Formalizing Limits of Knowledge Distillation Using Partial Information Decomposition

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Abstract

Knowledge distillation provides an effective method for deploying complex machine learning models in resource-constrained environments. It typically involves training a smaller student model to emulate either the probabilistic outputs or the internal feature representations of a larger teacher model. By doing so, the student model often achieves substantially better performance on a downstream task compared to when it is trained independently. Nevertheless, the teacher's internal representations can also encode noise or additional information that may not be relevant to the downstream task. This observation motivates our primary question: What are the information-theoretic limits of knowledge transfer? To this end, we leverage a body of work in information theory called Partial Information Decomposition (PID) that unravels the joint information contained in several input random variables about another target variable, e.g., the downstream task labels. Our main contribution is to quantify the distillable and distilled knowledge of a teacher's representation for a given downstream task. Moreover, we demonstrate that this metric can be practically used in distillation to address challenges caused by the complexity gap between the teacher and the student representations.

1 Introduction

Knowledge distillation can be used to compress a complex machine learning model (the teacher) by distilling it into a relatively simpler model (the student). The term "distillation" in this context means obtaining some assistance from the teacher during the training of the student, so that the student model performs much better than when it is trained alone. In one of its simplest forms, knowledge distillation involves the student trying to match the logits of the teacher network, in addition to the correct labels of the training examples [Hinton, 2015]. More advanced methods focus on distilling multiple intermediate representations of the teacher to the corresponding layers of the student [Romero et al., 2015, Ahn et al., 2019, Tian et al., 2020, Liang et al., 2023] (also see Gou et al. [2021], Sucholutsky et al. [2023] for a survey). Information theory has been instrumental in both designing [Ahn et al., 2019, Tian et al., 2020] and explaining [Zhang et al., 2022, Wang et al., 2022] knowledge distillation techniques. However, less attention has been given to characterizing the fundamental limits of the process from an information-theoretical perspective. Our goal is to bridge this gap by introducing a metric to quantify the distillable knowledge available in a teacher model, given a student model and a target task. As such, we bring in an emerging body of work named Partial Information Decomposition (PID) [Williams and Beer, 2010, Griffith et al., 2014, Bertschinger et al., 2014] to define the distillable knowledge as the "unique information about the task that is available only with the teacher, but not the student." As it follows, the quantification of distillable knowledge gives rise to a quantification of already distilled knowledge, leading to a metric

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³⁸th Conference on Neural Information Processing Systems (NeurIPS 2024).

that we can optimize during the distillation process. We further provide a novel knowledge distillation framework – Redundant Information Distillation (RID)– which optimizes this quantity and filters out the task-irrelevant information from the teacher. See Appendix A for a discussion on related works.

Background on PID: Partial Information Decomposition (PID), first introduced in Williams and Beer [2010], offers a way to decompose the joint information in two sources, say T and S, about another random variable Y (i.e., I(Y;T,S) where I(A;B) denotes the mutual information between A and B [Cover and Thomas, 2006]) into four components as follows:

- 1. Unique information $Uni(Y : T \setminus S)$ and $Uni(Y : S \setminus T)$: information about Y that each source uniquely contains
- 2. Redundant information Red(Y : T, S): the information about Y that both T and S share
- 3. Synergistic information Syn(Y : T, S): the information about Y that can be recovered only by using both T and S.

These PID components satisfy the relationships given below:

$$\begin{split} I(Y;T,S) &= Uni(Y:T\backslash S) + Uni(Y:S\backslash T) \\ &+ Red(Y:T,S) + Syn(Y:T,S) \quad (1) \\ I(Y;T) &= Uni(Y:T\backslash S) + Red(Y:T,S) \quad (2) \\ I(Y;S) &= Uni(Y:S\backslash T) + Red(Y:T,S). \quad (3) \end{split}$$

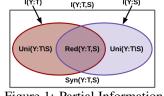
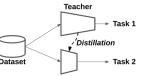


Figure 1: Partial Information Decomposition

While a unique definition for each term does not exist, defining only one of them is sufficient to define the rest. Consequently, a wide array of definitions exists, each based on different desired properties [Williams and Beer, 2010, Bertschinger et al., 2014, Griffith et al., 2014, Griffith and Ho, 2015]. Among these, the definition proposed in Bertschinger et al. [2014] is motivated with an operational interpretation of unique information in the context of decision theory. Moving on to the context of knowledge distillation, we map T to be the teacher representation, S to be the student representation, and Y to be the downstream task that the student is being trained for. That makes I(Y;T) and I(Y;S) be the total knowledge about Y that is in the teacher and in the student respectively.

Notation and problem setting: Upper-case letters denote random variables, except P and Q which represent probability distributions, C, H, W which represent the representation dimensions and K which represents the number of layers distilled. Lowercase letters are used for

vectors unless specified otherwise. Lowercase Greek letters denote parameters of neural networks. We consider a layer-wise distillation scheme where the teacher representation T(X) is distilled into the student representation $S_{\eta_s}(X)$, where X is the input. The target of the student is to predict the task Y from X. Both $T(\cdot)$ and $S_{\eta_s}(\cdot)$ are deterministic functions of X and the randomness is



and $S_{\eta_s}(\cdot)$ are deterministic functions of X and the randomness is due to the input being random. Note that the student representation depends on the parameters of the student network denoted by η_s and hence written as S_{η_s} . However, when this parameterization and dependence on X is irrelevant/obvious, we may omit both and simply write T and S. We denote the supports of Y, T and S by \mathcal{Y}, \mathcal{T} and S respectively.

Knowledge distillation is usually achieved by modifying the student loss function to include a distillation loss term in addition to the ordinary task-related loss as follows:

$$\mathcal{L}(\eta_s) = \lambda_1 \mathcal{L}_{\text{ordinary}}(Y, \hat{Y}(X)) + \lambda_2 \mathcal{L}_{\text{distill}}(Y, \hat{Y}(X), S_{\eta_s}, T) \qquad (\lambda_1, \lambda_2 > 0).$$
(4)

Since our experiments (in Section 4) are based on a classification task, in that case Y denotes the true class label and we use the cross entropy loss $\mathcal{L}_{CE}(Y, \hat{Y}) = -\mathbb{E}_{P_X} \left[\log P_{\hat{Y}(X)}(Y) \right]$ as the ordinary task-related loss for the student. Here, $\hat{Y}(X)$ is the student's final prediction of Y. The teacher network is assumed to remain unmodified during the distillation process.

2 Main Contribution: Quantifying Distillable and Distilled Knowledge

In this section, we propose information theoretic metrics to quantify both the task-relevant information that is available in the teacher for distillation, and the amount of information that has already been distilled to the student. Moreover, we discuss some favorable properties of the proposed metrics with examples that compare other candidate measures. Accordingly, we first define the amount of distillable information as follows:

Definition 2.1 (Distillable Knowledge). Let Y, S, and T be the target variable, student's intermediate representation, and the teacher's intermediate representation, respectively. The amount of knowledge distillable from T to S is defined as $Uni(Y : T \setminus S)$.

With the above definition, we see that the more the distillation happens, the more the $Uni(Y : T \setminus S)$ shrinks. Note that under the knowledge distillation setting, the total knowledge of the teacher I(Y : T) is constant since the teacher is not modified during the process. Since $I(Y;T) = Uni(Y : T \setminus S) + Red(Y : T, S)$ we therefore propose Red(Y : T, S) as a measure for knowledge that is already distilled.

Definition 2.2 (Distilled Knowledge). Let Y, S, and T be the target variable, student's intermediate representation, and the teacher's intermediate representation, respectively. The amount of distilled knowledge from T to S is defined as Red(Y : T, S).

We further propose using the unique and redundant information definitions due to Bertschinger et al. [2014] for an exact quantification.

Definition 2.3 (Unique and redundant information Bertschinger et al. [2014]).

$$Uni(Y:T\backslash S) = \min_{Q\in\Delta_P} I_Q(Y;T|S)$$
(5)

$$Red(Y:T,S) = I(Y;T) - \min_{Q \in \Delta_P} I_Q(Y;T|S)$$
(6)

where $\Delta_P = \{Q : Q(Y = y, T = t) = P(Y = y, T = t), Q(Y = y, S = s) = P(Y = y, S = s) \forall y \in \mathcal{Y}, t \in \mathcal{T} and s \in \mathcal{S} \}$ and P is the joint distribution of Y, T and S.

A multitude of knowledge distillation frameworks exists which are based on maximizing the mutual information between the teacher and the student (i.e., I(T; S)) Ahn et al. [2019], Tian et al. [2020], Chen et al. [2021], Miles et al. [2021]. While a distillation loss that maximizes I(T; S) can be helpful to the student when the teacher possesses task-related information, it creates a tension with the ordinary loss when the teacher has little or no task-relevant information. Moreover, even though the teacher contains task-related information, the limited capacity of the student may hinder a proper distillation when this kind of framework is used. The following examples provide an insight in this regard. The proposed measure Red(Y : T, S) resolves these cases in an intuitive manner.

Example 1: (Uninformative teacher) An uninformative teacher representation (i.e., T with I(Y;T) = 0) gives $Uni(T:T\setminus S) = Red(Y:T,S) = 0$ for any S, agreeing with the intuition. Hence, an algorithm that maximizes exactly the transferred knowledge Red(Y:T,S) will have a zero gradient over this term. In contrast, algorithms that maximize the similarity between S and T quantified by I(T;S) will force S to mimic the uninformative teacher, causing a performance worse than ordinary training without distillation. For example, let $U_1, U_2 \sim Ber(0.5)$ and $Y = U_1, T = U_2$. Then, the teacher cannot predict the intended task Y. Note that in this case, I(T:S) is not maximized when the student representation is S = Y. Instead, it is maximized when $S = U_2$.

Example 2: (Extra complex teacher) Let $U_1 \sim Ber(0.2), U_2 \sim Ber(0.5)$ and $Y = U_1, T = (U_1, U_2)$. Then, the teacher can completely predict the intended task Y. Assume the student is simpler than the teacher, and has only one binary output. In this situation, I(T : S) is not maximized when $S = U_1$ because $I((U_1, U_2) : U_1) \approx 0.72 < 1 = I((U_1, U_2) : U_2)$ where the right-hand side is achieved when $S = U_2$. However, $S = U_1$ is a maximizer for Red(Y : T, S) (i.e., $Red(Y : T, S) = Red(U_1 : T, U_1) = I(Y; T)$). Theorem 2.1 presents a more general case.

Theorem 2.1 (Teacher with nuisance). Let T = (Z, G) where Z contains all the task-related information (i.e., I(Y;T) = I(Y;Z)) and G does not contain any information about the task (i.e., I(Y;G) = 0). (G can be seen as a stronger version of nuisance defined in [Achille and Soatto, 2018, Section 2.2]). Let the student be a capacity-limited model as defined by $H(S) \le \max\{H(Z), H(G)\}$ where H(X) denotes the entropy of the random variable X. Then,

(i) I(T; S) is maximized when

$$S = \begin{cases} Z & ; & H(Z) > H(G) \\ G & ; & H(Z) < H(G) \end{cases}.$$
 (7)

(ii) Red(Y:T,S) is always maximized when S = Z.

In the above scenario, the task-related part of the student loss will have a tension with the distillation loss when H(Z) < H(G), in which case, the distillation actually affects adversely on the student. On the other hand, a distillation loss that maximizes Red(Y : T, S) will always be aligned with the task-related loss.

These examples show that the frameworks based on maximizing I(T; S) are not capable of selectively distilling the task-related information to the student. In an extreme case, they are not robust to being distilled from a corrupted teacher network. This is demonstrated in the experiments under Section 4. It may appear that using I(Y;T|S) as the metric for distillable knowledge resolves the cases similar to Example 1. However, Example 3 below provides a counter-example.

Example 3: (Effect of synergy) Consider a scenario similar to Example 1, where the teacher is uninformative regarding the interested task. For example, let $U_1, U_2 \sim Ber(0.5)$ and $Y = U_1, T = U_1 \oplus U_2$ where \oplus denotes the binary XOR operation. Suppose we were to consider conditional mutual information I(Y;T|S) as the measure of distillable information available in the teacher. Then, I(Y;T|S) = H(Y) when $S = U_2$, indicating non-zero distillable information in the teacher. This is unintuitive since in this case both I(Y;T) = I(Y;S) = 0 and neither the teacher nor the student can be used alone to predict Y. In contrast, the proposed measures $Uni(Y:T \setminus S) = Red(Y:T,S) = 0$ indicating no distillable or already distilled information available.

Next, we present Theorem 2.2 which highlights some important properties of the proposed metrics. These properties indicate that the proposed measures agree well with the intuition.

Theorem 2.2 (Properties). *The following properties hold for distillable and distilled knowledge defined as in Definition 2.1 and Definition 2.2 respectively.*

1. When $Uni(Y : T \setminus S) = 0$, the teacher has no distillable information. At this point, the student has the maximum information that any one of the representations T or S has about Y; i.e.,

$$\max\{I(Y;T), I(Y;S)\} = I(Y;S).$$
(8)

For a given student representation S and any two teacher representations T₁ and T₂ if there exists a deterministic mapping h such that T₁ = h(T₂), then Uni(Y : T₁\S) ≤ Uni(Y : T₂\S).
 Both Uni(Y : T\S) and Red(Y : T, S) are non-negative.

3 A Framework To Maximize Distilled Knowledge

In this section, we propose a distillation framework – Redundant Information Distillation (RID) – which maximizes the distilled knowledge quantified by Red(Y : T, S), targeting a classification problem. Accordingly, we first show that the framework directly maps to an alternative definition of redundant information (also called the I_{α} measure) denoted by $Red_{\Omega}(Y : T, S)$ [Griffith and Ho, 2015], under a certain assumption. Next, we show that $Red_{\Omega}(Y : T, S)$ is a lower-bound for Red(Y : T, S) by Bertschinger et al. [2014]. The definition of $Red_{\Omega}(Y : T, S)$ is given below:

Definition 3.1 (I_{α} measure [Griffith and Ho, 2015]).

$$Red_{\cap}(Y:T,S) = \max_{P(Q|Y)} I(Y:Q) \quad subject \text{ to } \quad I(Y;Q|f_t(T)) = I(Y;Q|f_s(S)) = 0.$$
 (9)

The proposed framework is based on selecting Q to be $Q = f_t(T)$, and parameterizing $f_t(\cdot)$ and $f_s(\cdot)$ using small neural networks. To denote the parameterization, we will occasionally use the elaborated notation $f_t(\cdot; \theta_t)$ and $f_s(\cdot; \theta_s)$, where θ_t and θ_s denote the parameters of f_t and f_s , respectively. With the substitution of $Q = f_t(T)$, Definition 3.1 results in the following optimization problem:

$$\max_{\theta_t, \theta_s, \eta_s} I(Y : f_t(T; \theta_t)) \quad \text{subject to} \quad I(Y; f_t(T; \theta_t) | f_s(S_{\eta_s}; \theta_s)) = 0.$$
(P1)

We divide the problem (P1) into two phases and employ gradient descent on two carefully designed loss functions to perform the optimization. In the first phase, we maximize the objective w.r.t. θ_t while θ_s and S are kept constant (recall that T is fixed in all cases because the teacher is not being trained during the process). For this, we append an additional classification head $g_t(\cdot; \phi_t)$ parametrized by ϕ_t to the teacher's task aware filter f_t . Then we minimize the loss function given below with respect to θ_t and ϕ_t using gradient descent.

$$\mathcal{L}_t(\theta_t, \phi_t) = \mathcal{L}_{CE}(Y, g_t(f_t(T; \theta_t); \phi_t)) + \sum_{c=1}^C \sum_{h=1}^H \sum_{w=1}^W \mathbb{E}_{P_X}\left[\frac{V_{c,h,w}^2}{\sigma_c}\right]$$
(10)

where $V_{c,h,w}$ denotes the corresponding element of $V = f_t(T(X); \theta_t) - f_s(S(X); \theta_s) \in \mathbb{R}^{C \times H \times W}$. Here, C, H, and W are the number of channels, height, and width of the outputs of f_s and f_t . $\sigma = [\sigma_1, \ldots, \sigma_C]^T$ is a stand-alone vector of weights that are optimized in the second phase. Minimizing the cross-entropy term $\mathcal{L}_{CE}(Y, g_t(f_t(T; \theta_t); \phi_t))$ of $\mathcal{L}_t(\theta_t, \phi_t)$ above amounts to maximizing $I(Y; f_t(T; \theta_t))$. The second term prohibits $f_t(T)$ from diverting too far from $f_s(S)$ during the process, so that the constraint $I(Y; f_t(T; \theta_t) | f_s(S; \theta_s)) = 0$ can be ensured.

During the second phase, we freeze θ_t and maximize the objective over θ_s , S_{η_s} and σ . The loss function employed in this phase is as follows:

$$\mathcal{L}(\theta_s, \sigma, \eta_s) = \lambda_1 \mathcal{L}_{CE}(Y, \hat{Y}_{\eta_s}) + \lambda_2 \underbrace{\left(||\sigma||^2 + \sum_{c=1}^C \sum_{h=1}^H \sum_{w=1}^W \mathbb{E}_{P_X} \left[\frac{V_{c,h,w}^2}{\sigma_c} \right] \right)}_{\mathcal{L}_s(\theta_s, \sigma, \eta_s)} \tag{11}$$

where λ_1 and λ_2 are scalar hyperparameters which determine the prominence of ordinary learning and distillation. V and σ are as defined earlier. \hat{Y}_{η_s} denotes the final prediction of the student network.

The first term of the loss function is the ordinary task-related loss. The next two terms correspond to the distillation loss, which is our focus in the following explanation. Consider phase 2 as an estimation problem that minimizes the σ -weighted mean squared error, where $Q = f_t(T)$ is the estimand and $f_s(\cdot)$ is the estimator. The magnitudes of the positive weights σ are controlled using the term $||\sigma||^2$. We observe that this optimization ensures $I(Y; Q|f_s(S)) = 0$ given that the following assumption holds.

Assumption: Let the estimation error be $\epsilon = f_t(T) - f_s(S)$. Assume $I(\epsilon; Y | f_s(S)) = 0$. In other words, given the estimate, the estimation error is independent of Y.

With the above assumption, we see that

 $I(Y; Q|f_s(S)) = I(Y; f_t(T)|f_s(S)) = I(Y; f_s(S) + \epsilon|f_s(S)) = I(Y; \epsilon|f_s(S)) = 0.$ (12) Therefore, the constraint in problem P1 is satisfied by this selection of random variables. Therefore, along with the maximization of I(Y; Q) during phase 1, the proposed framework can be seen as performing the optimization in Definition 3.1 in two steps.

Finally, we claim through Theorem 3.1 that $Red_{\cap}(Y : T, S)$ is a lower bound for Red(Y : T, S). **Theorem 3.1** (Distilled information lower bound). For any three random variables Y, T and S,

$$Red_{\cap}(Y:T,S) \le Red(Y:T,S)$$
 (13)

where $Red_{\Omega}(Y : T, S)$ is as per Definition 3.1 and Red(Y : T, S) is defined in Definition 2.3.

This completes our claim that the proposed framework maximizes a lower bound for the distilled knowledge. The framework is summarized in Algorithm 1. The advantage of this framework over the VID framework [Ahn et al., 2019] (which maximizes I(T; S)) can be observed in the experiments in Section 4. RID losses can be extended to multiple layers by simply summing up $\mathcal{L}_t^{(k)}(\theta_t^{(k)}, \phi_t^{(k)})$ and $\mathcal{L}_s^{(k)}(\theta_s^{(k)}, \sigma^{(k)}, \eta_s)$ corresponding to the representations $T^{(k)}$ and $S_{\eta_s}^{(k)}(k = 1, \ldots, K)$ in equations (10) and (11) respectively.

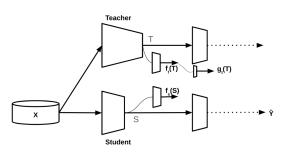


Figure 3: Redundant Information Distillation

Remark. We observe that the Task-aware Layer-wise Distillation (TED) framework [Liang et al., 2023] shares intuitive similarities with RID, with regard to distilling task-related knowledge. However, they take a heuristic approach to the design and the focus is on large language models. In fact, our mathematical formulation can explain the success of TED as detailed in Appendix C. In addition to the domain of application, the difference between TED and RID can mainly be attributed to the following: (i) During the first stage, TED trains both $f_t(\cdot)$ and $f_s(\cdot)$ whereas RID only trains $f_t(\cdot)$; (ii) In the second stage loss, TED includes an ordinary mean squared error term whereas RID includes a weighted (using σ) mean squared error term. To the best of our knowledge, our work is the first to information-theoretically quantify the actual task-relevant distilled knowledge and formally incorporate it into an optimization.

4 Experiments

We compare the performance of the proposed RID framework with that of the VID framework under two different conditions. In the first setting, the teacher network is fully trained with the complete training set, whereas in the second setting, the teacher is just randomly initialized without any training at all. Experiments are carried out on the CIFAR-10 dataset [Krizhevsky et al., 2009]. Additionally, we train a student without any knowledge distillation, which we label as BAS. We distill three teacher layers to the corresponding student layers. In all cases, we compute the PID components [Bertschinger et al., 2014] of the joint information of the innermost distilled layer using the estimation method in Liang et al. [2024a]. All the teacher models are WideResNet-(40,2) and all the student models are WideResNet-(16,1). More details on the experiments are given in Appendix D.

In the case of the trained (i.e., I(Y;T) > 0) teacher, we observe that $Uni(Y : T \setminus S)$ decreases with the increasing number of epochs. In the case of the untrained teacher (i.e., I(Y;T) = 0), $Uni(Y : T \setminus S) = 0$ as expected. Both BAS and RID models show an increase in I(Y;S) even under the untrained teacher. In this case, VID shows a very low I(Y;S) as expected, caused by the distillation loss forcing to mimic the teacher. The results are shown in Figure 4. Figure 5 in Appendix D shows the corresponding classification accuracies.

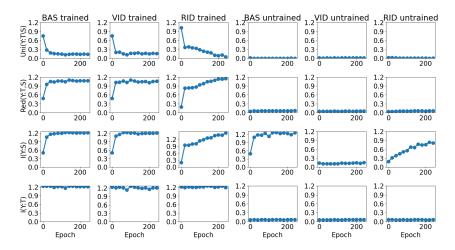


Figure 4: Information atoms of I(Y; T, S) for BAS, VID and RID when distilled using a trained and an untrained teacher. Values are shown for the innermost distilled layer. Notice how VID performs worse than BAS when the teacher is not trained.

5 Conclusion

We propose using $Uni(Y : T \setminus S)$ and Red(Y : T, S) to quantify distillable and distilled knowledge, corresponding to a given teacher-student pair regarding a given task. We show that knowledge distillation frameworks which use mutual information between the teacher and the student representations to quantify distillation have a fundamental problem. In contrast, through many examples we demonstrate that the proposed metric can correctly characterize the distillable and distilled knowledge. Moreover, we show the advantage of the proposed metric by implementing a new distillation framework – Redundant Information Distillation (RID) – and comparing its performance with the existing technique VID [Ahn et al., 2019]. While VID and RID perform similarly when the teacher is well-trained for the downstream task, VID performance degrades largely when the teacher is not trained. However, RID performs close to a student model that is trained independently, without knowledge distillation.

While the RID framework uses an alternative definition for redundant information, computation of exact Red(Y : T, S) during training can be computationally prohibitive due to the optimization over Δ_P . Extending the mathematical formulation in Section 3 to analyze other knowledge distillation frameworks is an interesting path for future research. Other potential research directions include: (i) distilling from an ensemble of teachers [Malinin et al., 2020] in a way that the adverse effects of corrupted teachers are mitigated; (ii) dataset distillation [Sucholutsky and Schonlau, 2021]; or (iii) distillation for model reconstruction from counterfactual explanations [Dissanayake and Dutta, 2024].

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A Related works

Multi-layer knowledge distillation was introduced in FitNets [Romero et al., 2015]. There onwards a large number of techniques, based on different statistics derived for matching a teacher-student pair, have been proposed. In particular, Ahn et al. [2019], Tian et al. [2020], Chen et al. [2021], Miles et al. [2021] leverage an information-theoretic perpective to arrive at a solution. We refer the reader to [Gou et al., 2021, Sucholutsky et al., 2023] for a thorough survey of different techniques used in knowledge distillation. In this article, we focus on Variational Information Distillation (VID, Ahn et al. [2019]) as a representative framework of the larger class of distillation frameworks which maximizes I(T; S) as the distillation strategy. We also discuss Task-aware Layer-wise Distillation (TED, Liang et al. [2023]) as a framework that filters out task-related information. Specifically, Liang et al. [2023] highlight the importance of distilling only the task-related information when there is a significant complexity gap between the teacher and the student. Towards this end, Zhu et al. [2022] points out the existence of undistillable classes due to the unmatched capacity of the student model. Kundu et al. [2021] presents a distillation. While TED uses intermediate representations of the teacher, Kundu et al. [2021] uses the penultimate layer.

Information theory has been instrumental in the attempts to explain the success of knowledge distillation. Wang et al. [2022] utilizes information bottleneck principles [Tishby et al., 2000, Tishby and Zaslavsky, 2015] to explain how a teacher model may assist the student to learn relevant features quickly. They reveal that a partially trained checkpoint of the teacher can help the student more than the fully converged teacher. [Zhang et al., 2022] observes the training process as systematically discarding knowledge from the input. Accordingly, the distillation helps the student to quickly learn what information to discard. Despite these attempts, we observe that there exists a gap in characterizing the fundamental limits of knowledge distillation which we seek to address using PID.

PID is also beginning to generate interest in other areas of machine learning [Dutta et al., 2020, 2021, Dutta and Hamman, 2023, Hamman and Dutta, 2024a, Liang et al., 2024a, b, Hamman and Dutta, 2024b, Tax et al., 2017, Ehrlich et al., 2022, Wollstadt et al., 2023, Mohamadi et al., 2023, Venkatesh et al., 2024, Halder et al., 2024]. However, it has not been leveraged in the context of knowledge distillation before. Additionally, while most related works predominantly focus on efficiently computing PID, e.g., Kleinman et al. [2021], Liang et al. [2024a], Halder et al. [2024], Pakman et al. [2021] that itself requires solving an optimization over the joint distribution, there are limited works that further incorporate it as a regularizer during model training. Dutta et al. [2021] leverages Gaussian assumptions to obtain closed-form expressions for the PID terms, enabling them to use unique information as a regularizer during training for fairness (also see Venkatesh and Schamberg [2022], Venkatesh et al. [2024] for more details on Gaussian PID). Our work makes novel connections between two notions of redundant information, and shows how PID can be integrated as a regularizer in a multi-level optimization without Gaussian assumptions, which could also be of independent interest outside the context of knowledge distillation.

B Proofs

B.1 Proof of Theorem 2.1

Theorem 2.1 (Teacher with nuisance). Let T = (Z, G) where Z contains all the task-related information (i.e., I(Y;T) = I(Y;Z)) and G does not contain any information about the task (i.e., I(Y;G) = 0). (G can be seen as a stronger version of nuisance defined in [Achille and Soatto, 2018, Section 2.2]). Let the student be a capacity-limited model as defined by $H(S) \le \max\{H(Z), H(G)\}$ where H(X) denotes the entropy of the random variable X. Then,

(i) I(T; S) is maximized when

$$S = \begin{cases} Z & ; & H(Z) > H(G) \\ G & ; & H(Z) < H(G) \end{cases}.$$
 (7)

(ii) Red(Y:T,S) is always maximized when S = Z.

Proof. To prove claim 1, observe that

$$I(T;S) = H(T) - H(T|S)$$
(14)

$$=H(Z,G)-H(Z,G|S)$$
(15)

$$= H(Z) + H(G) - H(Z, G|S).$$
(16)

Now, $S = Z \implies H(Z,G|S) = H(G)$ and $S = G \implies H(Z,G|S) = H(Z)$. Therefore,

$$I(T;S) = \begin{cases} H(Z) & ; S = Z \\ H(G) & ; S = G \end{cases}.$$
 (17)

Claim 1 follows from the above since $I(T; S) \le H(S) \le \max\{H(Z), H(G)\}$.

To prove claim 2, first observe that $I(Y;T) = I(Y;Z) \implies I(Y;G|Z) = 0$. Now consider the conditional mutual information I(Y;T|S):

$$I(Y;T|S) = I(Y;Z,G|S)$$
(18)

$$= I(Y;G|S) + I(Y;Z|G,S)$$
(19)

Note that the right-hand side above vanishes when S = Z. Therefore, $S = Z \implies I(Y;T|S) = 0$. Now since

$$Red(Y:T,S) = I(Y;T) - \underbrace{\min_{Q \in \Delta_P} I_Q(Y;T|S)}_{=0 \text{ with } Q = P \text{ when } S = Z}$$
(20)

and $Red(Y:T,S) \leq I(Y;T)$, setting S = Z achieves the maximum Red(Y:T,S).

B.2 Proof of Theorem 2.2

Theorem 2.2 (Properties). *The following properties hold for distillable and distilled knowledge defined as in Definition 2.1 and Definition 2.2 respectively.*

1. When $Uni(Y : T \setminus S) = 0$, the teacher has no distillable information. At this point, the student has the maximum information that any one of the representations T or S has about Y; i.e.,

$$\max\{I(Y;T), I(Y;S)\} = I(Y;S).$$
(8)

- 2. For a given student representation S and any two teacher representations T_1 and T_2 if there exists a deterministic mapping h such that $T_1 = h(T_2)$, then $Uni(Y : T_1 \setminus S) \leq Uni(Y : T_2 \setminus S)$.
- 3. Both $Uni(Y:T\setminus S)$ and Red(Y:T,S) are non-negative.

Proof of the first property is given below:

Proof.

$$\max\{I(Y;T), I(Y;S)\} = \max\{Red(Y:T,S) + \underbrace{Uni(Y:T\backslash S)}_{=0},$$
(21)

$$Red(Y:T,S) + Uni(Y:S\backslash T)\}$$
(22)

$$= Red(Y:T,S) + Uni(Y:S\backslash T)$$
(23)

$$=I(Y;S).$$
(24)

The second and third properties directly follow from Banerjee et al. [2018, Lemma 31] and Bertschinger et al. [2014, Lemma 5].

B.3 Proof of Lemma B.1

Lemma B.1. Let Y, T and S be any three random variables with supports \mathcal{Y}, \mathcal{T} and S respectively and $g(\cdot)$ be a deterministic function with domain S. Then

$$I(Y;T|g(S),S) = I(Y;T|S).$$
 (25)

Proof. By applying the mutual information chain rule to I(Y; T, S, g(S)) we get

$$I(Y;T,S,g(S)) = I(Y;S) + I(Y;T|S) + I(Y;g(S)|T,S)$$
(26)
$$I(Y;T,S) = I(Y;S) + I(Y;T|S) + I(Y;G(S)|T,S)$$
(26)

$$= I(Y;S) + I(Y;T|S) + \underbrace{H(g(S)|T,S)}_{=0} - \underbrace{H(g(S)|Y,T,S)}_{=0}$$
(27)

$$= I(Y;S) + I(Y;T|S).$$
(28)

Also, from a different decomposition, we get

$$I(Y;T,S,g(S)) = I(Y;S) + \underbrace{I(Y;g(S)|S)}_{=0} + I(Y;T|g(S),S)$$
(29)

$$= I(Y;S) + I(Y;T|g(S),S).$$
(30)

Combining the two right-hand sides yields the final result.

B.4 Proof of Theorem 3.1

Theorem 3.1 (Distilled information lower bound). For any three random variables Y, T and S,

$$Red_{\cap}(Y:T,S) \le Red(Y:T,S)$$
 (13)

where $Red_{\cap}(Y : T, S)$ is as per Definition 3.1 and Red(Y : T, S) is defined in Definition 2.3.

Proof. For a given set of random variables Y, T and S, let $f_t^*(T)$ and $f_s^*(S)$ achieve the maximum I(Y;Q) in Definition 3.1, i.e., $Red_{\cap}(Y:T,S) = I(Y;f_t^*(T))$ while $I(Y;f_t^*(T)|f_s^*(S)) = 0$. We first observe that $Red(Y:f_t^*(T),f_s^*(S)) = Red_{\cap}(Y:T,S) = I(Y;f_t^*(T))$ as shown below:

$$Red(Y: f_t^*(T), f_s^*(S)) = I(Y; f_t^*(T)) - \min_{Q \in \Delta_P} I_Q(Y; f_t^* | f_s^*(S))$$
(31)

$$= I(Y; f_t^*(T)) \quad (:: I(Y; f_t^*(T) | f_s^*(S)) = 0)$$
(32)

$$= Red_{\cap}(Y:T,S). \tag{33}$$

Next, we show that $Red(Y : f_t^*(T), f_s^*(S)) < Red(Y : T, S)$. In this regard, we use the following lemma due to Bertschinger et al. [2014].

Lemma B.2 (Lemma 25, Bertschinger et al. [2014]). Let $X, Y, Z_1, Z_2 \dots, Z_k$ and Z_{k+1} be a set of random variables. Then,

$$Uni(X:Y\backslash Z_1, Z_2..., Z_k) \ge Uni(X:Y\backslash Z_1, Z_2..., Z_k, Z_{k+1}).$$
(34)

Consider the set of random variable $Y, f_t^*(T), f_s^*(S)$ and S. From the above lemma we get

$$Uni(Y: f_t^*(T) \setminus f_s^*(S)) \ge Uni(Y: f_t^*(T) \setminus f_s^*(S), S)$$
(35)

$$= I(Y; f_t^*(T)) - I_{Q^*}(Y; f_t^*(T)|f_s^*(S), S)$$
(36)

where $Q^* = \arg \min_{Q \in \Delta_P} I_{Q^*}(Y; f_t^*(T) | f_s^*(S), S)$. Now, by applying Lemma B.1 to the righthand side we arrive at

$$Uni(Y: f_t^*(T) \setminus f_s^*(S)) \ge I(Y; f_t^*(T)) - I_{Q^*}(Y; f_t^*(T)|S)$$
(37)

$$= Uni(Y : f_t^*(T) \backslash S).$$
(38)

Next, observe that the following line arguments hold from Definition 2.3:

$$Uni(Y: f_t^*(T) \setminus f_s^*(S)) \ge Uni(Y: f_t^*(T) \setminus S)$$
(39)

$$\iff I(Y; f_t^*(T)) - Uni(Y: f_t^*(T) \setminus f_s^*(S)) \le I(Y; f_t^*(T)) - Uni(Y: f_t^*(T) \setminus S)$$
(40)

$$\iff Red(Y: f_t^*(T), f_s^*(S)) \le Red(Y: f_t^*(T), S).$$
(41)

Noting that Red(Y : A, B) is symmetric w.r.t. A and B, we may apply the previous argument to the pair $Red(Y : f_t^*(T), S)$ and Red(Y : T, S) to obtain

$$Red(Y: f_t^*(T), f_s^*(S)) \le Red(Y: f_t^*(T), S) \le Red(Y: T, S),$$
 (42)

concluding the proof.

C VID and TED frameworks

C.1 Variational Information Distillation (VID)

The VID framework [Ahn et al., 2019] is based on maximizing a variational lower bound to the mutual information I(T; S). It finds a student representation S which minimizes the following loss function:

$$\mathcal{L}_{VID}(\eta_s, \mu) = \mathcal{L}_{CE}(Y, \hat{Y}_{\eta_s}) + \lambda \sum_{c=1}^{C} \sum_{h=1}^{H} \sum_{w=1}^{W} \left(\log \sigma_c + \mathbb{E}_{P_X} \left[\frac{(T_{c,h,w} - \mu_{c,h,w}(S_{\eta_s}))^2}{2\sigma_c^2} \right] \right).$$
(43)

Here, C, H and W are the number of channels, height and width of the representation T respectively (i.e., $T \in \mathbb{R}^{C \times H \times W}$). μ is a deterministic function parameterized using a neural network and learned during the training process. $\sigma = [\sigma_1, \ldots, \sigma_c]^T$ is a vector of independent positive parameters, which is also learned during the training process. \hat{Y}_{η_s} is the final prediction of the student model of the target label Y.

C.2 Task-aware Layer-wise Distillation (TED)

The TED framework Liang et al. [2023] fine-tunes a student in two stages. During the first stage, task-aware filters appended to the teacher and the student are trained with task-related heads while the student and the teacher parameters are kept constant. In the next step, the task-related heads are removed from the filters and the student is trained along with its task-aware filter while the teacher and its task-aware filter is kept unchanged. We observe that each of these steps implicitly maximizes the redundant information under Definition 3.1. To see the relationship between the TED framework and the above definition of redundant information, let Q be parameterized using the teacher's task-aware filter as $Q = f_t(T)$. Now consider the first stage loss corresponding to the teacher's task-aware filter which is given below:

$$\mathcal{L}_t(T,\theta_t) = \mathbb{E}_{x \sim \mathcal{X}} \left[\ell(f_t(T;\theta_t)) \right]. \tag{44}$$

Here, $\ell(\cdot)$ is the task specific loss, f_t is the task-aware filter parameterized by θ_t . During the first stage, this loss is minimized over θ_t . A similar loss corresponding to the student (i.e., $\mathbb{E}_{x \sim \mathcal{X}} \left[\ell(f_s(S; \theta_t)) \right]$) is minimized in order to train the student's task aware filter. Note that during this process, both $I(Y; f_t(T))$ and $I(Y; f_s(S))$ are increased.

During stage 2, the distillation loss which is given below is minimized over θ_s and S while θ_t and T being held constant.

$$\mathcal{D}_{TED}\left(T,S\right) = \mathbb{E}_{x \sim \mathcal{X}}\left[\left|\left|f_t(T;\theta_t) - f_s(S;\theta_s)\right|\right|^2\right].$$
(45)

Consider stage 2 as an estimation problem which minimizes the mean square error, where $Q = f_t(T)$ is the estimand and $f_s(\cdot)$ is the estimator. We observe that this optimization ensures $I(Y; Q|f_s(S)) = 0$ given that the same assumption as in Section 3 holds. Following similar steps as in Section 3, we see that TED framework maximizes a lower bound for the distilled knowledge, quantified as in Definition 2.2.

The main difference of this scheme w.r.t. the RED framework is two-fold. First, in RED we optimize $f_t(\cdot)$ in addition to $f_s(\cdot)$ and S during stage 2. In contrast, TED does not modify the teacher's filter during the second stage. Second, RED distillation loss employs a weighting parameter similar to that of VID.

D Experiments

Dataset: We use the CIFAR-10 dataset [Krizhevsky et al., 2009] with 60000 32x32 colour images belonging to 10 classes, with 6000 images per class. The training set consists of 50000 images (5000 per class) and the test set is 10000 images (1000 per class). The PID values are evaluated over the same test set.

Redundant Information Distillation algorithm: We distill from multiple teacher layers $T^{(1)}, \ldots, T^{(K)}$ to corresponding student layers $S^{(1)}, \ldots, S^{(K)}$. Each teacher layer $T^{(k)}$ has its own filter $f_t^{(k)}$ parameterized with $\theta_t^{(k)}$. Student filters are parameterized in a similar manner. Moreover, each teacher filter $f_t^{(k)}(\cdot)$ has its own classification head $g^{(k)}(\cdot)$ parameterized with $\phi^{(k)}$. All the student representations are parameterized by the complete weight vector η_s . In the beginning, the teacher filters are trained for n_w number of warm-up epochs with just the cross-entropy loss $\sum_{k=1}^{K} \mathcal{L}_{CE}(Y, g_t^{(k)}(f_t^{(k)}(T^{(k)}; \theta_t^{(k)}); \phi_t^{(k)})))$. Then, the optimization alternates between the first and second stages, with each cycle taking q epochs in total. Within a cycle, phase 1 is carried out for $r \times q$ epochs followed by phase 2 for rest of the epochs (See Algorithm 1).

Algorithm 1: Redundant Information Distillation

Models and hyperparameters: Teacher models are WideResNet-(40,2) and the student models are WideResNet-(16,1). For the VID distillation, the value for λ was set to 100. Learning rate was 0.05 at the beginning and was reduced to 0.01 and 0.002 at 150th and 200th epochs respectively. Stochastic Gradient Descent with a weight decay=0.0005 and momentum=0.9 with Nesterov momentum enabled was used as the optimiser. We choose three intermediate layers for distillation from the last three blocks of both the teacher and student models. The function $\mu(\cdot)$ for each layer is parameterized using a sequential model with three convolutional layers, ReLU activations and batch normalization in between the layers. A similar architecture and a training setup was used for the basline (BAS, no distillation) and the RID models. In case of the RID models, the filters $f_s(\cdot)$ and $f_t(\cdot)$ were parameterized using 2-layer convolutional network with a batch normalization layer in the middle. The classification head $g_t(\cdot)$ is a linear layer. We set $n_w = 30, q = 30, r = 1/4$ and the total number of epochs $n + n_w = 300$. Teacher, Baseline and VID models are trained for 300 epochs. In both cases of VID and RID, the independent parameter vector σ has a dimension equal to the number of channels in the outputs of functions μ , f_s or f_t . All the training was carried out on a computer with an AMD Ryzen Threadripper PRO 5975WX processor and an Nvidia RTX A4500 graphic card.

PID computation: We compute the PID components of the joint information of innermost distilled layers I(Y; T, S), using the framework proposed in Liang et al. [2024a] as follows:

- 1. Representations are individually flattened
- 2. Compute PCA on each set of representations
- 3. Cluster representations to discretize
- 4. Compute the joint distribution p(Y, T, S)
- 5. Compute PID components using the joint distribution

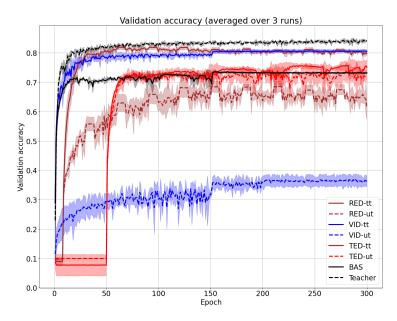


Figure 5: Classification accuracy for CIFAR10 dataset of BAS, VID, TED and RID when distilled using a trained and an untrained teacher. The suffixes "tt" stands for a trained teacher and "ut" stands for an untrained teacher. Graphs show the average over 3 runs and the shaded areas indicate mean \pm standard deviation regions.

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