



Contrastive learning: Big Data Foundations and Applications

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ABSTRACT

Contrastive learning (CL) has exploded in popularity due to its ability to learn effective representations using vast quantities of unlabelled data across multiple domains. CL underlies some of the most impressive applications of generative AI for the general public. We will review the fundamentals and applied work on contrastive learning representations focusing on three main topics: 1) CL in supervised, unsupervised and self-supervised setup and its revival in AI research as an instance discriminator. In this part, we will focus on learning about the nuts and bolts, such as different augmentation techniques, loss functions, performance evaluation metrics, and some theoretical understanding of contrastive loss. We will also present the methods supporting DALL-E 2, a popular generative AI. 2) Learning contrastive representations across vision, text, time series, tabular data and knowledge graph modalities. Specifically, we will present the literature representative of solution approaches regarding new augmentation techniques, modification in the loss function, and additional information. The first two parts will also have small hands-on session on the application shown and some of the methods learned. 3) Discussing the various theoretical and empirical claims for CL's success, including the role of negative examples. We will also present some work that challenges the shared information assumption of CL and propose alternative explanations. Finally, we will conclude with some future directions and applications for CL.

CCS CONCEPTS

• **Computing methodologies** → **Unsupervised learning; Knowledge representation and reasoning.**

KEYWORDS

contrastive learning, multi-view, multi-modal, augmentations, time-series, graphs, tabular datasets, distillation, clustering, noise estimation loss

ACM Reference Format:

Sandhya Tripathi and Christopher R. King. 2024. Contrastive learning: Big Data Foundations and Applications. In *7th Joint International Conference on Data Science & Management of Data (11th ACM IKDD CODS and 29th COMAD) (CODS-COMAD 2024)*, January 04–07, 2024, Bangalore, India. ACM, New York, NY, USA, 5 pages. <https://doi.org/10.1145/3632410.3633291>



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CODS-COMAD 2024, January 04–07, 2024, Bangalore, India
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ACM ISBN 979-8-4007-1634-8/24/01.
<https://doi.org/10.1145/3632410.3633291>

1 BACKGROUND

Traditionally learning paradigms have been understood in the context of supervised, semi-supervised and unsupervised learning where the presence of supervision refers to the availability of annotations. However, annotation can be time-consuming, cost-ineffective or erroneous. To circumvent this issue, self-supervised learning provides a framework (of pretraining) where the goal is to learn good feature representations without annotations. These representations can then be used for various downstream tasks in both discriminative and generative forms.

Recently, multi-view self-supervised learning (MVSSL) where the goal is to learn similar representations for the different views of the same data has gained a lot of attention due to its success demonstrated in computer vision [1], speech recognition [2] and other domains. Three main categories of MVSSL are: 1) contrastive loss-based where a suitable similarity metric between the representations of two views from the same example should be maximized and from different examples should be minimized [7], 2) clustering-based where the clusters assignments for one view are to be predicted from the representations of another view [6], 3) distillation-based where a teacher-student model approach is taken for while training [17]. In this tutorial, our focus is on contrastive learning methods across a variety of modalities. In particular, we focus on how different components of contrastive learning vary across modalities in terms of their unique and shared properties.

2 GOALS AND RELEVANCE

Our goal is to review foundations and applied practices in multi-modal contrastive learning for representation learning. We present the major breakthroughs in the following modalities: 1) vision, 2) text, 3) time series, 4) tabular data, and 5) knowledge graphs. To complement the theory, we also provide a code base for the presented work¹.

Self-supervised and semi-supervised learning have long been important for learning representations from big data. While auto-encoder models are successful in some domains, contrastive approaches learning to discriminate encoded representations have exploded in their applicability and power in many domains, especially in those where generative models and loss functions on objects are difficult. However, most available applications are in the image and text domains; other modalities that stand to benefit from CL-based encoders include tabular databases, clinical times series in Electronic Health Records (EHRs), and structured (graph-encoded) data. This strategy is fundamental to several state-of-the-art generative methods. Our tutorial will provide a summary of state-of-the-art solutions and open problems.

¹https://github.com/sandhyat/ContrastiveLearning_Tutorial

3 GENERAL DESCRIPTION OF TUTORIAL CONTENT

Contrastive learning (CL) is a self-supervised strategy to learn a dense numeric representation of a given feature space, usually by discriminating augmentations of a sample (positive pairs) versus other samples (negative pairs). CL methods differ based on the strategy for generating augmentations, strategy for selecting negative pairs, and loss function. By manipulating the contrastive task, differentiating corrupted versions of the same object from other objects will train embedding functions to represent the major features of the feature space. Because paired representations of the same object in different domains (such as text description of an image) can be used as the positive pair, multimodal representation learning in the same space is possible without significant modifications. Although the concept of contrastive losses was introduced by [18], it was not broadly used by ML community until the InfoNCE loss was defined [34] and found to work well as an instance discriminator [50]. In the computer vision and natural language processing domain, the CLIP model [35] shows the potential of contrastive learning by pre-training representations of images and text that are zero-shot transferred to generative methods. Due to CL's real world popularity in vision and language, the existing survey papers and tutorials (Neurips'21, ECCV'22, NAACL'22) focus on these domains. We will present a comprehensive overview of CL foundations and applications outside of images and text.

The goal of data augmentation is to increase the variability of the data and expose the model to different perspectives for learning similar or dissimilar representations. Data augmentation techniques in CL are modality-specific, and hence each data type has its own particular strategies which may not apply elsewhere. For example, there is obviously workable analogy of "color distortion" from images into text. Common data augmentation techniques include cropping, flipping, rotation, adding noise, and random trimming in sequences. In addition to pre-determined augmentations, one can also create augmentations adaptively [31]. Specific augmentation techniques are also available in time series [11, 23, 57] and tabular data [3, 44, 54]. Learning contrastive representation over graphs has focused on downstream task performance [19] and the need for better augmentations [55, 56].

In new data modalities, the optimal augmentation is difficult to identify; in those cases, the loss function selected becomes more important [33]. Some loss functions are optimized for a particular modality, such as in images [58] and time series [33, 49, 52]. Generally, there are a variety of loss functions that are available for CL, the main ones being 1) contrastive loss that maximizes the similarity between positive pairs, 2) InfoNCE loss that treats CL as a binary classification problem between positive and negative pairs, 3) triplet loss which relies on the relative distance between the examples.

Unlike most supervised learning methods, forming batches in an appropriate way is a key step in the contrastive learning framework. Because the examples selected into a particular step of the loss function can make the underlying discriminative task easier or harder, "hard negative mining" of example pairs which force the embedding to represent more subtle features is a long-standing approach [21, 22, 37, 45]. However, some variations are successful

with no negative examples at all [8, 58, 59]. Alternatively, large batch sizes can make likely that at least some negative pairs are "hard" and improve performance [50]. To circumvent the computational complexity and optimization instability of these algorithms, approaches which cluster examples based on an intermediate representation or an auxiliary network can accomplish much the same goal [6, 17]. Batch selection is therefore intimately tied to the optimization strategy, which can have a large impact on the quality of representations. For example, large memory banks [50], momentum encoders as in MoCo [20], and simple agreement maximization on large batch sizes for a longer time as in SimCLR [7] were found to work well in images, but may not be as important in tabular data. Most CL methods assume that positive pairs (from augmentations or views) share underlying information and maximize the agreement between the latent representation as training progresses. FactorCL [29] challenges this assumption and demonstrates that there exist cases where task-relevant information can be factorized into shared and unique representation.

The two views in contrastive learning can be augmented views (noisy images) of the same data point [7, 20], two different views (images from different angles) of a source of information [38, 42], or two different sources of information about the same object (image and its text description) [14, 62]. In addition to contrasting in the native input space, similar to VAEs, one can implement contrastive loss on the perturbations of embeddings [26, 56].

Understanding why CL is so successful in some cases is still an active area of research. Some work has elucidated the relationship between mutual information and CL via InfoNCE [43]. Another line of work explores the geometry of embeddings being on a hypersphere [45] and of the modality gap between views [30]. The network architecture and training algorithm are also important variables in the success of CL; this is especially important in less investigated modalities [39]. A popular use case of contrastive learning, DALL·E 2, which generates images from a text prompt, is a prominent example which illustrates the working of the above components together to form a highly performant representation used in a complex downstream task [35, 36].

4 OUTLINE

- (1) Part 1: Overview of contrastive learning foundations and applications
 - Contrastive learning in different paradigms, history and popularity [18, 34, 50]
 - Different data augmentation techniques: cutout, adding noise, trimming, etc.
 - Different loss functions: InfoNCE, Triplet loss, NT-Xent loss, etc.
 - Performance evaluation methods: linear methods, transfer learning abilities
 - Theoretical understanding of contrastive learning in terms of inductive biases [39], geometry of embedding [46], mutual information and entropy [16]
 - Understanding CLIP [35] and UnCLIP [36] that led to DALL·E 2 (AI artist)
- (2) Part 2: How contrastive learning differs in different data modalities?

- Need of modality-specific augmentations and loss functions.
 - Contrastive learning methods for visual representations that rely on
 - optimization parameters (large batch size, more training steps etc[7], adding a momentum encoder [20]) or using a memory bank [50]
 - using embeddings from nearest neighbour set [12]
 - Contrastive learning methods for text representations
 - earliest work modified noise contrastive estimation [32]
 - based on classification task [15, 51], text generation task [27] or pretraining task [41]
 - Contrastive learning methods for time series representations
 - using another source of information in addition to the temporal one: temporal and context [13], temporal and spatial [25], temporal and frequency [61]
 - modifying the loss function using the neighbourhood information [52] or expert feature information [33]
 - utilizing data augmentation techniques [23, 49, 57]
 - Contrastive learning methods for tabular data representation
 - augmentations created based on addition of noise [3, 54], some use complex models such as transformers [40, 47]
 - modelling as a multiview problem by subsetting the features [44]
 - Contrastive learning methods for graph based representations: whether the augmentations are needed or not [55, 56], modelling the real world structures [24]
 - Hands-on experience on one method for each data modality
- (3) Part 3: What works and why? Further possibilities for CL!
- Decoupling and debiased contrastive loss functions [10, 53]
 - (Un)Importance of negative samples in contrastive learning [21, 22, 37, 45, 59, 60]
 - Learning in the presence of noisy views by proposing a noise-robust loss function [9], in the presence of noisy labels by selecting confident pairs [28]
 - Multi-modal contrastive learning [14, 35, 62]
 - Importance of shared and unique information in multi-modal CL [29], Connecting pairs of modalities [48]
 - Possible attacks [5] and mitigation strategies on multi-modal CL [4]
 - Non-contrastive (without negative examples) methods: BYOL [17], using stop gradient [8], using correlation metric [58]; clustering to improve the representations[6]
 - CL for learning joint representations from two databases for feature matching task
 - CL application in healthcare AI and implementation challenges

5 AUDIENCE, REQUISITES AND DURATION

The tutorial duration will be 1.5 hours. The tutorial could be useful for researchers, students, and practitioners interested in adding

CL-based methods to experiments and applications. Audience background can be intermediate with knowledge of neural network training (loss functions, gradient descent) and widely used architectures (CNN, RNN, transformers). Some topics will be more valuable to those with prior exposure (graph neural networks).

6 TUTORIAL PRESENTERS

- Dr. Christopher Ryan King, MD, PhD is an assistant professor in the Department of Anesthesiology at Washington University School of Medicine. His PhD in biostatistics from the University of Chicago focused on the analysis of rare variants in whole-genome sequencing. His current research centers on the applied use of artificial intelligence for clinical decision support. Email id: christopherking@wustl.edu
- Sandhya Tripathi, PhD is a postdoctoral research associate in the Department of Anesthesiology at Washington University School of Medicine. Her PhD at IIT Bombay, India focused on developing solutions for label noise (incorrect annotations) problems in classification and interpretable subset selection method using Shapley value. Currently, she has been interested in developing and applying machine learning models for real-world clinical problems, such as combining EHRs across hospitals and evaluating fairness. Email id: sandhyat@wustl.edu

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