What is Hard Negative Sample?

2022. 11. 11

Data Mining & Quality Analytics Lab.

채고은

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- Data Mining & Quality Analytics Lab. (김성범 교수님)
- 석 · 박사 통합 과정 (2022. 03 ~ Present)

❖ Research Interest

- Self-Supervised Learning
- Hard Negative Sampling in Contrastive Learning
- Explainable AI

❖ Contact

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아래의 식물들을 어떻게 분류할까?


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아래의 식물들을 어떻게 분류할까?

각 식물의 **Label** 을 알 수 없다면?

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아래의 식물들을 어떻게 분류할까?

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아래의 식물들을 어떻게 분류할까?

Label 이 없는 식물이 **아주 많다**면?

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아래의 캐릭터들을 어떻게 분류할까?

Introduction

Background

아래의 캐릭터들을 어떻게 분류할까?

분류가 어렵고 & **Label** 이 없는 데이터가 **아주 많다**면?

Introduction

Background

Data	Label	Data	Label
	Dave		Kevin?
	Bob		
	Stuart		

Introduction

Background

Data	Label	Data	Label
	Dave		Kevin
	Bob		Phil?!
	Stuart		

Introduction

Background

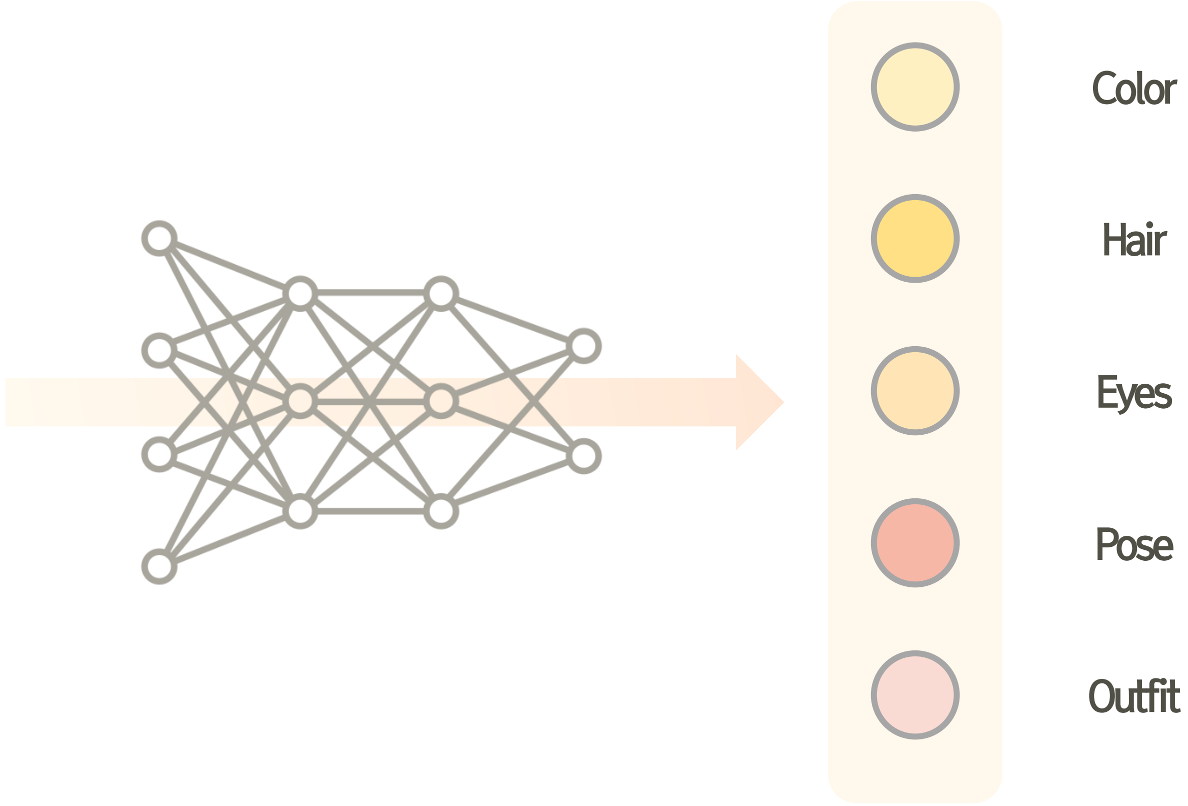
Labeling 없이 데이터 자체의 특징을 학습할 수는 없을까?

Introduction

Self-Supervised Learning

❖ What is Self-Supervised Learning?

- Representation Learning 의 특별한 유형
- Unlabeled Dataset 에서 좋은 Data Representation 구축하여 학습 가능



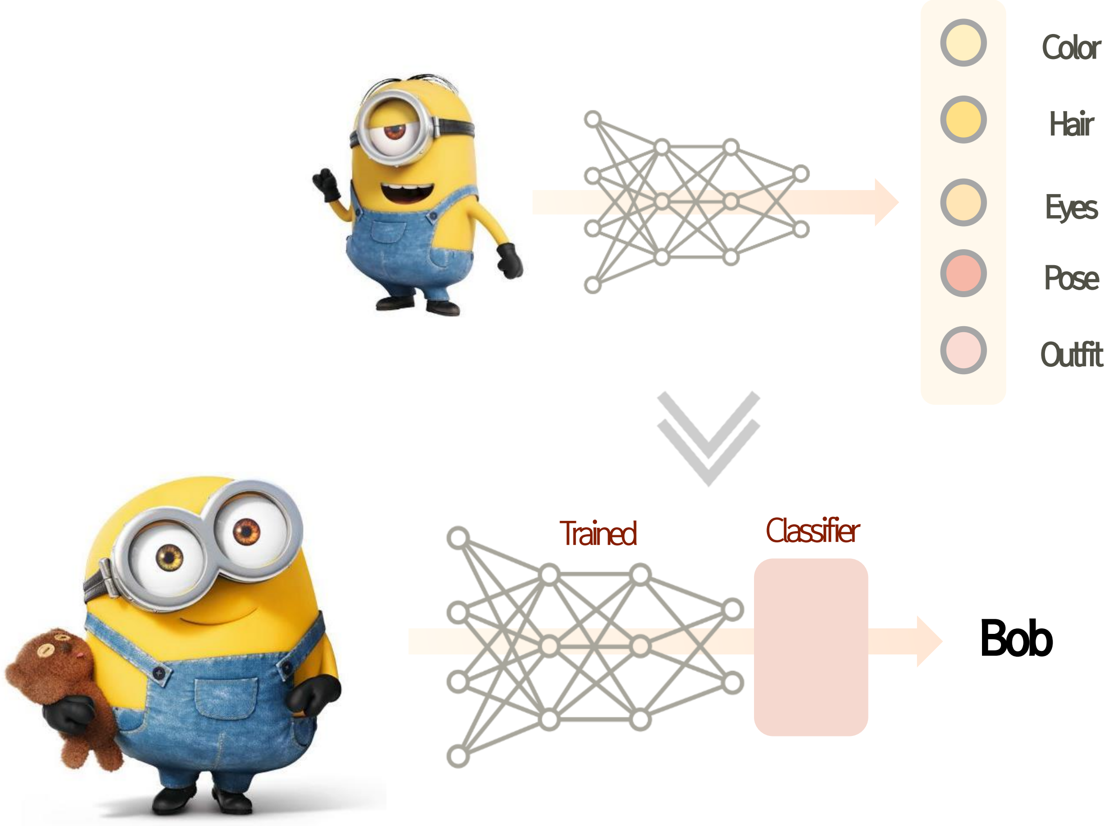
Introduction

Self-Supervised Learning

❖ Why Do We Need Self-Supervised Learning?

- Data Labeling 에 많은 노동과 비용 필요 & Labeling 과정에서 작업자의 Bias 존재
- 학습한 Representations 을 다양한 Downstream Task 에 적용 가능

구체적으로 풀고자 하는 Task



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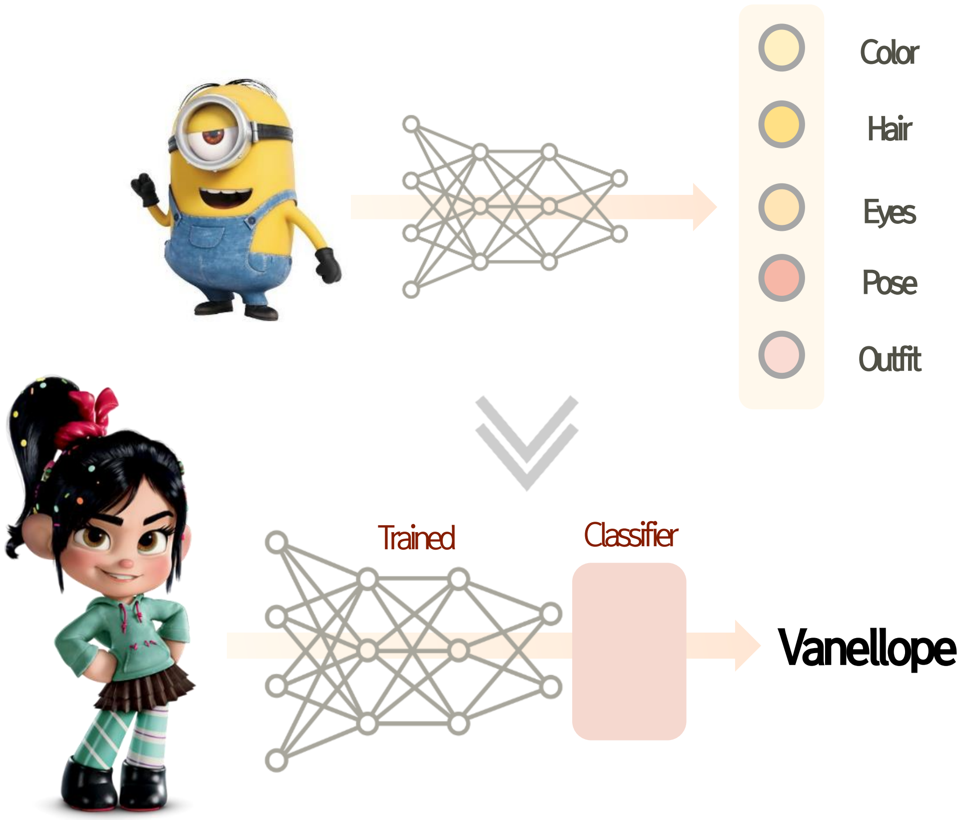

Introduction

Self-Supervised Learning

❖ Self-Supervised Learning: Taxonomy

- Self-Supervised Learning은 방법론에 따라 4가지의 카테고리로 분류 가능

Self-Supervised Learning

1. Generative Model	주어진 학습 데이터의 분포를 따르는 유사한 데이터 생성 데이터의 본질을 발견하고 효율적인 내부화 필요	VAE, GAN, Autoregressive, Flow-based, Diffusion
2. Self-Prediction Model	개별 데이터 샘플 내에서 예측 작업 수행 데이터 샘플에서 다른 부분이 샘플의 한 부분 예측	Masked Prediction Channel Shuffling
3. Innate Relationship	데이터 샘플을 변화시켜도 원래 정보를 유지하는 가설 기반	Image Rotation Feature Counting
4. Contrastive Learning	주어진 데이터 샘플 내에서 그들 사이의 관계를 예측 Embedding 공간 학습이 목표	Instance Discrimination Augmented Views

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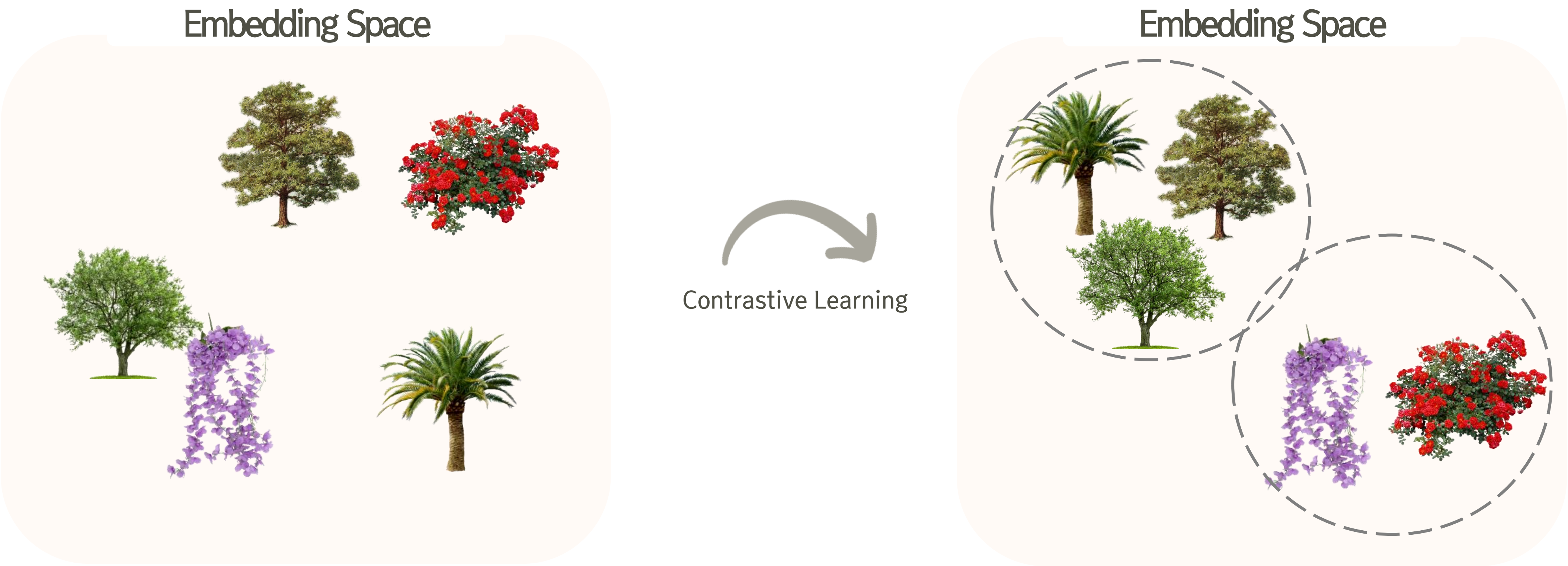
2. Contrastive Learning

Contrastive Learning

Basic Definition

❖ Contrastive Learning

- 주어진 데이터 샘플 내에서 그들 사이의 관계를 예측
- 목표: 유사한 샘플 Pair 가 가까이 있고, 다른 샘플 Pair 가 멀리 있는 Embedding Space 학습

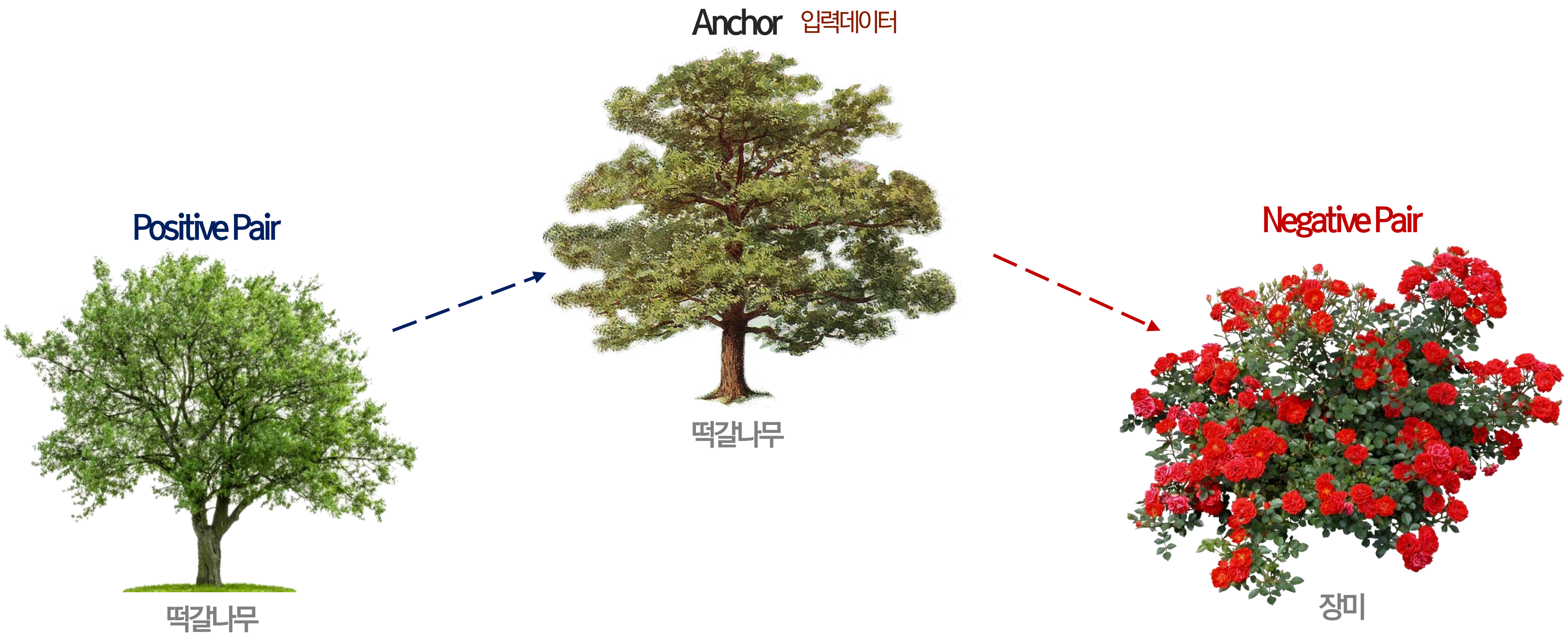


Contrastive Learning

Basic Definition

❖ Contrastive Learning

- Anchor 를 기준으로 Positive Pair, Negative Pair 정의
- Positive Pair 는 가까워지도록, Negative Pair 는 멀어지도록 학습



Contrastive Learning

SimCLR

❖ A Simple Framework for Contrastive Learning of Visual Representations (ICML, 2020)

- 2022년 11월 기준 6946회 인용
- Contrastive Visual Representation Learning 을 위한 새로운 Framework SimCLR 제안

A Simple Framework for Contrastive Learning of Visual Representations

Ting Chen [1] **Simon Kornblith** [1] **Mohammad Norouzi** [1] **Geoffrey Hinton** [1]

Abstract

This paper presents *SimCLR*: a simple framework for contrastive learning of visual representations. We simplify recently proposed contrastive self-supervised learning algorithms without requiring specialized architectures or a memory bank. In order to understand what enables the contrastive prediction tasks to learn useful representations, we systematically study the major components of our framework. We show that (1) composition of data augmentations plays a critical role in defining effective predictive tasks, (2) introducing a learnable nonlinear transformation between the representation and the contrastive loss substantially improves the quality of the learned representations, and (3) contrastive learning benefits from larger batch sizes and more training steps compared to supervised learning. By combining these findings, we are able to considerably outperform previous methods for self-supervised and semi-supervised learning on ImageNet. A linear classifier trained on self-supervised representations learned by SimCLR achieves 76.5% top-1 accuracy, which is a 7% relative improvement over previous state-of-the-art, matching the performance of a supervised ResNet-50. When fine-tuned on only 1% of the labels, we achieve 85.8% top-5 accuracy, outperforming AlexNet with 100× fewer labels. [1]

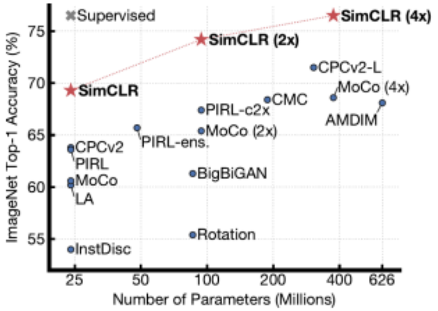


Figure 1. ImageNet Top-1 accuracy of linear classifiers trained on representations learned with different self-supervised methods (pretrained on ImageNet). Gray cross indicates supervised ResNet-50. Our method, SimCLR, is shown in bold.

However, pixel-level generation is computationally expensive and may not be necessary for representation learning. Discriminative approaches learn representations using objective functions similar to those used for supervised learning, but train networks to perform pretext tasks where both the inputs and labels are derived from an unlabeled dataset. Many such approaches have relied on heuristics to design pretext tasks (Doersch et al., 2015; Zhang et al., 2016; Noroozi & Favaro, 2016; Gidaris et al., 2018), which could limit the generality of the learned representations. Discriminative

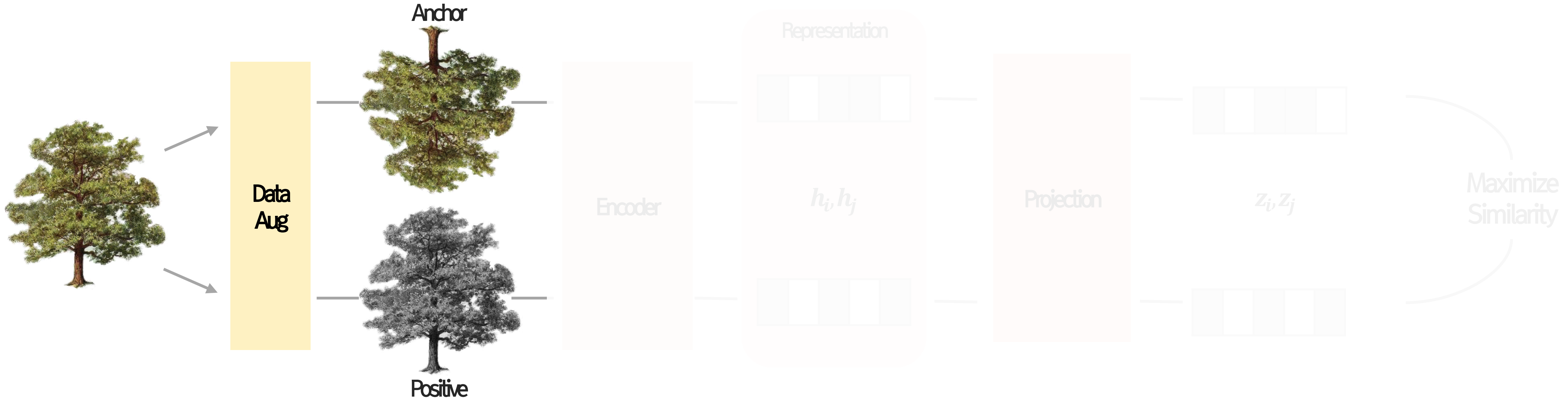
[2] Chen, T., Kornblith, S., Norouzi, M., & Hinton, G. (2020, November). A simple framework for contrastive learning of visual representations. In International conference on machine learning (pp. 1597-1607). PMLR.

Contrastive Learning

SimCLR

❖ A Simple Framework for Contrastive Learning of Visual Representations

- 한 Sample 에 대해 다르게 Augmented 된 두 결과를 Anchor, Positive pair 로 정의
- Latent Space 에서 Contrastive Loss 를 통해 Anchor-Positive 유사도 최대화



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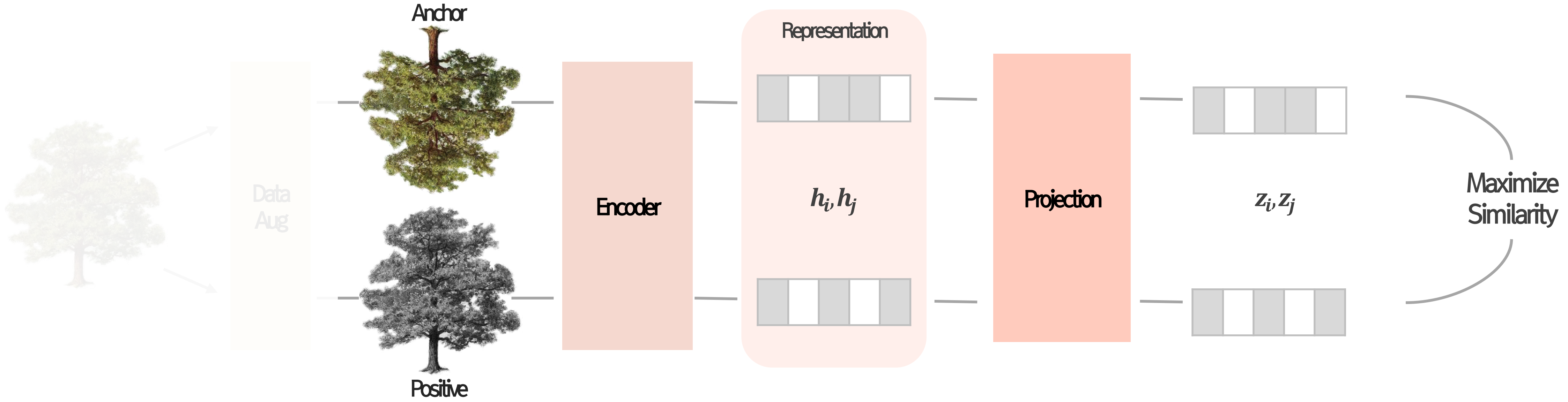

Contrastive Learning

SimCLR

❖ A Simple Framework for Contrastive Learning of Visual Representations

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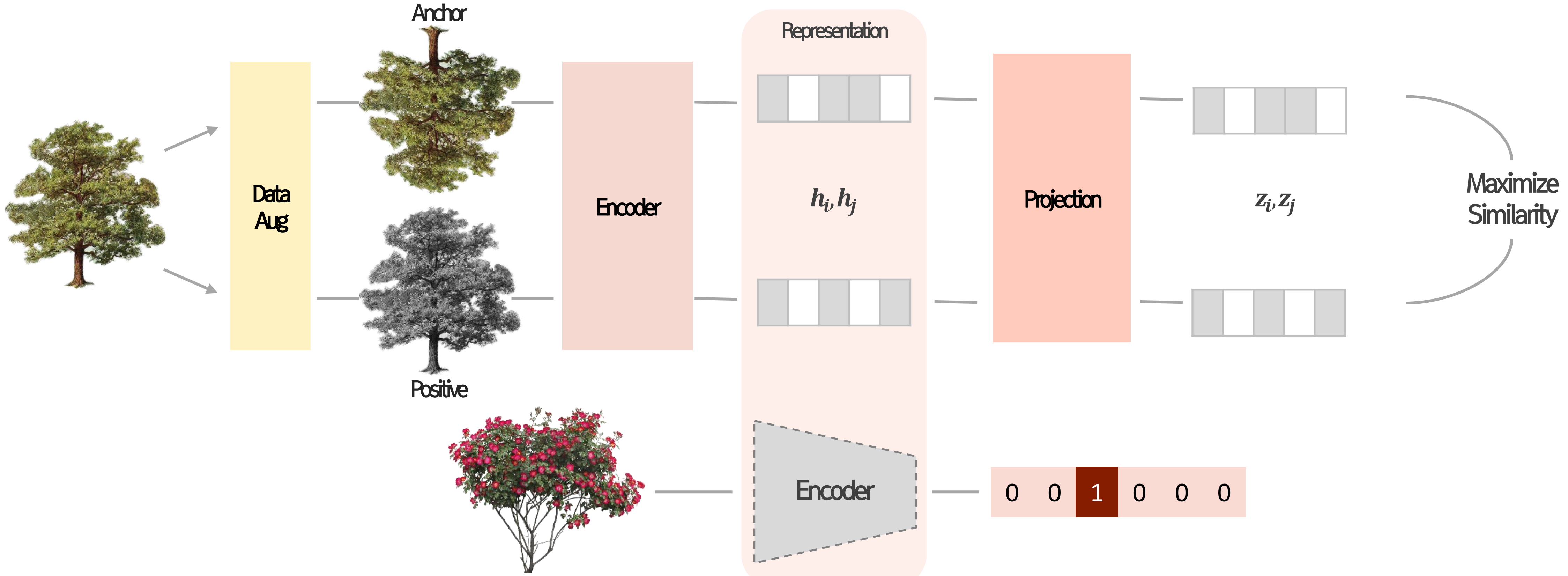
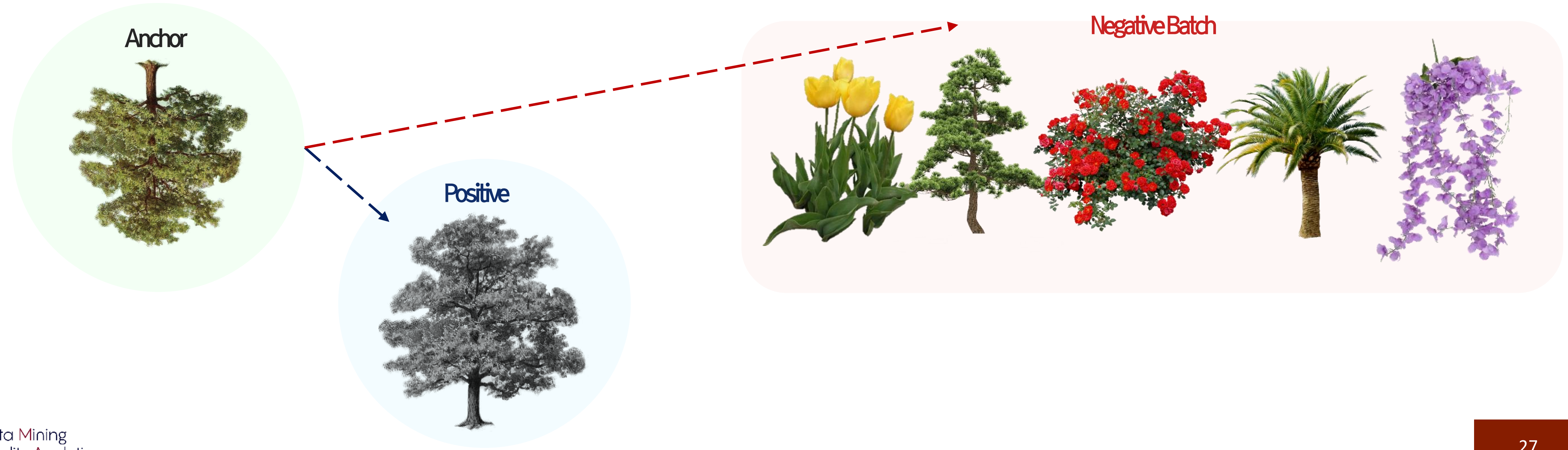


Contrastive Learning

SimCLR

❖ A Simple Framework for Contrastive Learning of Visual Representations

- 다양한 Data Augmentation 기법 활용 (Random Crop + Color Distortion)
- 깊은 Embedding Layers & 큰 Batch Size



Contrastive Learning

SimCLR

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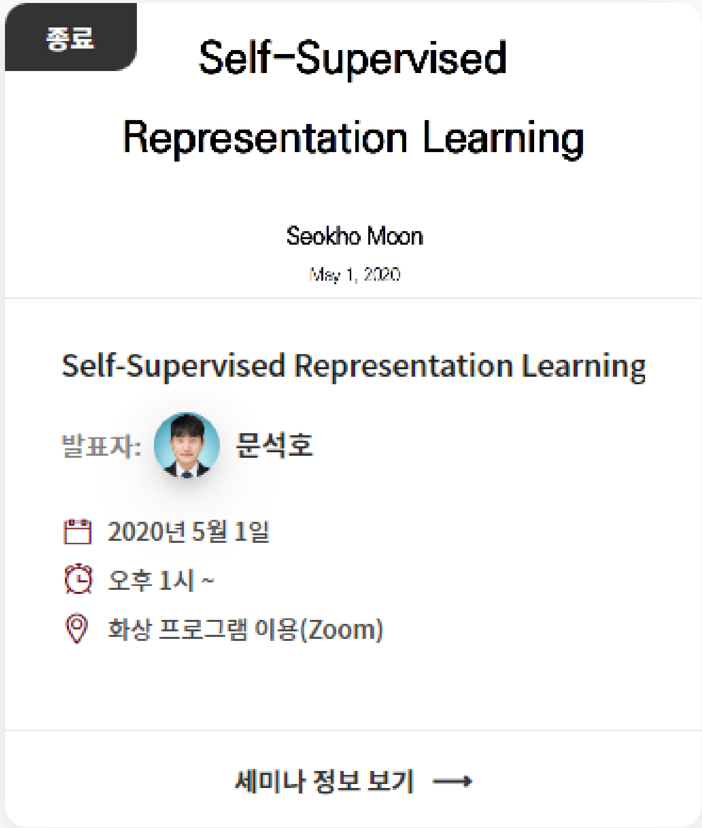
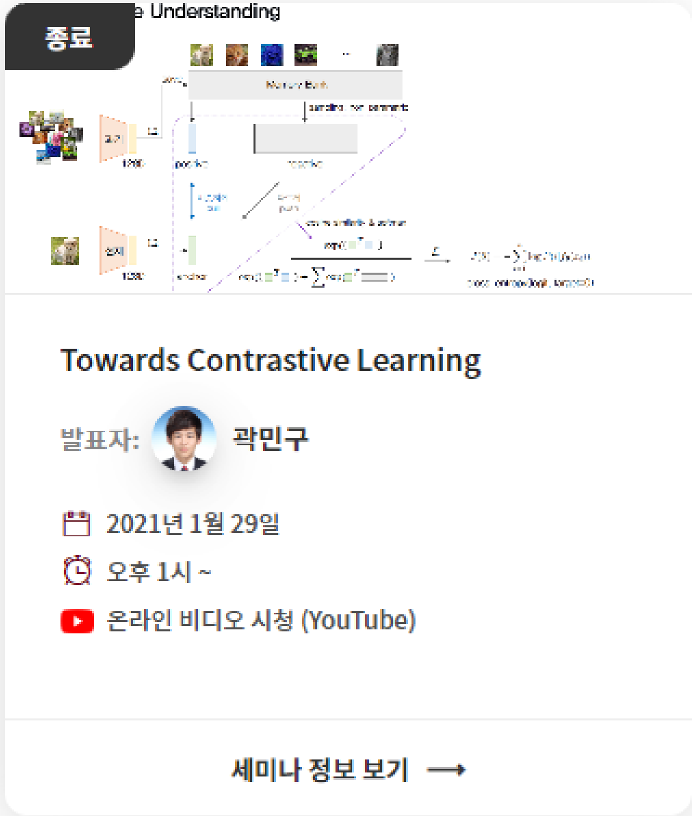
관련 DMQA Open Seminar





Contrastive Learning

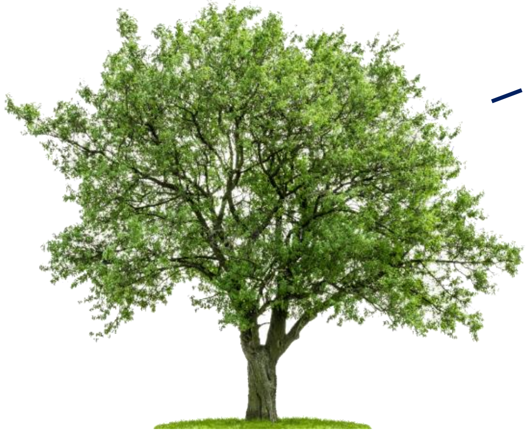
❖ Contrastive Learning

- Anchor와 유사한 특성을 가지는 Sample의 경우에는?

Anchor

떡갈나무

Positive Pair



떡갈나무

Negative Pair

장미

Contrastive Learning

❖ Contrastive Learning

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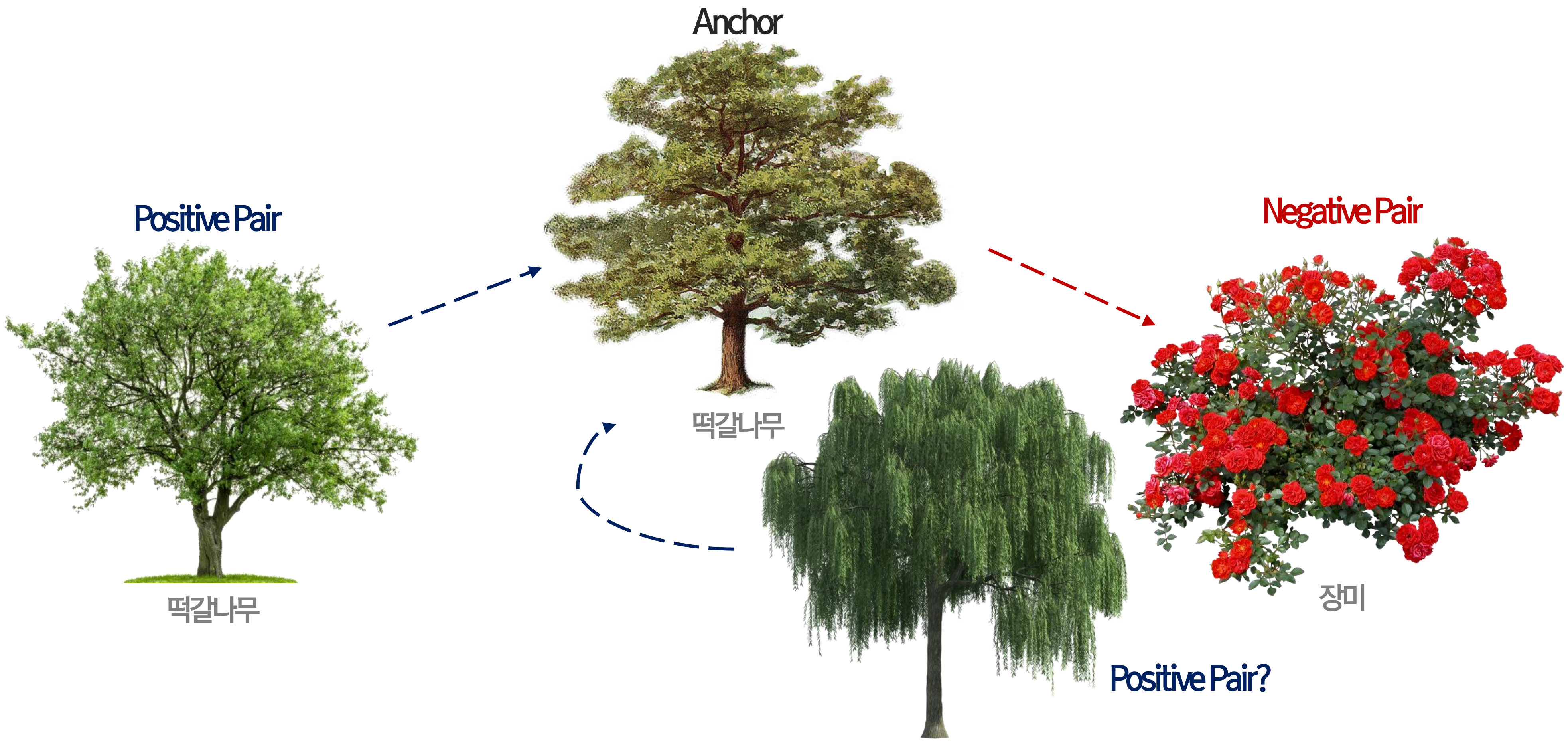

Contrastive Learning

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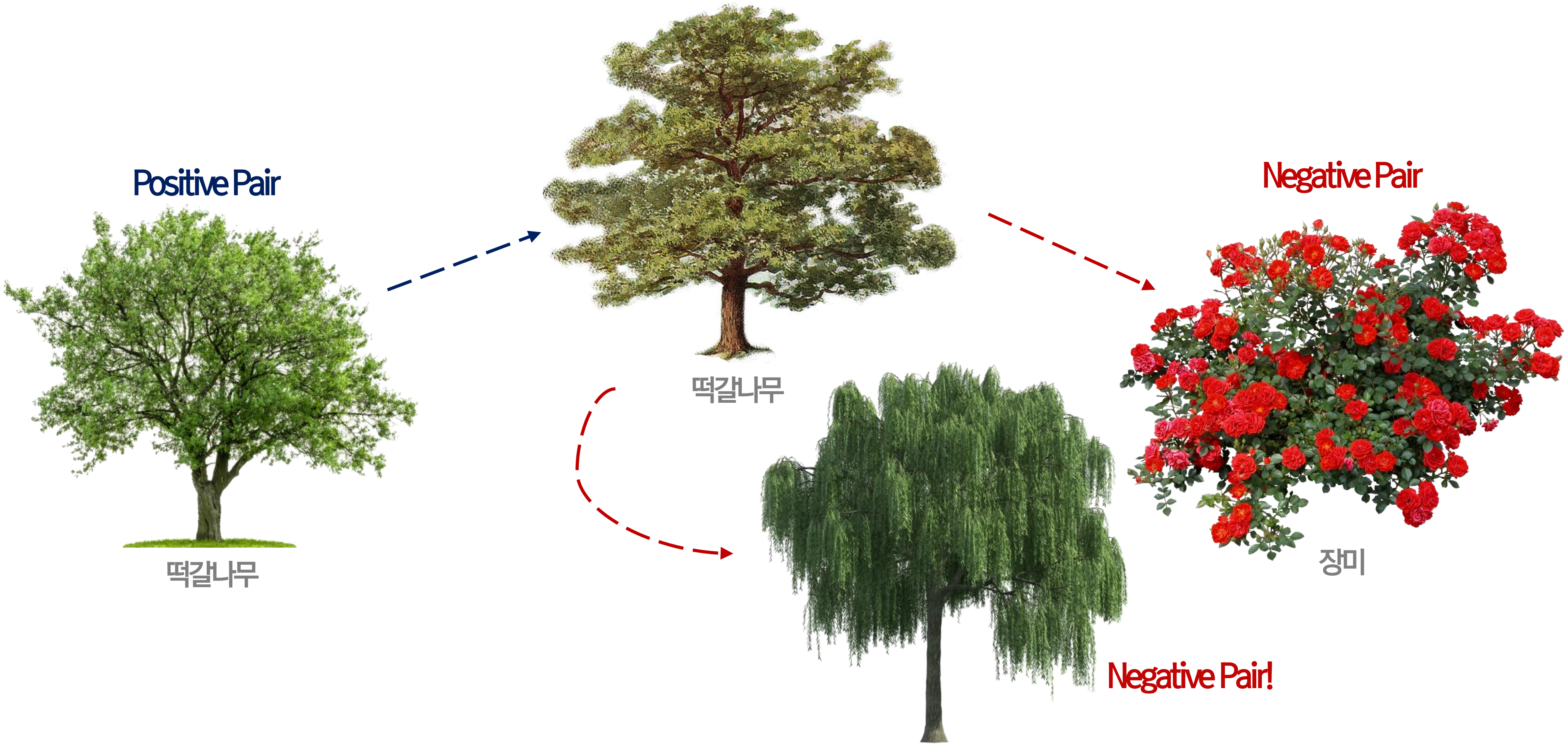
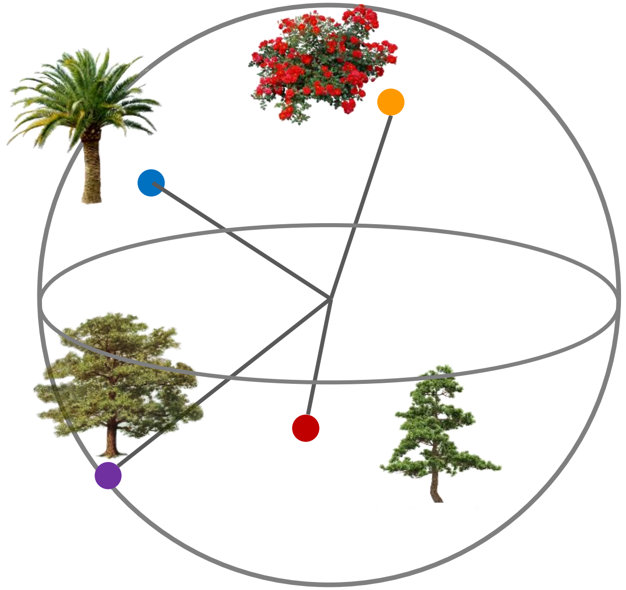
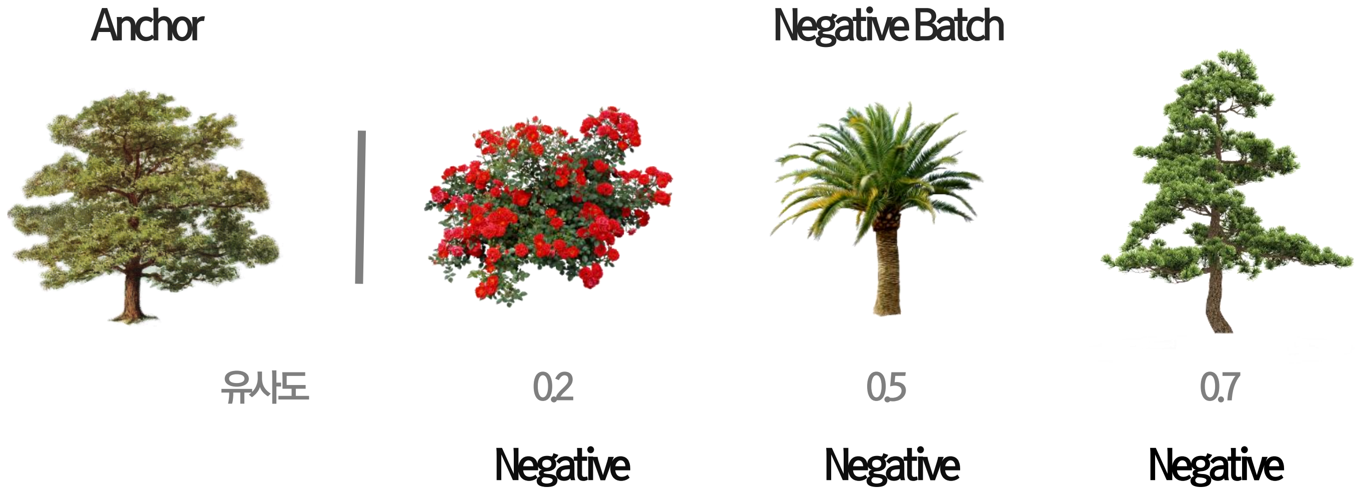


Contrastive Learning

❖ SimCLR

- Negative Batch 안에서 Anchor 와의 유사도 반영 부족





Contrastive Learning

❖ SimCLR

- Negative Batch 안에서 Anchor 와의 유사도 반영 부족

Negative Batch 중 Anchor 와 유사한 것을 학습할수록

모델이 더 좋은 표현을 학습할 수 있지 않을까?

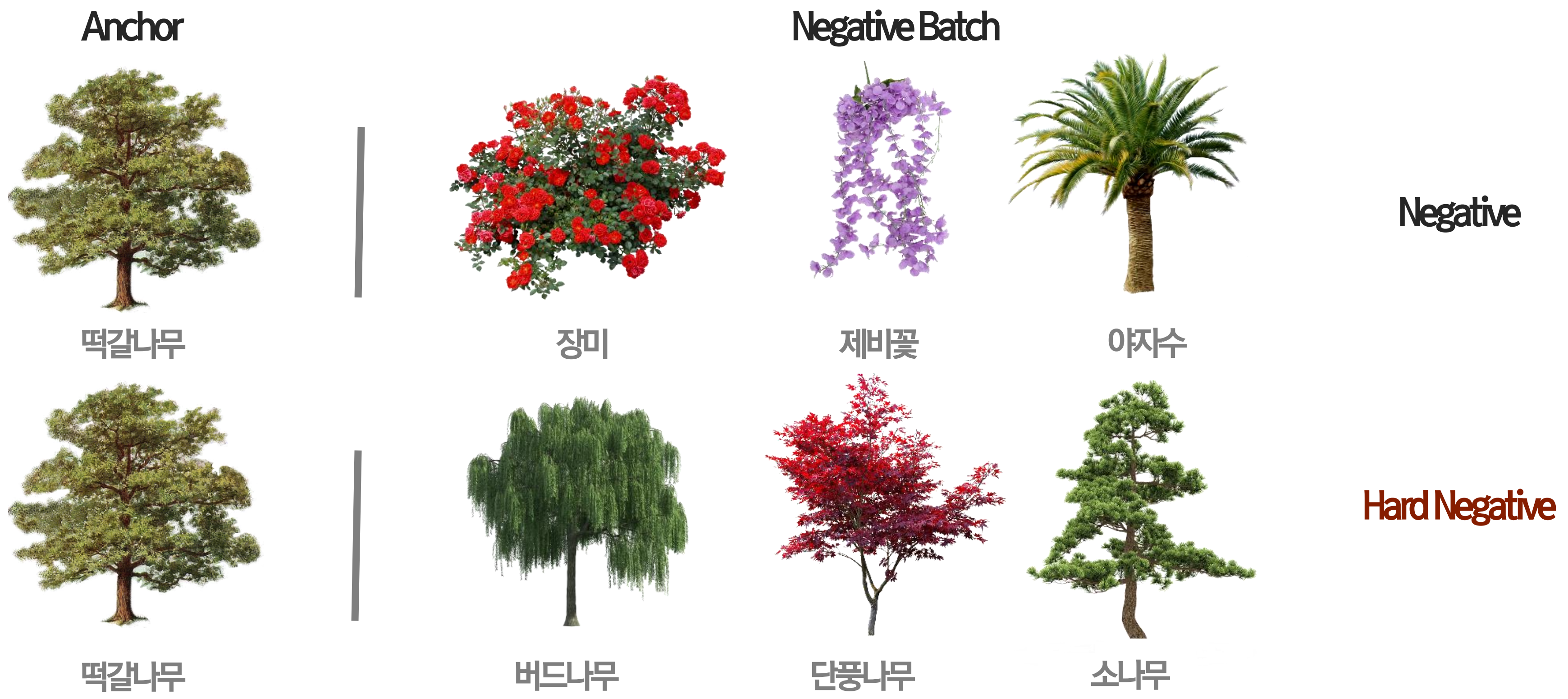
3. Hard Negative Sample

Hard Negative Sample

Basic Definition

❖ Hard Negative Sample

- Anchor 와 다른 Label : True Negative
- Anchor 와 다른 Label & Anchor 와 유사한 특징 : Hard Negative



Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Contrastive Learning With Hard Negative Samples (ICLR, 2021)

- 2022년 11월 기준 228회 인용
- 사용자가 Hardness를 제어할 수 있는 Hard Negative Samples 선택을 위한 방법론 제안

CONTRASTIVE LEARNING WITH HARD NEGATIVE SAMPLES

Joshua Robinson, Ching-Yao Chuang, Suvrit Sra, Stefanie Jegelka
Massachusetts Institute of Technology
Cambridge, MA, USA
{joshrob, cychuang, suvrit, stefje}@mit.edu

ABSTRACT

How can you sample good negative examples for contrastive learning? We argue that, as with metric learning, contrastive learning of representations benefits from hard negative samples (i.e., points that are difficult to distinguish from an anchor point). The key challenge toward using hard negatives is that contrastive methods must remain unsupervised, making it infeasible to adopt existing negative sampling strategies that use *true* similarity information. In response, we develop a new family of unsupervised sampling methods for selecting hard negative samples where the user can control the hardness. A limiting case of this sampling results in a representation that tightly clusters each class, and pushes different classes as far apart as possible. The proposed method improves downstream performance across multiple modalities, requires only few additional lines of code to implement, and introduces no computational overhead.

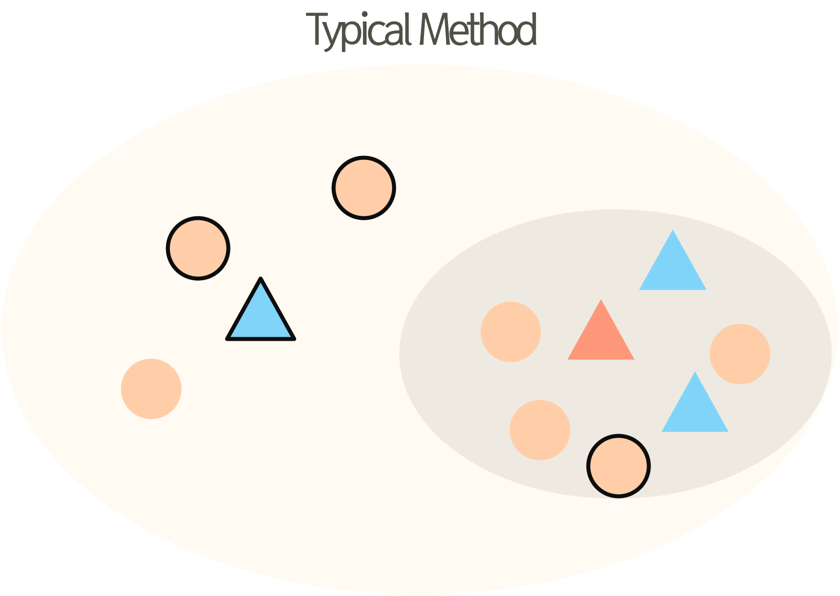
[3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

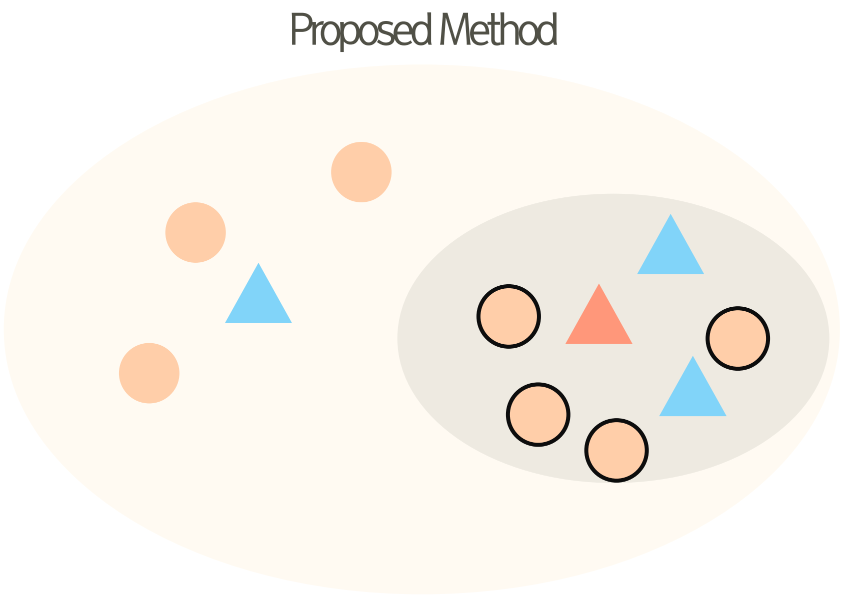
Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Contrastive Learning With Hard Negative Samples (ICLR, 2021)

- Positive, Negative Pairs 의 구성에 따라 Contrastive Learning 의 성공 결정
- Informative Negative Samples: 직관적으로는 근처에 위치한다고 생각하지만, 사실은 멀리 떨어져야 하는 Pairs





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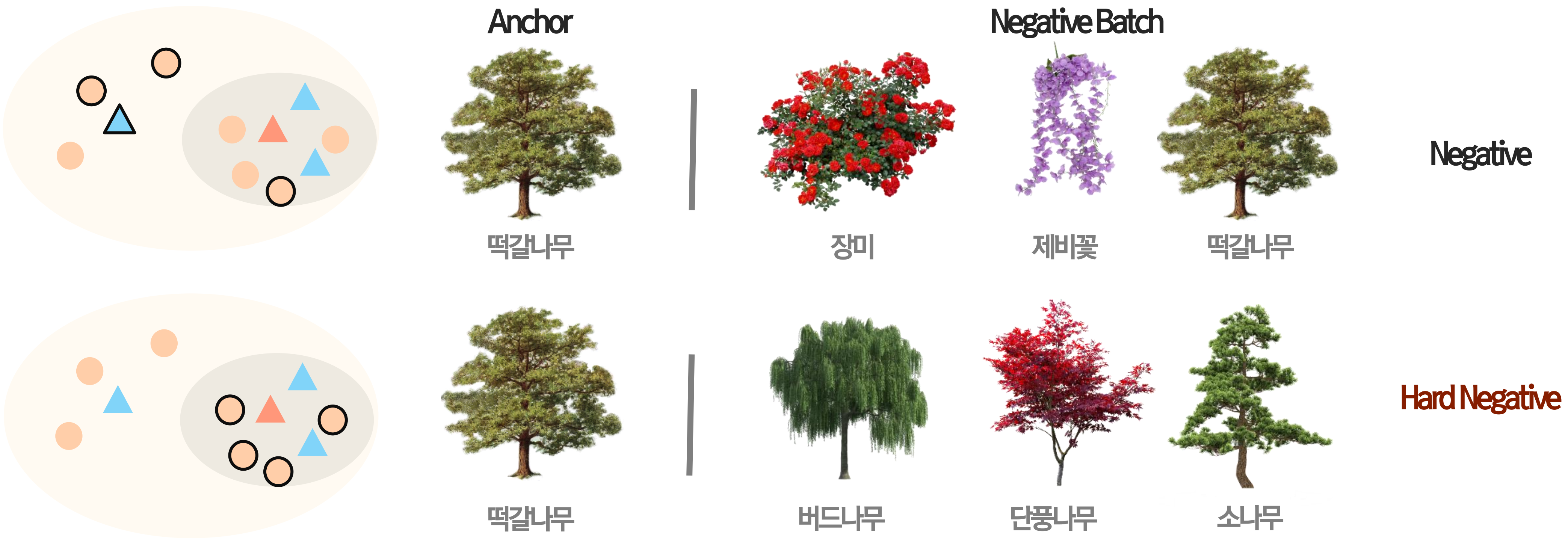
Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Challenges

- 모든 True Similarity/ Dissimilarity 에 대한 정보 없음
- Tunable Distribution 에 대한 효율적인 샘플링 전략 필요



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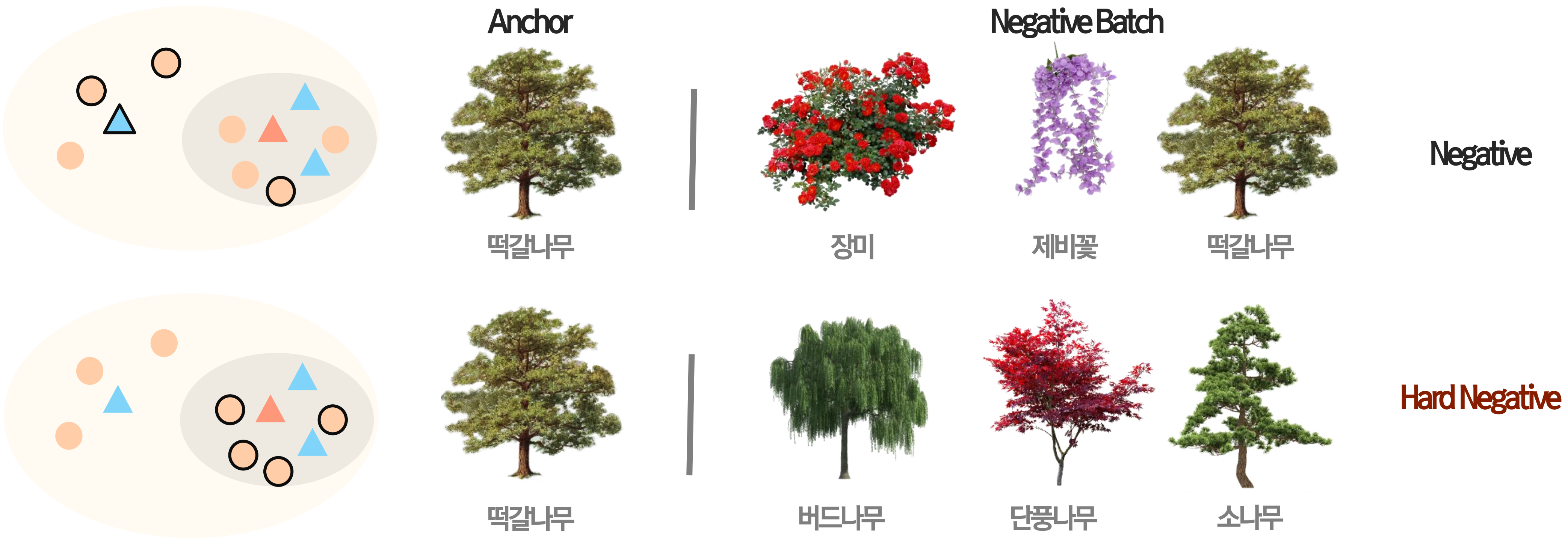
Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Challenges

- 모든 True Similarity/ Dissimilarity 에 대한 정보 없음 -> Positive-Unlabeled Learning 아이디어 참고
- Tunable Distribution 에 대한 효율적인 샘플링 전략 필요 -> 계산 복잡성 낮은 중요도 샘플링 전략 구축



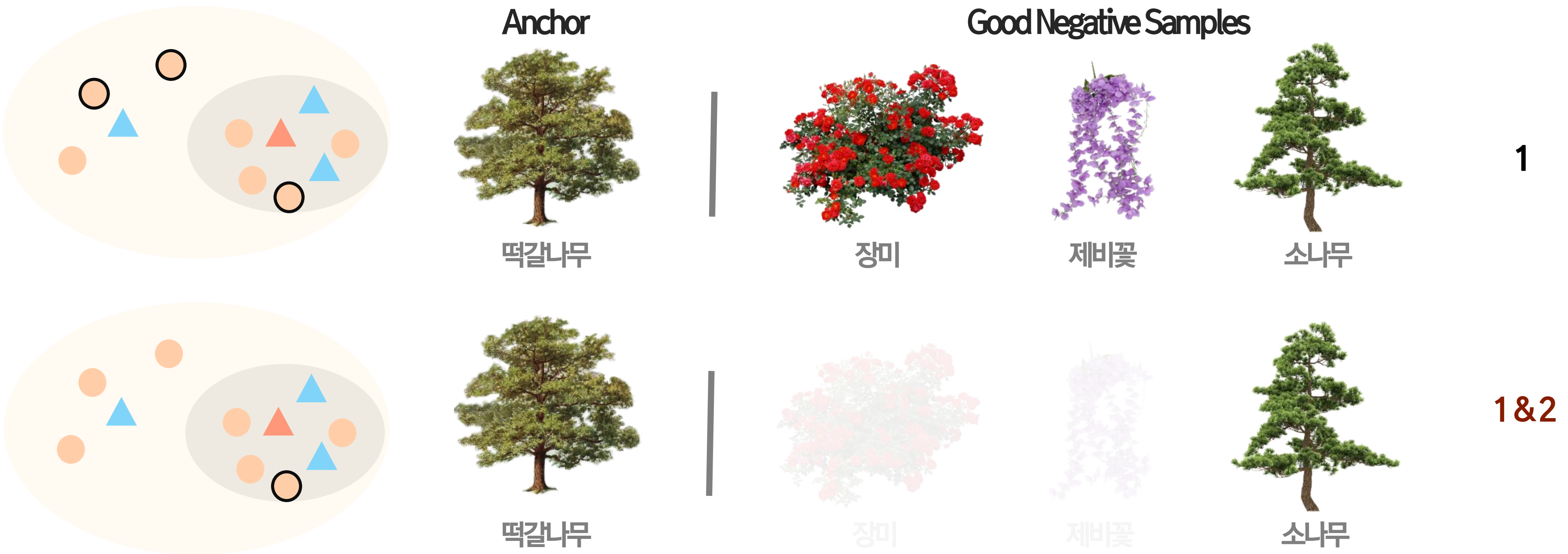
Data Mining Quality Analytics [3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ What Makes A Good Negative Sample?

- Principal 1) Anchor x 와 다른 Label 을 가지는 True Negatives x_i^- 추출
- Principal 2) 가장 유용한 Negative Sample 은 Embedding Space 가 현재 Anchor 와 유사하다고 믿는 것



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Hard Negative 로 부터 얻은 발전된 표현

↕

False Negative 에서 오는 학습의 어려움

Anchor 와 동일함에도 Negative 로 분류

Trade- Off 존재

Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Sampling Negatives From The Distribution q_β^-

- Principal 1) Anchor x 와 다른 Label 을 가지는 True Negatives x_i^- 추출
- Principal 2) 가장 유용한 Negative Sample 은 Embedding Space 가 현재 Anchor 와 유사하다고 믿는 것
- 목표: Embedding f 와 Anchor x 에 따른 χ 의 분포 q 설계, q 에서 Negative Batch Sampling

$$q_\beta^-(x^-) := q_\beta(x^- | h(x) \neq h(x^-)), \text{ where } q_\beta(x^-) \propto e^{\beta f(x)^T f(x^-)} \cdot p(x^-), \text{ for } \beta \geq 0$$

x, x^- 가 다른 Latent Class 를 가지는 조건

Principal 1 만족

[3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

Hard Negative Sample

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$$\boldsymbol{q_\beta^-(x^-) \coloneqq q_\beta(x^- | h(x) \neq h(x^-))}, where\ q_\beta(x^-) \propto e^{\beta f(x)^T f(x^-)} \cdot p(x^-), for\ \beta \geq 0$$

β: concentration parameter

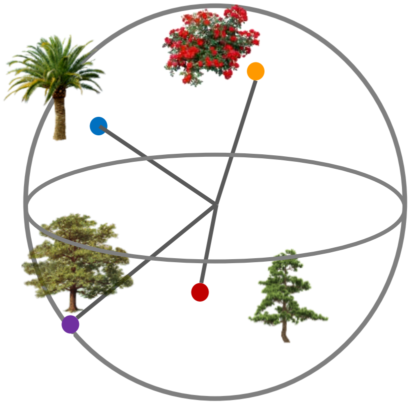
Anchor x 와 유사도가 높은 x^- 선택하는 정도 조절

Principal 2 만족

유사도: Inner Products

f 가 반지름 1/t 인 Hypersphere 표면이므로,

큰 Inner Product = 짧은 Euclidean 거리



Embedding Space

[3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Sampling Negatives From The Distribution q_β^-

- Principal 1) Anchor x 와 다른 Label 을 가지는 True Negatives x_i^- 추출
- Principal 2) 가장 유용한 Negative Sample 은 Embedding Space 가 현재 Anchor 와 유사하다고 믿는 것
- 목표: Embedding f 와 Anchor x 에 따른 χ 의 분포 q 설계, q 에서 Negative Batch Sampling

$$q_\beta^-(x^-) := q_\beta(x^- | h(x) \neq h(x^-)), \; where \; q_\beta(x^-) \propto e^{\beta f(x)^T f(x^-)} \cdot p(x^-), for \; \beta \geq 0$$

β: concentration parameter

유사도: Inner Products

Principal 2 만족

큰 Inner Product = 짧은 Euclidean 거리

Principal 1& 2 만족하는 q_β^- 구축 완료,

어떻게 효율적으로 샘플링 할까?

Hard Negative Sample

Contrastive Learning With Hard Negative Samples

❖ Sampling Negatives From The Distribution q_β^-

- 구축한 Distribution q_β 에 PU-Learning Viewpoint 적용 후, 식 (1) 구축 ($h(x) = h(x^-)$조건 만족)
- Importance Sampling 접근법 사용 Rejection Sampling 도 사용 가능 하지만, Sampling Batches 가 계속 변형되어 알고리즘이 복잡해짐
- Negative Sampling Distribution q_β^- 에 대해 식(2) 로 변형 가능

$$\boldsymbol{q_\beta(x^-) = \tau^- q_\beta^-(x^-) + \tau^+ q_\beta^+(x^-)} \text{ , } where\ q_\beta(x^-) \propto e^{\beta f(x)^T f(x^-)} \cdot p(x^-), for\ \beta \geq 0 \quad \text{식 (1)}$$

$$\boldsymbol{q_\beta^-(x^-) = (q_\beta(x^-) - \tau^+ q_\beta^+(x^-))/\tau^-} \quad \text{식 (2)}$$

[3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

Hard Negative Sample

Conditional Negative Sampling For Contrastive Learning Of Visual Representations

❖ Conditional Negative Sampling For Contrastive Learning Of Visual Representations (2020)

- 2022년 11월 기준 32회 인용
- Positive Samples 와 가깝지만, 너무 가깝지는 않은 Negatives 선택을 위한 Ring Model 제안

CONDITIONAL NEGATIVE SAMPLING FOR CONTRASTIVE LEARNING OF VISUAL REPRESENTATIONS

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Department of Computer Science[1], Psychology[2], and Philosophy[3]
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ABSTRACT

Recent methods for learning unsupervised visual representations, dubbed contrastive learning, optimize the noise-contrastive estimation (NCE) bound on mutual information between two views of an image. NCE uses randomly sampled negative examples to normalize the objective. In this paper, we show that choosing difficult negatives, or those more similar to the current instance, can yield stronger representations. To do this, we introduce a family of mutual information estimators that sample negatives conditionally – in a "ring" around each positive. We prove that these estimators lower-bound mutual information, with higher bias but lower variance than NCE. Experimentally, we find our approach, applied on top of existing models (IR, CMC, and MoCo) improves accuracy by 2-5% points in each case, measured by linear evaluation on four standard image datasets. Moreover, we find continued benefits when transferring features to a variety of new image distributions from the Meta-Dataset collection and to a variety of downstream tasks such as object detection, instance segmentation, and keypoint detection.

[4] Wu, M., Mosse, M., Zhuang, C., Yamins, D., & Goodman, N. (2020). Conditional negative sampling for contrastive learning of visual representations. arXiv preprint arXiv:2010.02037.

Hard Negative Sample

Conditional Negative Sampling For Contrastive Learning Of Visual Representations

❖ Conditional Negative Sampling For Contrastive Learning Of Visual Representations (2020)

- 가설: Negatives 를 잘 선택하면 높은 Quality 의 Representations 학습 가능
- 나무를 다른 Class 와 구분하는 것 보다 나무 안에서 종을 구분하는 것이 더 어려움
  - ✓ Granular & Semantic Information 에 집중 필요

Harder

떡갈나무

↔

장미

〈

떡갈나무

↔

소나무

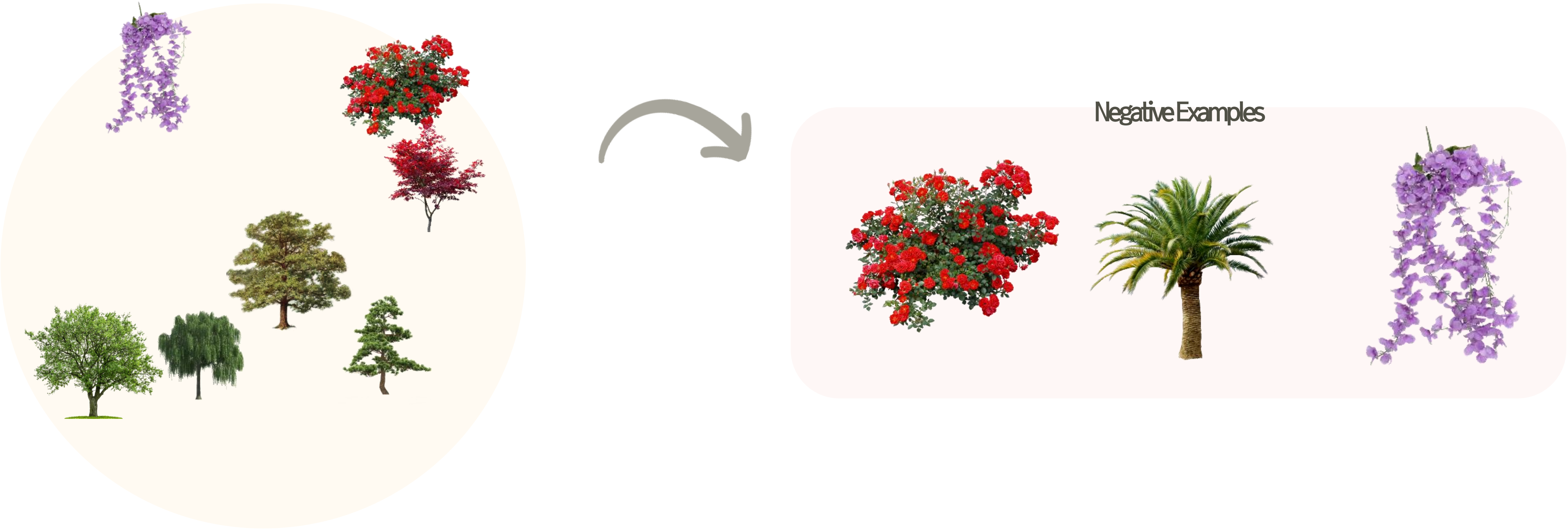
[4] Wu, M., Mosse, M., Zhuang, C., Yamins, D., & Goodman, N. (2020). Conditional negative sampling for contrastive learning of visual representations. arXiv preprint arXiv:2010.02037.

Hard Negative Sample

Conditional Negative Sampling For Contrastive Learning Of Visual Representations

❖ Noise-Contrastive Estimation (NCE)

- NCE: Positive 는 가깝게, Negative 는 멀리 위치하도록 하는 Representations 학습 Loss
- NCE 에서 Negative Examples 는 Marginal Distribution 으로 부터 i.i.d 하게 샘플링 independently and identically distributed
  - ✓ 좋은 Representation 을 학습하기 위한 최선의 Negative Samples 선택 방법은 아님



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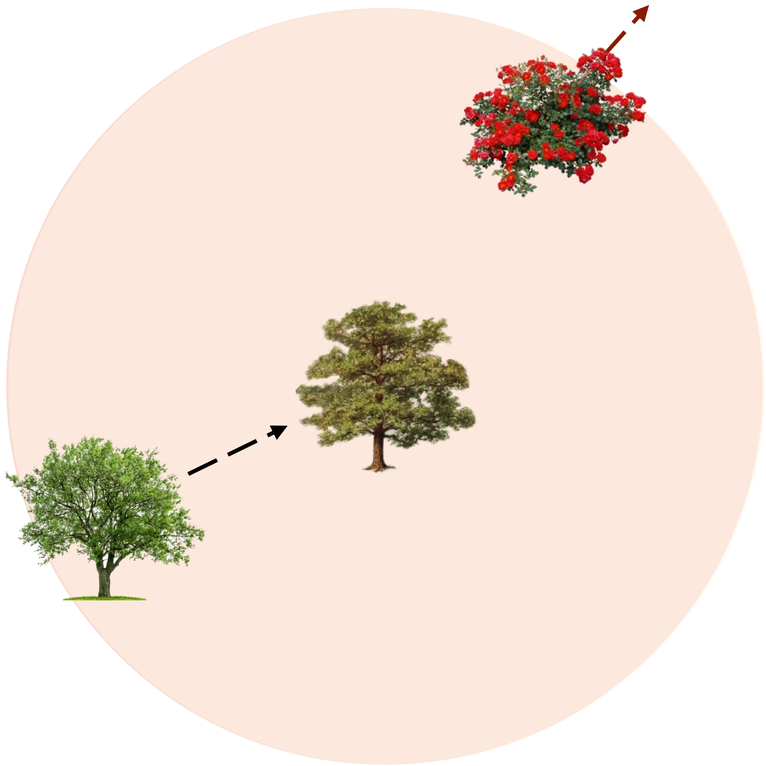
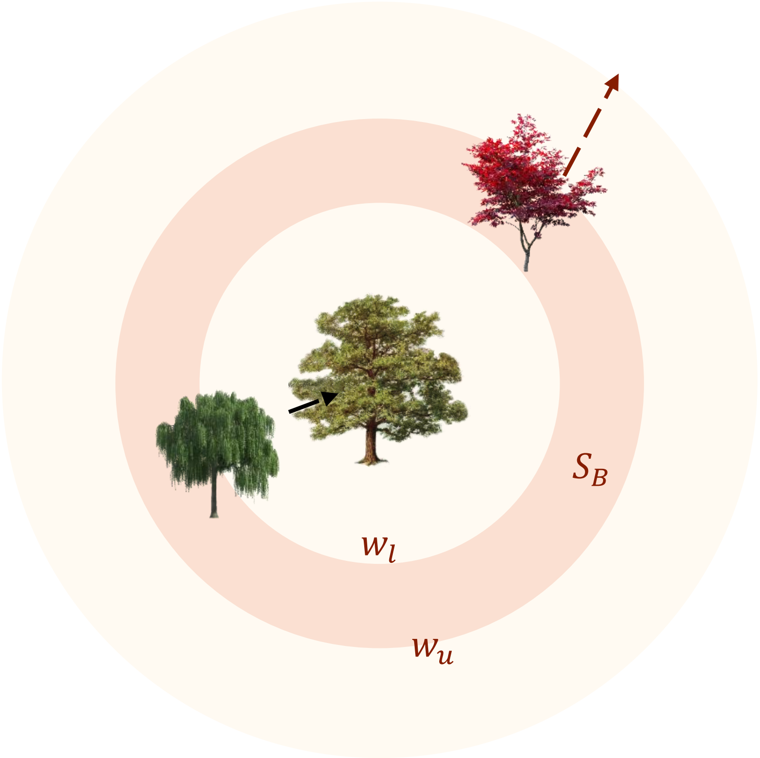
Hard Negative Sample

Conditional Negative Sampling For Contrastive Learning Of Visual Representations

❖ Conditional Noise Contrastive Estimator (CNCE) i번째 예시에 대해 percentile 선택 (w_l, w_u)

- Representation 이 Anchor와 매우 유사해서 Positive 로 분류되지 않는 것 (not too hard)
- Anchor 와 적당히 유사한 특징을 가지는 것 (not too easy)





[4] Wu, M., Mosse, M., Zhuang, C., Yamins, D., & Goodman, N. (2020). Conditional negative sampling for contrastive learning of visual representations. arXiv preprint arXiv:2010.02037.

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Ring Discrimination Algorithm

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Hard Negative Sample

Conditional Negative Sampling For Contrastive Learning Of Visual Representations

❖ Annealing Policy

- Representations 가 잘 구축되지 않은 초기에 Ring 적용은 Poor Representation 야기
- 학습과정에서 S_B의 크기를 줄여가는 Annealing Policy 사용 Annealing Thresholds 가 매우 중요

[4] Wu, M., Mosse, M., Zhuang, C., Yamins, D., & Goodman, N. (2020). Conditional negative sampling for contrastive learning of visual representations. arXiv preprint arXiv:2010.02037.

4. Conclusion

Conclusions

What is Hard Negative Sample?

❖ Self-Supervised Learning 의 필요성과 종류

- Unlabeled Data 에서 데이터 특징을 학습하여 사용자가 풀고자 하는 문제 수행

❖ Contrastive Learning 의 정의와 특징

- Anchor 를 기준으로 Positive 와 Negative 를 정의하여 가까워지고, 멀어지도록 학습 진행
- SimCLR

❖ Hard Negative Samples

- Negative Batch 안에서 유사도 반영을 위해 필요
- Anchor 와 다른 Latent Class 로 분류되지만 유사한 특징을 가지는 Examples
- Sampling Negatives From q_{β}^{-} / Ring Discriminination

5. Reference

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[2] Chen, T., Kornblith, S., Norouzi, M., & Hinton, G. (2020, November). A simple framework for contrastive learning of visual representations. In International conference on machine learning (pp. 1597-1607). PMLR.

[3] Robinson, J., Chuang, C. Y., Sra, S., & Jegelka, S. (2020). Contrastive learning with hard negative samples. arXiv preprint arXiv:2010.04592.

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Thank You