ and $\mathcal{L}_{\mathrm{KL}}(\theta)$ 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 1.8 by a general Rényi divergence of order α. Thus, the loss function 1.6 is replaced by

$$\mathcal{L}(\theta) = (1 - \beta)\mathcal{L}_{\mathrm{CE}}(\theta) + \beta\mathcal{L}_{\alpha}(\theta), \tag{1.10}$$

where

$$\begin{aligned}\mathcal{L}_{\alpha} &= \frac{T^2}{\alpha}\sum_{i=1}^{N} D_{\alpha}(P(x_i, \theta_t)\|P(x_i, \theta_s)),\\ &= \frac{T^2}{\alpha}\sum_{i=1}^{N}\sum_{j=1}^{n} \frac{1}{\alpha - 1}\log p_j(x_i, \theta_t)^{\alpha} p_j(x_i, \theta_s)^{1-\alpha}.\end{aligned}$$

What remains to shown is how the T^2 term from 1.8 is affected. Firstly, we compute the derivatives of $D_{\alpha}(P\|Q)$ with respect to the logits of Q. We have

$$\frac{\partial D_{\alpha}(P\|Q)}{\partial z_j} = \frac{\partial}{\partial z_j}\frac{1}{\alpha - 1}\log\sum_{i=1}^{n} p_i^{\alpha}\left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}}\right)^{1-\alpha},$$

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

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

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

$$
\begin{aligned}
\frac{\partial Z}{\partial z_j} =& \frac{\partial}{\partial z_j} \sum_{i=1}^{n} p_i^\alpha \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{1-\alpha}, \\
=& \frac{\partial}{\partial z_j} p_j^\alpha \left(\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{1-\alpha} + \frac{\partial}{\partial z_j} \sum_{i \neq j}^{n} p_i^\alpha \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{1-\alpha}, \\
=& p_j^\alpha (1-\alpha) \left(\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{-\alpha} \frac{\frac{1}{T} \sum_{k=1}^{n} e^{\frac{z_k}{T}} e^{\frac{z_j}{T}} - \frac{1}{T} e^{\frac{z_j}{T}} e^{\frac{z_j}{T}}}{(\sum_{k=1}^{n} e^{\frac{z_k}{T}})^2} \\
& - \sum_{i \neq j}^{n} p_i^\alpha \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{-\alpha} (1-\alpha) \frac{e^{\frac{z_i}{T}}}{(\sum_{k=1}^{n} e^{\frac{z_k}{T}})^2} e^{\frac{z_j}{T}} \frac{1}{T}, \\
=& \frac{1-\alpha}{T} \left[p_j^\alpha \left(\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{1-\alpha} \frac{\sum_{k=1}^{n} e^{\frac{z_k}{T}} - e^{\frac{z_j}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right. \\
& \left. - \sum_{i \neq j}^{n} p_i^\alpha \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right)^{1-\alpha} \frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^{n} e^{\frac{z_k}{T}}} \right], \\
=& \frac{1-\alpha}{T} \left[p_j^\alpha q_j^{1-\alpha} (1-q_j) - \sum_{i \neq j}^{n} p_i^\alpha q_i^{1-\alpha} q_j \right], \\
=& \frac{1-\alpha}{T} \left[p_j^\alpha q_j^{1-\alpha} - q_j \sum_{i=1}^{n} p_i^\alpha q_i^{1-\alpha} \right], \\
=& \frac{1-\alpha}{T} (p_j^\alpha q_j^{1-\alpha} - q_j Z).
\end{aligned}
$$

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

$$
\frac{\partial D_\alpha(P\|Q)}{\partial z_j} = \frac{1}{T} \left(q_j - \frac{p_j^\alpha q_j^{1-\alpha}}{\sum_{i=1}^{n} p_i^\alpha q_i^{1-\alpha}} \right), \tag{1.11}
$$

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 $\frac{q_j}{T}$ if $p_j = 0$, or to $\frac{q_j - 1}{T}$ if $p_j = 1$. This holds for any choice of α, which is why we do not modify the $\mathcal{L}_{\text{CE}}$ term in knowledge distillation.

From the result in Equation 1.11, we must derive an analogous expression to Equation 1.9, using previously established notation and assumption of centered logits. Moreover, we approximate the exponential function using a Taylor polynomial, but here, unlike before, the temperature must be high compared to both the magnitude of the logits and the value of α. We derive

$$
\begin{aligned}
\frac{\partial D_\alpha(P\|Q)}{\partial z_j} =& \frac{1}{T}\left[\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}} - \left(\frac{e^{\frac{v_j}{T}}}{\sum_{k=1}^n e^{\frac{v_k}{T}}}\right)^\alpha \left(\frac{e^{\frac{z_j}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}}\right)^{1-\alpha}\right. \\
&\left.\left(\sum_{i=1}^n \left(\frac{e^{\frac{v_i}{T}}}{\sum_{k=1}^n e^{\frac{v_k}{T}}}\right)^\alpha \left(\frac{e^{\frac{z_i}{T}}}{\sum_{k=1}^n e^{\frac{z_k}{T}}}\right)^{1-\alpha}\right)^{-1}\right], \\
\approx& \frac{1}{T}\left[\frac{1+\frac{z_j}{T}}{n+\sum_{k=1}^n \frac{z_k}{T}} - \frac{1+\frac{\alpha v_j}{T}}{\left(n+\sum_{k=1}^n \frac{v_k}{T}\right)^\alpha}\frac{1+\frac{(1-\alpha)z_j}{T}}{\left(n+\sum_{k=1}^n \frac{z_k}{T}\right)^{1-\alpha}}\right. \\
&\left.\left(\sum_{i=1}^n \frac{1+\frac{\alpha v_i}{T}}{\left(n+\sum_{k=1}^n \frac{v_k}{T}\right)^\alpha}\frac{1+\frac{(1-\alpha)z_i}{T}}{\left(n+\sum_{k=1}^n \frac{z_k}{T}\right)^{1-\alpha}}\right)^{-1}\right], \\
=& \frac{1}{T}\left[\frac{1+\frac{z_j}{T}}{n} - \frac{1+\frac{\alpha v_j}{T}+\frac{(1-\alpha)z_j}{T}+\frac{\alpha(1-\alpha)v_j z_j}{T^2}}{n}\right. \\
&\left.\left(\frac{1}{n}\sum_{i=1}^n 1+\frac{\alpha v_i}{T}+\frac{(1-\alpha)z_i}{T}+\frac{\alpha(1-\alpha)v_i z_i}{T^2}\right)^{-1}\right].
\end{aligned}
$$

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 $\frac{\alpha(1-\alpha)v_j z_j}{T^2} \approx 0$.

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 (1.9), except that it is multiplied by α.

2. Title of the second chapter

2.1 Title of the first subchapter of the second chapter

2.2 Title of the second subchapter of the second chapter

Conclusion

Bibliography

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A. Attachments

A.1 First Attachment