How Information Bottleneck Helps Representation Learning: From the Rate Distortion Theory to VAEs

Yichao Cai

yichao.cai@adelaide.edu.au

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Abstract

This blog is on the topic of Information Bottleneck (IB) principle, clarifying its connection with rate-distortion theory, exploring different optimization strategies for IB, and discussing the application of the Variational Information Bottleneck (VIB) and β-VAE within the context of representation learning. Designed as both a personal reference and a resource for others, this blog aims to provide a holistic view understanding of the IB principle. Due to the breadth of concepts covered, some mathematical details are not included here. Readers seeking more in-depth exploration are encouraged to consult the references provided.

Contents

1 Preliminaries: Information Measures

Information measures are pivotal to this topic and essential for the majority, if not all, learning objectives aimed at optimizing machine learning models. Consequently, the author is compelled to outline some fundamental definitions and the intuitive implementations of these concepts. Given their foundational nature, readers may opt to proceed directly to section 2.
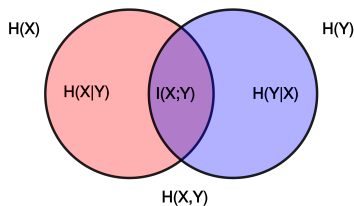

Figure 1: Venn diagram showing relations of information measures (figure taken from wikipedia).

1.1 Entropy Measures

1.1.1 Information Entropy

Given a discrete random variable X, taking values from $\mathcal{X}$ with probability mass function (pmf) $p_X : \mathcal{X} \to [0,1]$, the information entropy is

$$H(X) = -\sum_{x \in \mathcal{X}} p_X(x) \log p_X(x) = \mathbb{E}_{p_X}[-\log p_X(x)]. \tag{1}$$

The entropy measures the average amount of information contained in the random variable X, with values ranging from $0 \leq H(X) \leq log|\mathcal{X}|$. The entropy takes the minimum value 0, when X is a deterministic event, meaning there is no uncertainty about its outcome; and it reaches its maximum value when X is uniformly distributed across its support set, indicating maximum uncertainty or randomness in its outcomes. This maximum uncertainty necessitates more information to represent X, as each outcome is equally likely and no predictions can be made based on probabilities skewed toward particular outcomes.

1.1.2 Joint Entropy

Given a pair of random variables (X, Y) with pmf $p_X : \mathcal{X} \to [0,1]$, $p_Y : \mathcal{Y} \to [0,1]$ and joint probability $p_{X,Y} : \mathcal{X} \times \mathcal{Y} \to [0,1]$, the joint entropy is given by

$$H(X,Y) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_{X,Y}(x,y) \log p_{X,Y}(x,y) = \mathbb{E}_{p_{X,Y}}[-\log p_{X,Y}(x,y)]. \tag{2}$$

The joint entropy measures the uncertainty with a set of (X, Y), which indicates how much information we need to represent both X and Y. Clearly, as shown in fig. 1, we know that $\max[H(X), H(Y)] \leq H(X,Y) \leq H(X)+H(Y)$, where the minimum is met when one variable is the subevent of the other while the maximum value is met when two variables are independent.

It is worth noting that the term cross entropy, $H(p,q) = \mathbb{E}_{x \sim p_X}[-\log q_X(x)]$, is a distinct concept from joint entropy, which measures the information needed for encoding two different distributions, i.e., $p_X : \mathcal{X} \to [0,1]; q_X : \mathcal{X} \to [0,1]$, over the same underlying set $\mathcal{X}$.

1.1.3 Conditional Entropy

The conditional entropy $H(Y|X)$ quantifies the amount of information required to describe Y when X is known. It is defined as:

$$H(Y|X) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_{X,Y}(x,y) \log \frac{p_{X,Y}(x,y)}{p_X(x)} = \mathbb{E}_{p_{X,Y}}[-\log p_{Y|X}(y|x)]. \tag{3}$$

We have $H(Y|X) = H(X,Y) - H(X)$. If Y is completely determined by X, then $H(Y|X) = 0$, indicating no remaining uncertainty about Y once X is known. Conversely, if X and Y are independent variables, then $H(Y|X) = H(Y)$, as knowledge of X provides no information about Y. It is important to note that conditional entropy is not symmetric, meaning $H(Y|X)$ is not necessarily equal to $H(X|Y)$.

1.1.4 Kullback–Leibler Divergence

Kullback-Leibler (KL) divergence, also known as relative entropy, quantifies the difference between two probability distributions, p_X and q_X, over the same set $\mathcal{X}$. It is defined as:

$$D_{KL}(p_X \| q_X) = \sum_{x \in \mathcal{X}} p_X(x) \log \frac{p_X(x)}{q_X(x)} = \mathbb{E}_{p_X}[\log \frac{p_X(x)}{q_X(x)}]. \tag{4}$$

KL divergence is non-negative, not upper-bounded, and asymmetric. Formally, it can be expressed as the difference between the cross entropy of p_X with respect to q_X and the entropy of p_X, i.e., $D_{KL}(p_X \| q_X) = H(p_X, q_X) - H(p_X)$.

1.2 Mutual Information

The mutual information (MI) between two variables X and Y quantifies the information gained about one variable through observing the other, reflecting their mutual dependence. It is given by:

$$I(X;Y) = D_{KL}(p_{X,Y} \| p_X \otimes p_Y) = \mathbb{E}_{p_{X,Y}}[\log \frac{p_{X,Y}(x,y)}{p_X(x) \cdot p_Y(y)}]. \tag{5}$$

Mutual information is inherently non-negative and equals zero specifically when X and Y are independent variables. Intuitively, mutual information measures the amount of information shared between two variables: it quantifies how much knowing one variable reduces uncertainty about the other.

Building on these definitions, mutual information can also be related to entropy in the following ways:

$$I(X;Y) = H(Y) - H(Y|X) = H(X,Y) - H(X|Y) - H(Y|X). \tag{6}$$

2 Rate Distortion Theory

The problem of lossy compression investigates how to minimize the quantization rate—thereby maximizing compression—by encoding a signal X into a representation $\tilde{X}$ while maintaining minimal distortion. We define the distortion function[1] $d : \mathcal{X} \times \tilde{\mathcal{X}} \to \mathbb{R}^+$. The compression of X, through a mapping $p(\tilde{x}|x)$, results in an *expected distortion* given by:

$$\langle d(x, \tilde{x}) \rangle_{p(x, \tilde{x})} = \sum_{x \in \mathcal{X}} \sum_{\tilde{x} \in \tilde{\mathcal{X}}} p(x, \tilde{x}) \cdot d(x, \tilde{x}). \tag{7}$$

The rate function is quantified by the mutual information (MI) between X and $\tilde{X}$, denoted as $I(X; \tilde{X})$. According to its definition, a lower MI corresponds to a reduced quantization rate (greater compression).
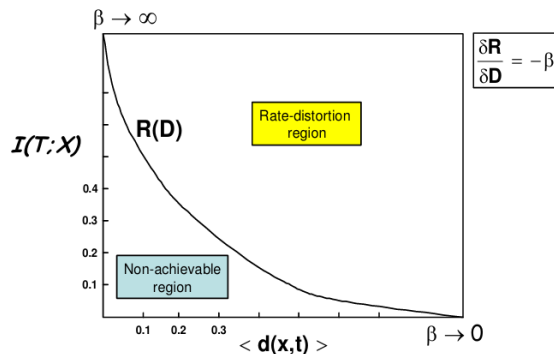
Figure 2: An example of rate distortion curve (figure taken from Slonim_PhD.pdf). The notations T and t mean $\tilde{X}$ and $\tilde{x}$ in this blog.

There exists a monotonic trade-off between these two objectives: the higher the rate, the lower the achievable distortion. Figure 2 illustrates this relationship with a representative case.

The *Rate-Distortion Theorem* elucidates the trade-off between compression rate and distortion by establishing a constraint D, through a expected distortion function. The corresponding rate-distortion (R-D) functional is defined as:

$$R(D) = \min_{p(\tilde{x}|x):\langle d(x,\tilde{x})\rangle \leq D} I(X;\tilde{X}). \tag{8}$$

To solve this functional, one can introduce a Lagrange multiplier, β, associated with the expected distortion term, transforming the objective into minimizing the following variational functional:

$$\mathcal{L}_{RD}[p(\tilde{x}|x)] = I(X;\tilde{X}) + \beta\langle d(x,\tilde{x})\rangle_{p(x,\tilde{x})}. \tag{9}$$

This formulation fundamentally seeks to determine the smallest quantization rate achievable under the constraint that the expected distortion does not exceed D. The optimal trade-off is realized at the minimum point of $\mathcal{L}_{RD}$.

2.1 Solution for the R-D functional

To minimize the rate-distortion functional $\mathcal{L}_{RD}$, the derivative is taken with respect to the conditional probability distribution $p(\tilde{x}|x)$ such that $\frac{\delta\mathcal{L}_{RD}}{\delta p(\tilde{x}|x)} = 0$, under the assumption of *normalized distributions* $p(\tilde{x}|x)$. This leads to:

$$p(\tilde{x}|x) = \frac{p(\tilde{x})}{Z(x,\beta)} \exp[-\beta d(x,\tilde{x})], \tag{10}$$

where $Z(x,\beta) = \sum_{\tilde{x}} p(\tilde{x}) \exp[-\beta d(x,\tilde{x})]$ functions as a normalization factor. Intuitively, $Z(x,\beta)$ determines how the input data X is divided into intervals to form the encoded $\tilde{X}$. Furthermore, the parameter β is determined by the required distortion level, such that $\frac{\delta R}{\delta D} = -\beta$, indicating a positive value due to the concavity of the R-D function, as demonstrated in Figure 2.

2.2 Optimization with Blahut-Arimoto Algorithm

To optimize the rate-distortion functional effectively, we aim to satisfy both equations of $p(\tilde{x})$ and $p(\tilde{x}|x)$ simultaneously at the minimum of the R-D functional, expressed as:

$$\min_{p(\tilde{x})} \min_{p(\tilde{x}|x)} \mathcal{L}_{RD}[p(\tilde{x}|x)]. \tag{11}$$

The Blahut-Arimoto (BA) algorithm provides a systematic method to address this optimization challenge:

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[1]Note that the distortion function here is a general form, which could be various specific criteria.

1. *Initialization.* Begin with an initial guess for the marginal distribution $p(\tilde{x})$ based on the data points.

2. *R-D optimization.* Optimize the marginal and conditional distributions *independently* through iterative processing. Let t represent the time step:

$$\begin{cases} p_{t+1}(\tilde{x}) = \sum_x p(x)p_t(\tilde{x}|x) \\ p_t(\tilde{x}|x) = \frac{p_t(\tilde{x})}{Z_t(x,\beta)} \exp[-\beta d(x,\tilde{x})] \end{cases} \tag{12}$$

3. *Iteration.* Calculate the normalization function $Z_t(x,\beta)$ and repeat the optimization until convergence is achieved.

At the convergence of the optimization, the learning object converges to a unique minimum of $\mathcal{L}_{RD}$ within the convex sets of the two distributions. However, the trajectories and the final distributions are not unique, indicating that the model solution is not unique.

The BA algorithm is adept at dividing a data set X into groups or partitions based on an optimality criterion but does not address the selection of the best representatives for each group. Beyond merely partitioning the data, it is essential to select the optimal representatives for each partition to retain *relevant information* for specific tasks related to a variable Y.

3   The Information Bottleneck Principle

The application of rate-distortion theory in practical scenarios is often limited due to the challenge of defining an appropriate distortion function. To overcome this, the Information Bottleneck (IB) method offers a direct and effective approach by focusing on preserving relevant information about another variable Y. This variable Y is assumed to be statistically dependent on X, evidenced by a mutual information (MI) measure $I(X;Y) > 0$. Furthermore, it is assumed access to the joint distribution $p(x,y)$ is available, enabling supervised learning with labeled data. By definition, $I(\tilde{X};Y) \leq I(X;Y)$, indicating no new information is generated during the encoding process; equivalence occurs when the representation does not lose any relevant information about Y.

The core trade-off involves maximizing the use of the minimum bit rate to represent features (*compressing representation*), while simultaneously preserving as much relevant information related to Y as possible (*preserving relevant information*). This trade-off is addressed by minimizing the following functional:

$$\mathcal{L}_{IB}[p(\tilde{x}|x)] = I(\tilde{X};X) - \beta I(\tilde{X};Y), \tag{13}$$

where β is a Lagrange multiplier that emphasizes the importance of preserving meaningful information. This multiplier also helps maintain the normalization of the mapping $p(\tilde{x}|x)$ for each x. By adjusting the hyper-parameter β, one can explore the balance between information preservation and compression.

The intuition behind the Information Bottleneck (IB) principle is clear and compelling: by imposing constraints on the preservation of relevant information, the method encourages simpler and potentially sparser representations. This simplification acts to prevent complicated relationships within the representations, aiding in the causal relationships of semantic information (in this case, disentanglement can be achieved by Markovian factorization), which in the original data is usually deeply intertwined and complex. By minimizing extraneous information while maximizing the retention of relevant information, the IB principle enhances the clarity and utility of the resulting representations, making them more manageable and insightful for further analysis.

3.1   Solution for IB

The IB method presents a more complex solution compared to the traditional Rate-Distortion (R-D) function, primarily because the constraints weighted by β are directly tied to the encoding model.[2] However, a formal

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[2]In the context of this blog, which adopts a representational perspective, the conditional distribution $p(\tilde{x}|x)$ is sometimes referred to as the encoding model or encoder.

solution for minimizing the functional can be achieved. By establishing the Markovian relation $\tilde{X} \leftrightarrow X \leftrightarrow Y$ and assuming β and $p(x, y)$ are given, the conditional $p(t|x)$ reaches a stationary point if and only if,

$$p(\tilde{x}|x) = \frac{p(\tilde{x})}{Z(x, \beta)} \exp(-\beta D_{KL}[p(y|x)\|p(y|\tilde{x})]), \forall \tilde{x} \in \tilde{\mathcal{X}}, \forall x \in \mathcal{X}, \tag{14}$$

where $Z(x, \beta)$ is a normalization function ensuring that $\sum_{\tilde{x}} p(\tilde{x}|x) = 1$ for each x. *It is critical to clarify that the Markovian relation is not a modeling assumption about the latent variable model or the underlying causal structure.* Rather, it defines the problem setting—establishing a linkage between $\tilde{X}$ and Y through X so that the marginal distribution over $p(x, y, \tilde{x})$ relative to X and Y remains consistent with the input distribution $p(x, y)$, indicating that the encoding process does not modify the distribution of inputs[3].

The IB functional can be viewed as a specific, effective R-D function, where the distortion criterion $d(x, \tilde{x}) = D_{KL}[p(y|x)\|p(y|\tilde{x})]$ is guided by the target variable Y but not assumed a priori. Contrary to traditional R-D theory, where encoding is performed through partitioning alone, the IB method focuses on conditional distributions $p(y|\tilde{x})$, highlighting not only the optimal partitioning but also the selection of representatives, emphasizing how the encoded representation actively involves choices concerning the portrayal of the representatives.

3.2 Iteration algorithm for IB

The optimization target, i.e., minimizing the functional, is outlined as follows:

$$\mathcal{L}_{IB}[p(\tilde{x}|x); p(\tilde{x}); p(y|\tilde{x})] = -\langle \log Z(x, \beta) \rangle_{p(x)} = I(X; \tilde{X}) + \beta \langle D_{KL}[p(y|x)\|p(y|\tilde{x})] \rangle_{p(x,\tilde{x})}, \tag{15}$$

With the known joint distribution $p(x, y)$, trade-off parameter β, and convergence criterion ε, this minimization can be conducted independently over the convex sets of the normalized distributions $\{p(\tilde{x}|x)\}$, $\{p(\tilde{x})\}$, and $\{p(y|\tilde{x})\}$.

The iterative optimization process involves:

1. **Initialization.** Randomly initialize $p(\tilde{x}|x)$.

2. **Iteration.** Denote by t the iteration step:

$$\begin{cases} p_t(\tilde{x}|x) = \frac{p_t(\tilde{x})}{Z_t(x,\beta)} \exp(-\beta D_{KL}[p(y|x)\|p_t(y|\tilde{x})]) \\ p_{t+1}(\tilde{x}) = \sum_x p(x)p_t(\tilde{x}|x) \\ p_{t+1}(y|\tilde{x}) = \frac{1}{p_{t+1}(\tilde{x})} \sum_x p_t(\tilde{x}|x)p(y|x)p(x) \end{cases} \tag{16}$$

3. **Evaluate.** If $\mathcal{L}_{IB} \leq \varepsilon$, terminate; otherwise, continue the iteration.

As shown in fig. 3, the solutions to these self-consistent equations correspond to a family of annealing curves, all starting from the trivial point $(0, 0)$ in the information plane with infinite slope, parameterized by the value of β. Increasing the value of β allows exploration along convex curves in the information plane, analogous to rate-distortion curves, which exist for every choice of the cardinality of $\tilde{X}$. Interestingly, every two curves in this family separate (bifurcate) at some finite (critical) point through a second-order phase transition. These transitions create a hierarchy of relevant quantizations for different cardinalities of $\tilde{X}$. Similar to R-D theory, the trajectory to the stationary point is independently optimized for the three convex sets, thus the solution is not unique.

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[3]In many representation learning scenarios, the latent variable corresponding to the representation is considered a confounder between X and Y. This complicates the model significantly because it challenges the assumption that marginal distributions remain invariant.
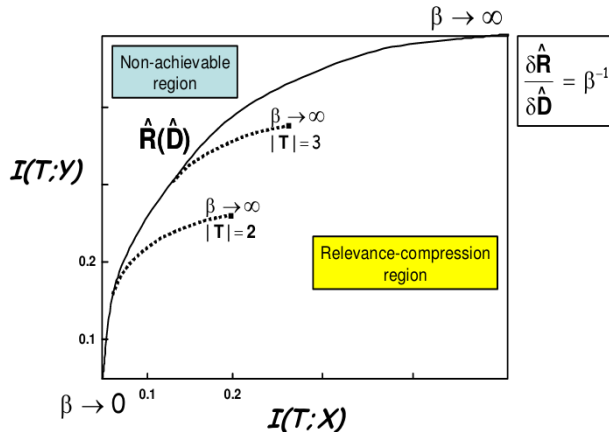
Figure 3: An example of information-compression curve of IB (figure taken from Slonim_PhD.pdf).

4 VAEs through an IB Perspective

Variation Autoencoders (VAEs) and their extensions (e.g., β-VAE and annealing VAE) form a fundamental framework in representation learning. VAEs can be interpreted through the lens of the Information Bottleneck (IB) principle, which emphasizes controlling the information flow between the input data and latent variables to balance compression with representation fidelity.

4.1 ELBO and Vanilla VAE

VAEs maximize the Evidence Lower Bound (ELBO), comprising a reconstruction term and a regularization term (KL divergence) that enforces the closeness between the approximate posterior $q(z|x)$ and the prior $p(z)$. The objective for a vanilla VAE is:

$$\mathcal{L} = \mathbb{E}_{q(z|x)}[\log p(x|z)] - D_{KL}(q(z|x) \parallel p(z)). \tag{17}$$

The regularization term encourages the latent variables z to encode a compressed representation of the input x. From an IB perspective, this objective balances the mutual information $I(X;Z)$ between the input X and latent variables Z with reconstruction accuracy. The prior, $p(z)$, acts as a regularizing force in the latent space, defining our assumptions about the distribution of latent variables. Intuitively, this prior helps structure the latent space by guiding the representations of z toward configurations that align with desired properties, such as simplicity and smoothness. This promotes generalization by encouraging representations that are less specific to individual training examples and more robust to variations in data. Thus, $p(z)$ aids in learning representations that are transferable and likely to generalize well to unseen data.

By minimizing the KL divergence, the model limits the amount of information Z retains about X, promoting simpler, more generalizable representations. Meanwhile, the reconstruction term encourages the latent variables to retain essential information needed to accurately reconstruct the input X. However, without strict control over this trade-off, vanilla VAEs may suffer from poor latent space structure or limited expressiveness, as the KL term often dominates the reconstruction term, leading to over-regularization.

4.2 β-VAE

To address the above issue, the β-VAE introduces a hyperparameter β to the regularization term in the ELBO. The objective becomes:

$$\mathcal{L}_\beta = \mathbb{E}_{q(z|x)}[\log, p(x|z)] - \beta D_{KL}(q(z|x) \parallel p(z)). \tag{18}$$

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From an IB perspective, the trade-off between information compression and reconstruction fidelity is controlled by varying β. A larger β enforces stronger compression (by pushing the KL divergence to be smaller), creating a tighter bottleneck that reduces the mutual information $I(X; Z)$, which can encourage disentangled representations but risks losing detail in the reconstruction. Conversely, a smaller β allows more information to pass through the bottleneck, resulting in better reconstruction accuracy but potentially poorer generalization.

Therefore, adjusting β becomes essential to retain only the most relevant features, aligning well with the IB principle's focus on capturing minimal yet sufficient information. However, finding an optimal trade-off is challenging—too large a β can lead to underfitting, where Z lacks sufficient information to accurately reconstruct X.

5 Time-Varying Information Bottleneck

5.1 Annealing VAE

In contrast to using a constant β, annealing VAEs apply a dynamic β during training. They start with a small β value (close to zero) and gradually increase it over the course of training, or they may use a cyclical schedule, as shown in fig. 4.
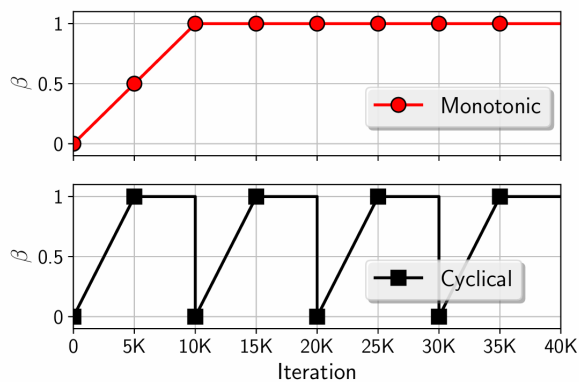

Figure 4: Two annealing schedules in annealing VAE. Picture taken from (Fu, et al, 2019)

This approach allows for a time-varying information bottleneck. For instance, with a gradually increasing β, the model is encouraged to initially focus on accurately reconstructing X before imposing stronger constraints on Z.

Intuitively, easing into regularization prevents the sharp reduction in information that a high β value would impose from the start, which can lead to premature loss of important details. Annealing stabilizes training, promoting a gradual learning of relevant latent factors and resulting in representations that retain essential features of the data.

5.2 Information Bottleneck Diffusion Models

Diffusion models are optimized by predicting the Gaussian noise added to images at different time steps, with the noise strength controlled by a varying β. The learning objective can be expressed as an ELBO:

$$\mathcal{L}_{VLB} = -\mathbb{E}_{q(X_{0:T})}[\log \frac{q(X_{1:T}|X_0)}{p_\theta(X_{0:T})}]$$

$$= \underbrace{\log p_\theta(X_0|X_1)}_{L_0} - \sum_{t=2}^{T} \underbrace{D_{KL}(q(x_{t-1}|X_t, X_0) \parallel p_\theta(X_{t-1}|X_t))}_{\mathcal{L}_{t-1}} - \underbrace{\mathbb{E}_q[D_{KL}(q(X_T|X_0) \parallel p_\theta(X_T))]}_{\mathcal{L}_T} \quad (19)$$

$$\leq \mathbb{E}_{q(x_0)}\log p_\theta(X_0).$$

Each KL divergence term is optimized via the reparameterization trick with a standard Gaussian prior. Each D_{KL} term in the objective indicates an information bottleneck with different strengths across time steps. Different time schedules can be applied to control the time-varying regularization term β, resulting in different KL divergence trends, as shown in fig. 5.
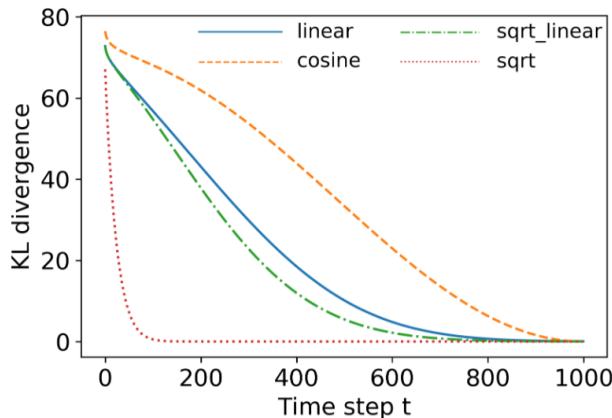

Figure 5: KL divergence curves with different time schedules. Picture taken from (Yang, et al, 2024)

Intuitively, an increasing KL divergence suggests that the information carried by X_{t-1} grows, leading to a progressively looser information bottleneck over X_{t-1}. This varying information bottleneck encourages the model to learn simplified yet effective representations, potentially improving disentanglement performance.

6 Discussion

In summary, the Information Bottleneck (IB) principle is a foundational tool for understanding unsupervised representation learning. By leveraging appropriate information measures, controlling the information bottleneck facilitates a desirable trade-off between simplicity and sufficiency in representations. However, significant gaps remain in achieving an optimal balance. For example:

1. **Does the prior matter?** Current methods typically use a Gaussian prior to simplify the estimation of the KL divergence and to stabilize gradient flow during variational inference. However, literature in causal representation learning and non-linear Independent Component Analysis (ICA) suggests that a Gaussian prior may hinder the identifiability of latent models and affect disentanglement quality. Additionally, some works argue that an unconditional prior may limit effective compression, potentially impeding the recovery of intrinsic causal structures in the latent space without overly restrictive assumptions on the function classes.

2. **Is there an efficient method to incorporate additional inductive biases?** Discovering and effectively using inductive biases remains both challenging and essential for enhancing model performance. Appropriate inductive biases could guide the learning process toward more interpretable and generalizable representations, facilitating convergence to useful latent features.

3. **Is it necessary to include variational inference?** Variational inference, used in models like VAEs and to optimize the Evidence Lower Bound (ELBO), is central for structuring latent variables with a chosen prior to improve generalization. However, estimating information measures like KL divergence requires approximating two distributions, which can be complex and computationally demanding. This raises the question of whether alternative approaches to mutual information estimation could enable efficient gradient-based optimization without depending on variational inference. Additionally, variational inference offers the advantage of sampling-based training, which helps to build a more generalized decoder. A related question is whether potential alternatives could retain this advantage in training generalized decoders as well.

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