

Applied Deep Learning



Beyond Supervised Learning



November 27th, 2024

<http://adl.miulab.tw>



**National
Taiwan
University**
國立臺灣大學

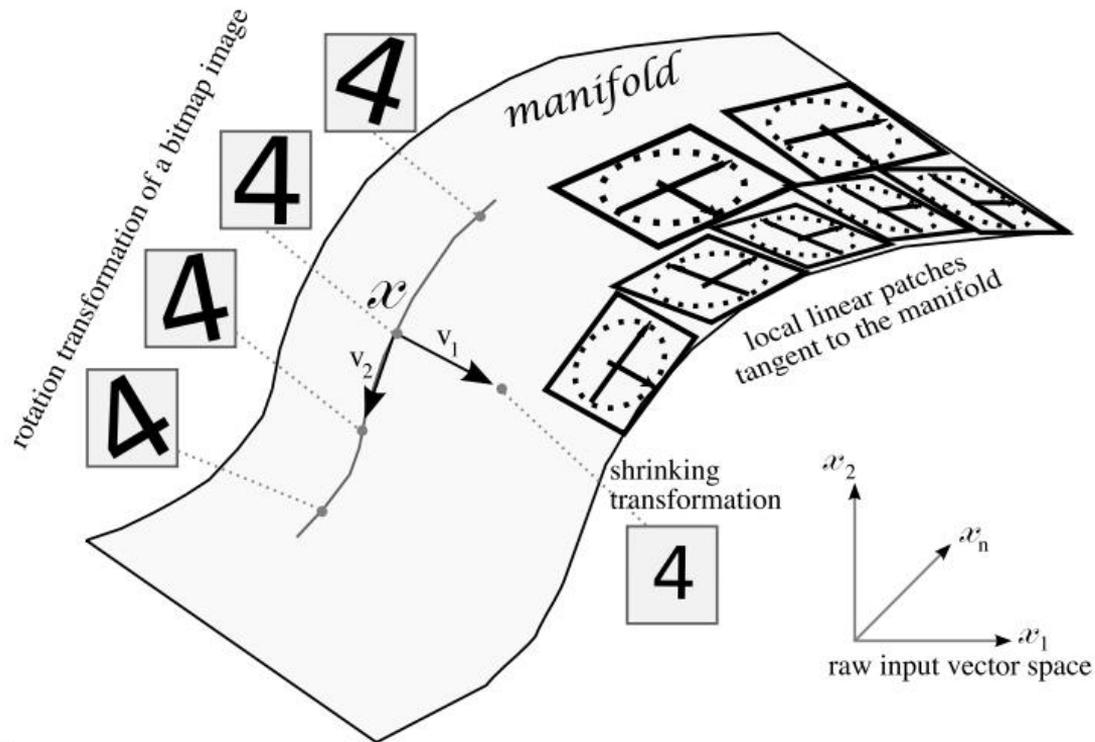
Introduction

- Big data \neq Big annotated data
- Machine learning techniques include:
 - Supervised learning (if we have labelled data)
 - Reinforcement learning (if we have an environment for reward)
 - Unsupervised learning (if we do not have labelled data)

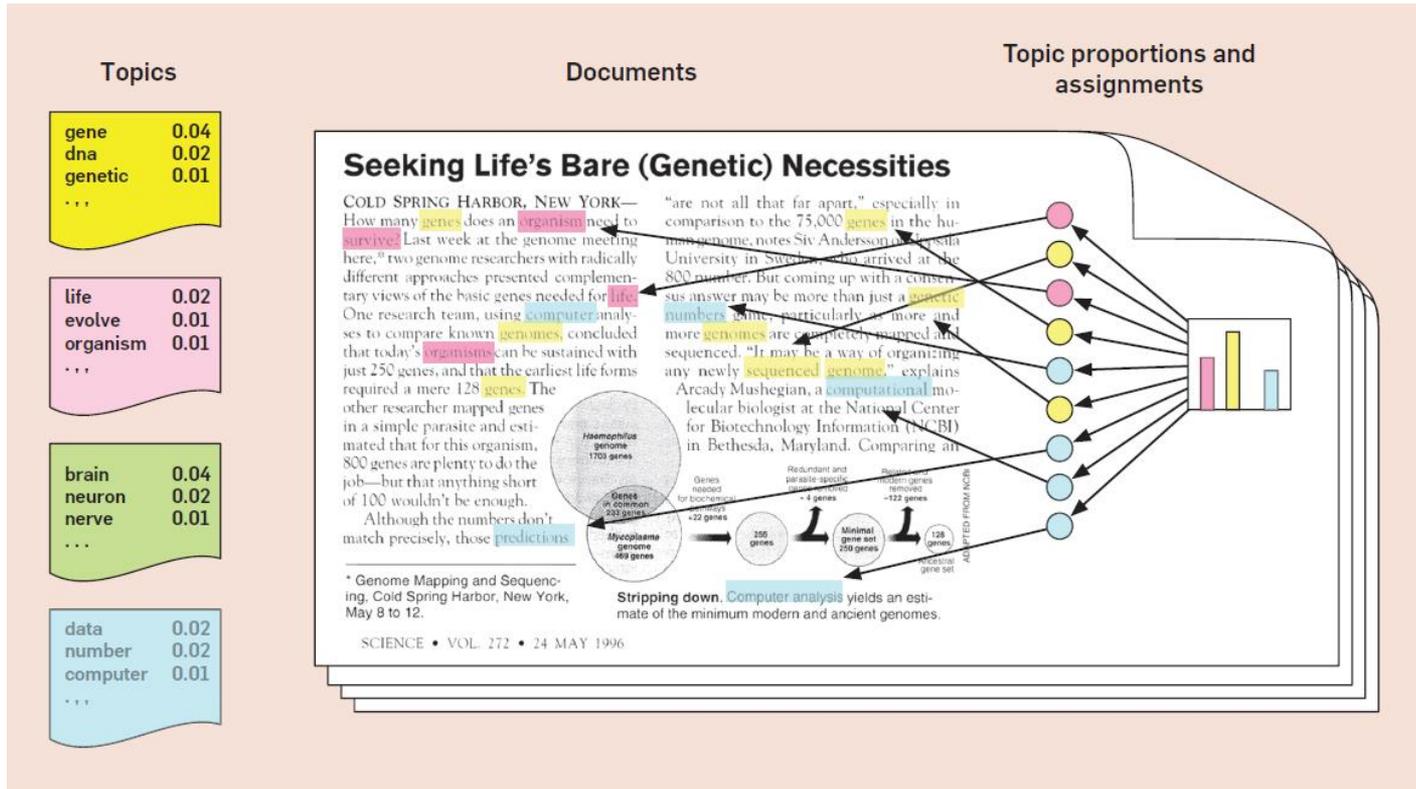
Why does unlabeled and unrelated data help the tasks?

Finding latent factors that control the observations

Latent Factors for Handwritten Digits



Latent Factors for Documents



Latent Factors for Recommendation System



單純呆



傲嬌



Latent Factors for Recommendation Systems



推理類

韓劇

美劇



浪漫愛情

金秀賢

實境秀

韓劇



推理類

韓劇

實境秀



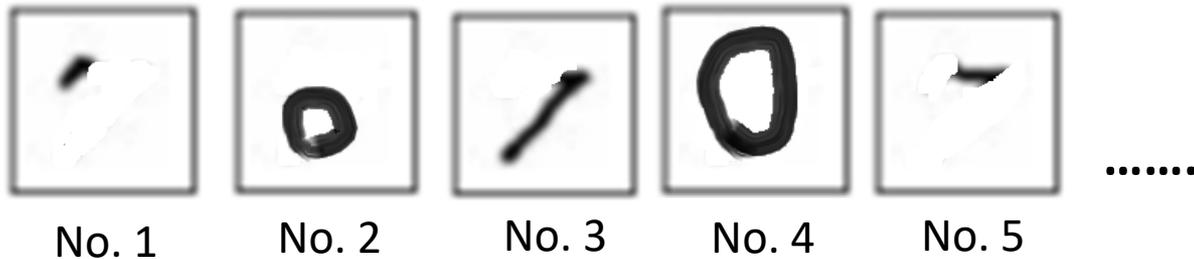
7 Latent Factor Exploitation

- Handwritten digits



The handwritten images are composed of **strokes**

Strokes (Latent Factors)



Discriminative vs. Generative

- ⦿ **Discriminative:** calculate the probability of output given input $P(Y|X)$
- ⦿ **Generative:** calculate the probability of a variable $P(X)$, or multiple variables $P(X, Y)$

Variable Types

- Observed vs. Latent:
 - Observed: something we can see from our data, e.g. X or Y
 - Latent: a variable that we assume exists without a given value
- Deterministic vs. Random:
 - Deterministic: variables calculated directly via deterministic functions
 - Random (stochastic): variables obeying a probability distribution
- A latent variable model is a probability distribution over two sets of variables

$$p(\mathbf{x}, \mathbf{z}; \theta)$$

Observed Latent

Latent Variable Types $p(x, z; \theta)$

Latent

- Latent continuous vector
 - Auto-encoder
 - Variational auto-encoder
- Latent discrete vector
 - Topic model
- Latent structure
 - HMM
 - Tree-structured model

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Auto-Encoder

Representation Learning

Auto-Encoder

- An observed output x
- A latent variable z
- A function (network) f parameterized by θ maps from z to x

$$\underset{\text{Observed}}{x} = f(\underset{\text{Latent}}{z}; \theta)$$

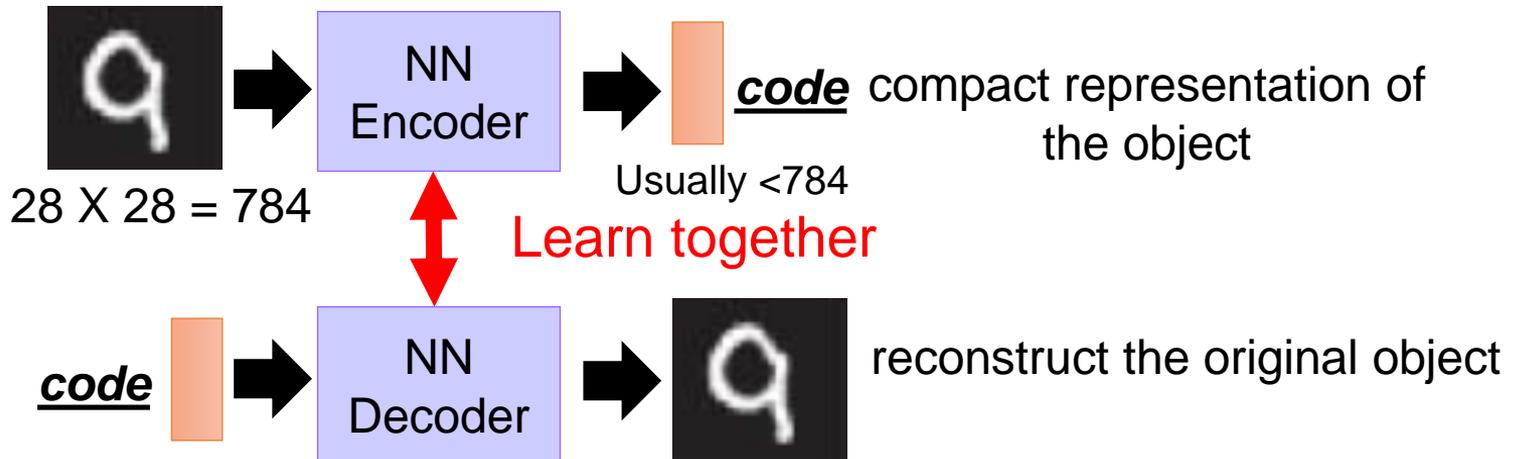
Idea: represent the output in a more compact way (latent codes)

Auto-Encoder

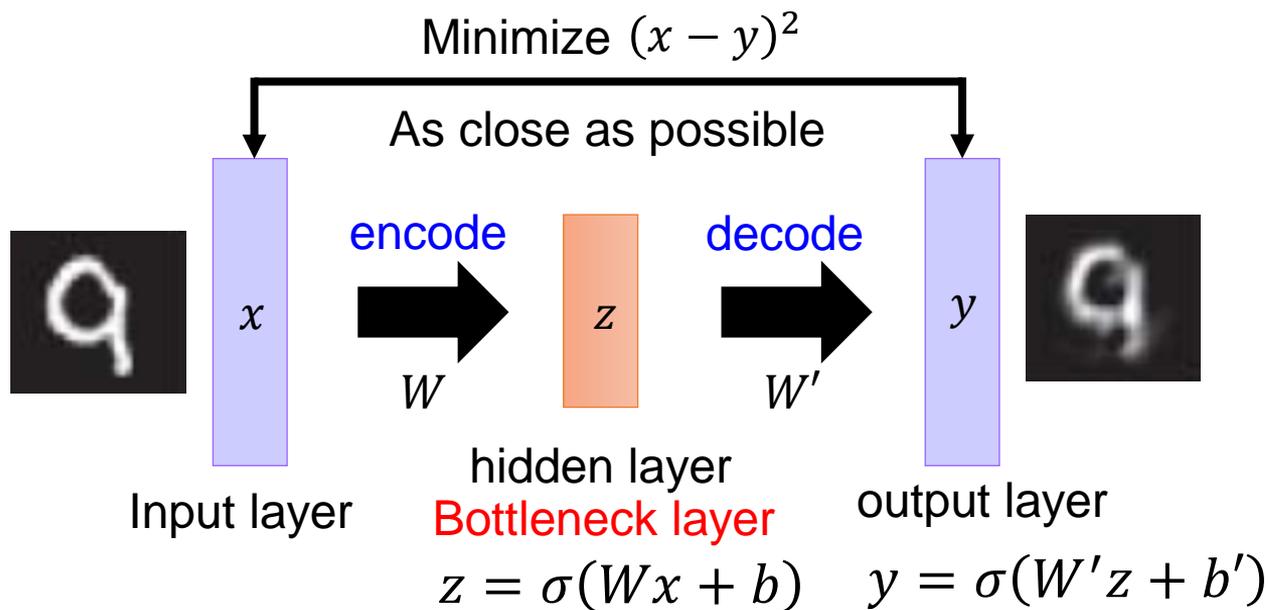


- Represent a digit using 28 X 28 dimensions
- Not all 28 X 28 images are digits

Idea: represent the images of digits in a more compact way



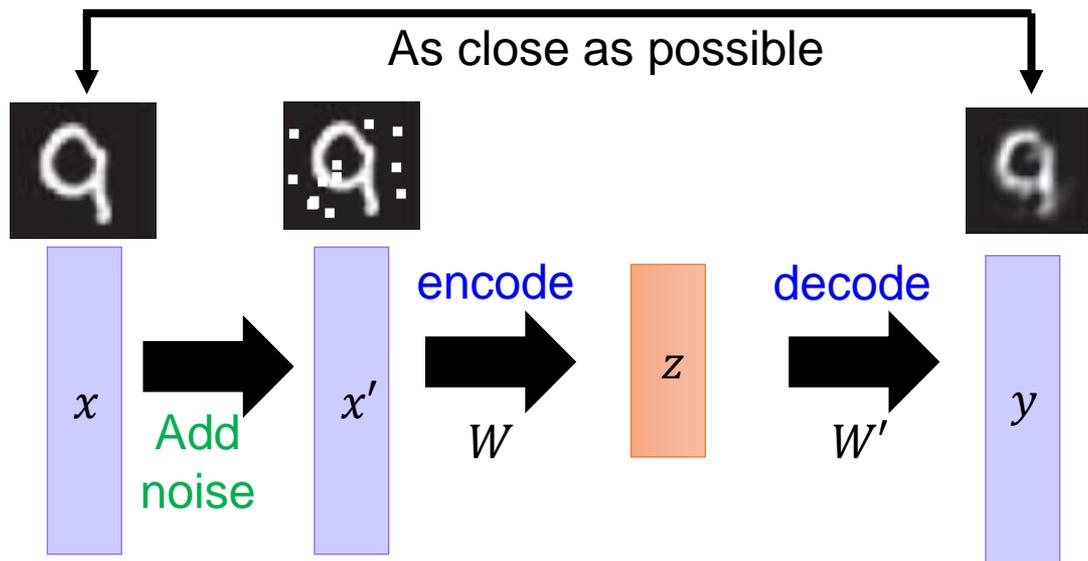
Auto-Encoder



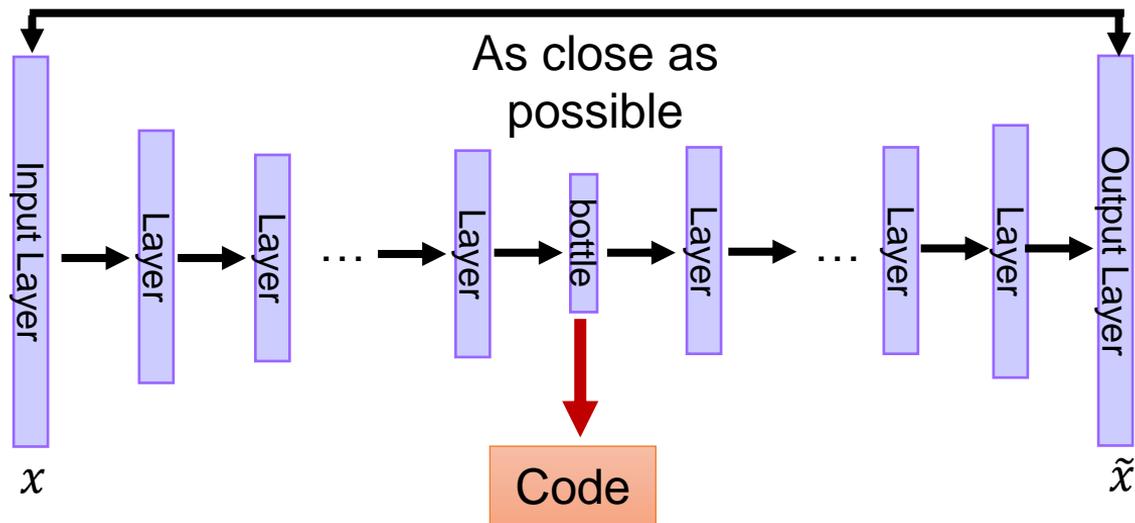
Output of the hidden layer is the code

Denoising Auto-Encoder

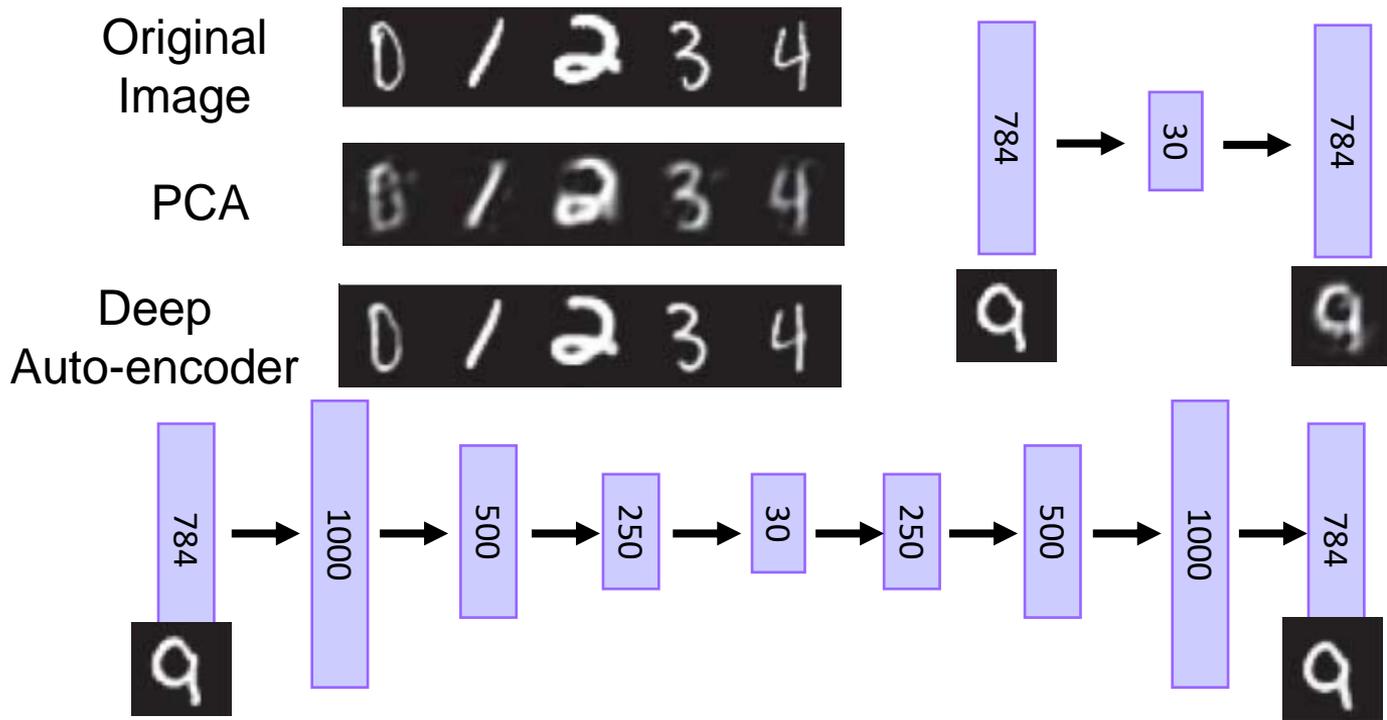
- Improve robustness of a latent variable



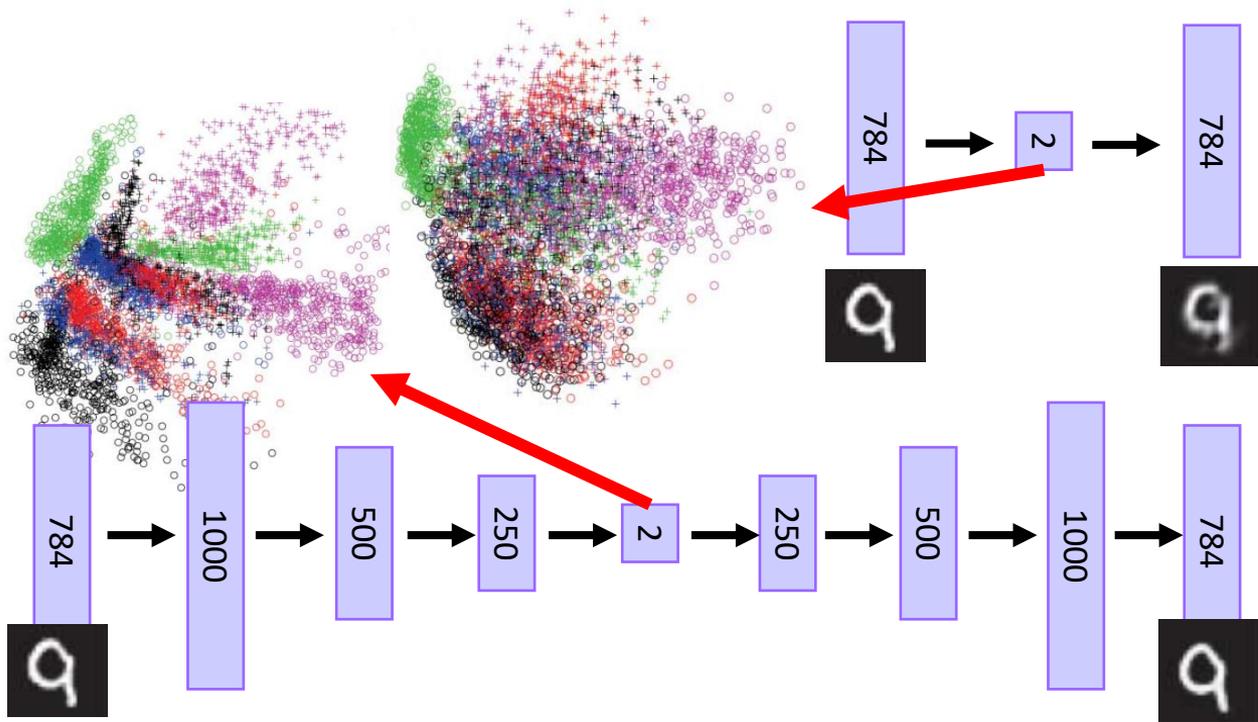
Deep Auto-Encoder



Deep Auto-Encoder



Feature Representation

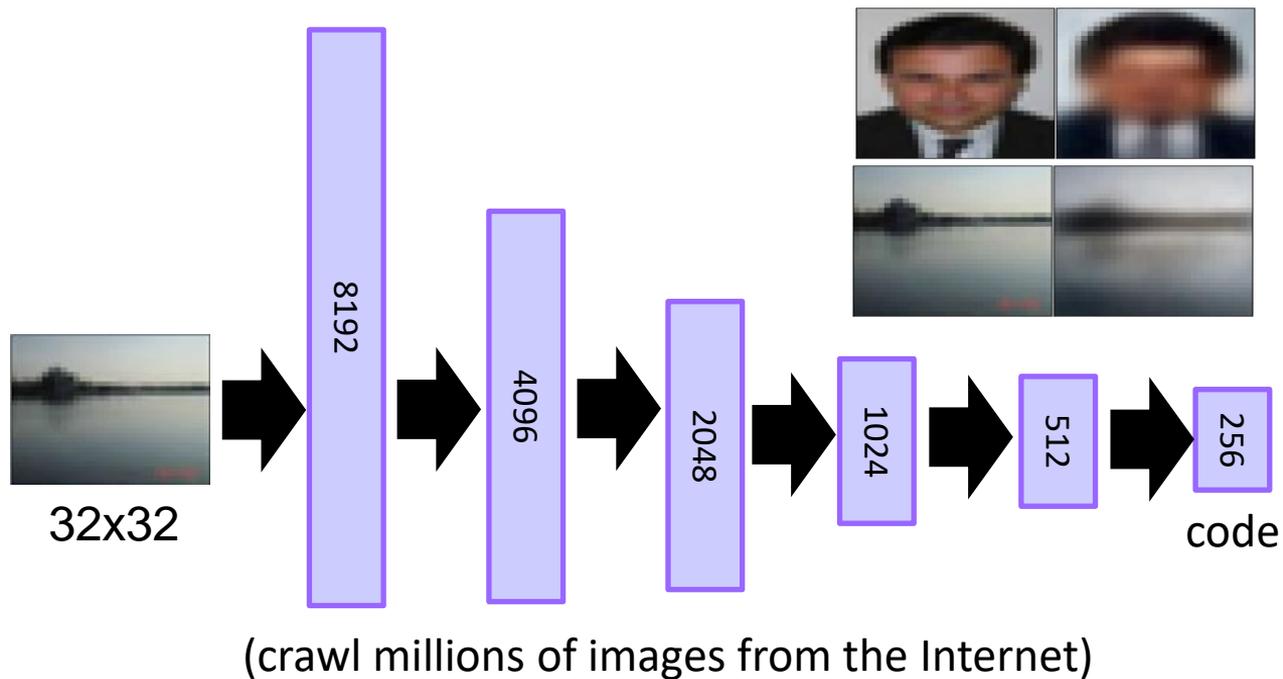


Auto-Encoder – Similar Image Retrieval

- Retrieved using Euclidean distance in pixel intensity space

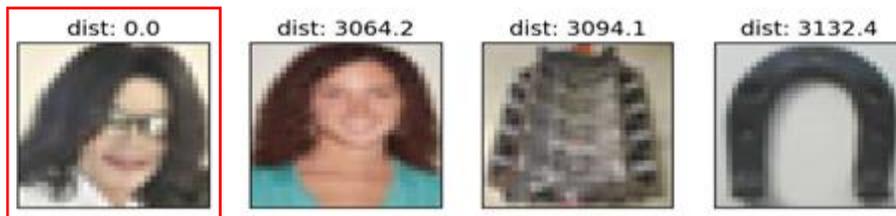


Auto-Encoder – Similar Image Retrieval

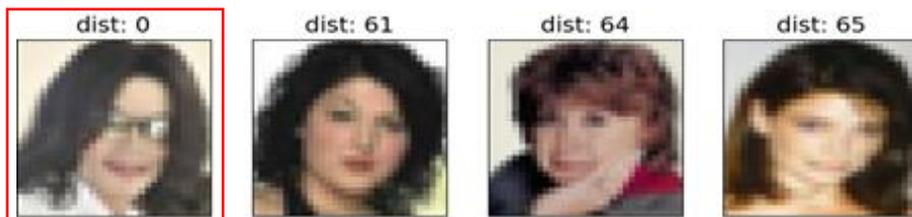


Auto-Encoder – Similar Image Retrieval

- Images retrieved using Euclidean distance in pixel intensity space



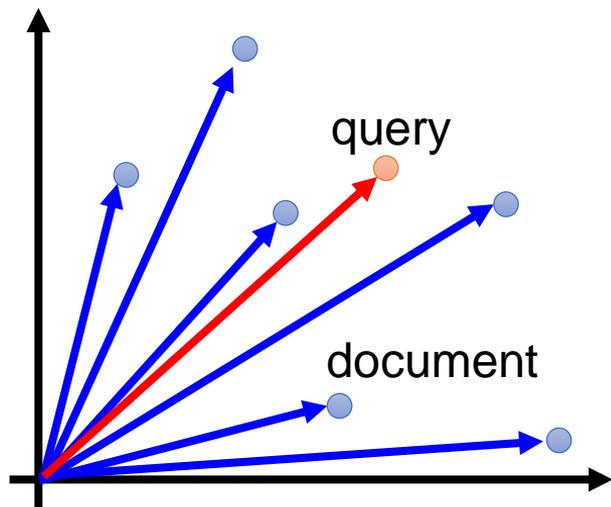
- Images retrieved using 256 codes



Learning the useful latent factors

Auto-Encoder – Text Retrieval

Vector Space Model

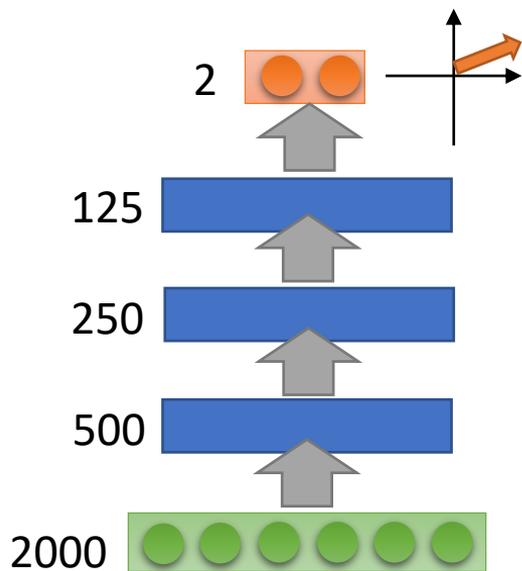


Bag-of-words word string: "This is an apple"

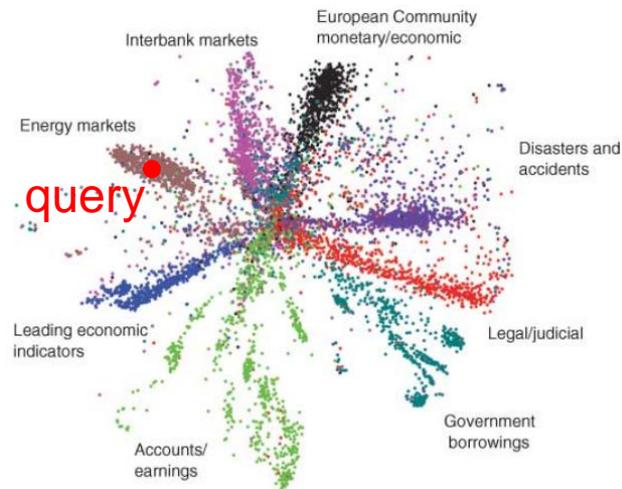
this	●	1
is	●	1
a	●	0
an	●	1
apple	●	1
pen	●	0
⋮	⋮	

Semantics are not considered

Auto-Encoder – Text Retrieval



Bag-of-words (document or query)



The documents talking about the same thing will have close code

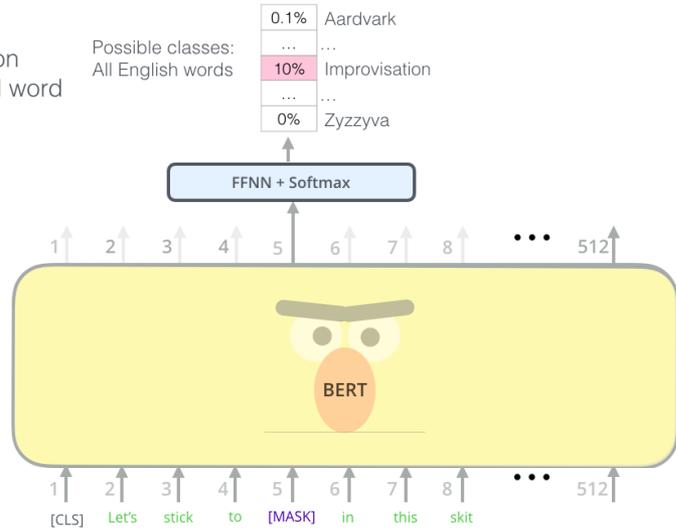
Denosing Auto-Encoding

Objective: reconstructing \bar{x} from \hat{x}

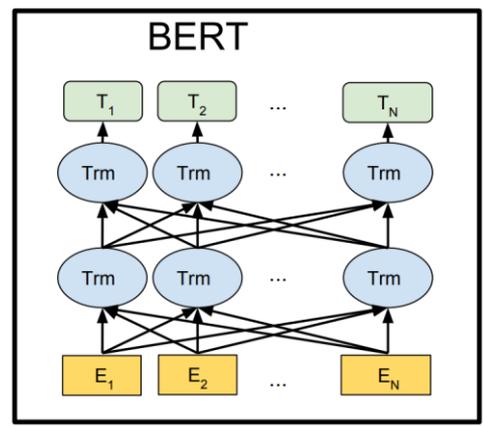
$$\max_{\theta} \log p_{\theta}(\bar{x} | \hat{x}) \approx \sum_{t=1}^T m_t \log p_{\theta}(x_t | \hat{x}) = \sum_{t=1}^T m_t \log \frac{\exp(H_{\theta}(\hat{x})_t^{\top} e(x_t))}{\sum_{x'} \exp(H_{\theta}(\hat{x})_t^{\top} e(x'))}$$

dimension reduction or denosing (masked LM)

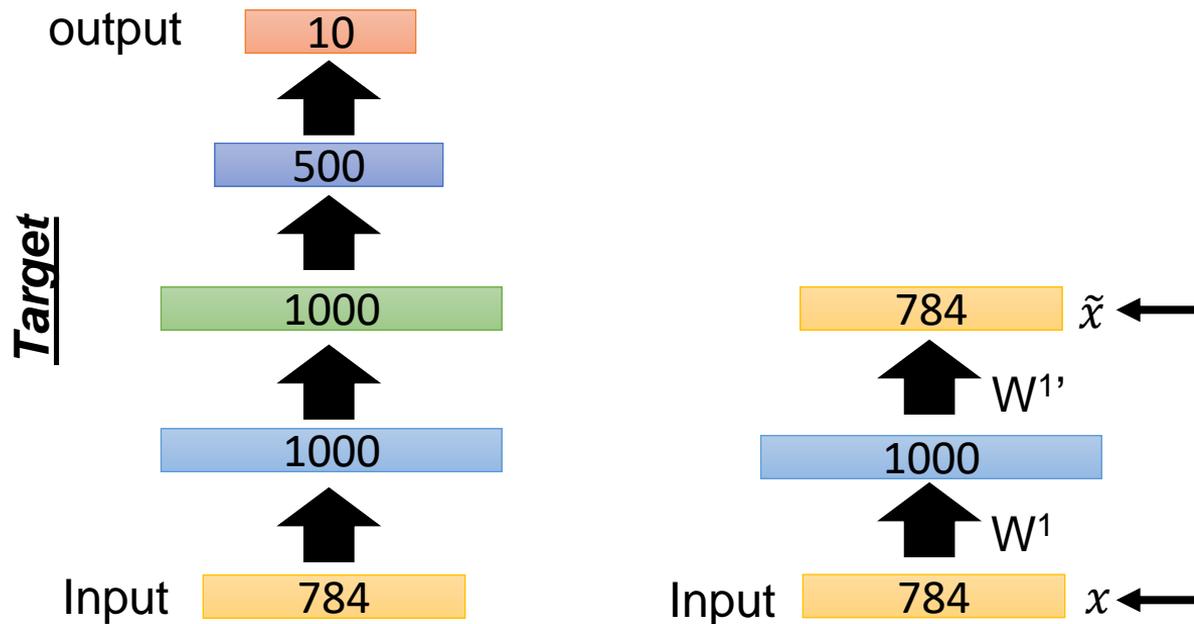
Use the output of the masked word's position to predict the masked word



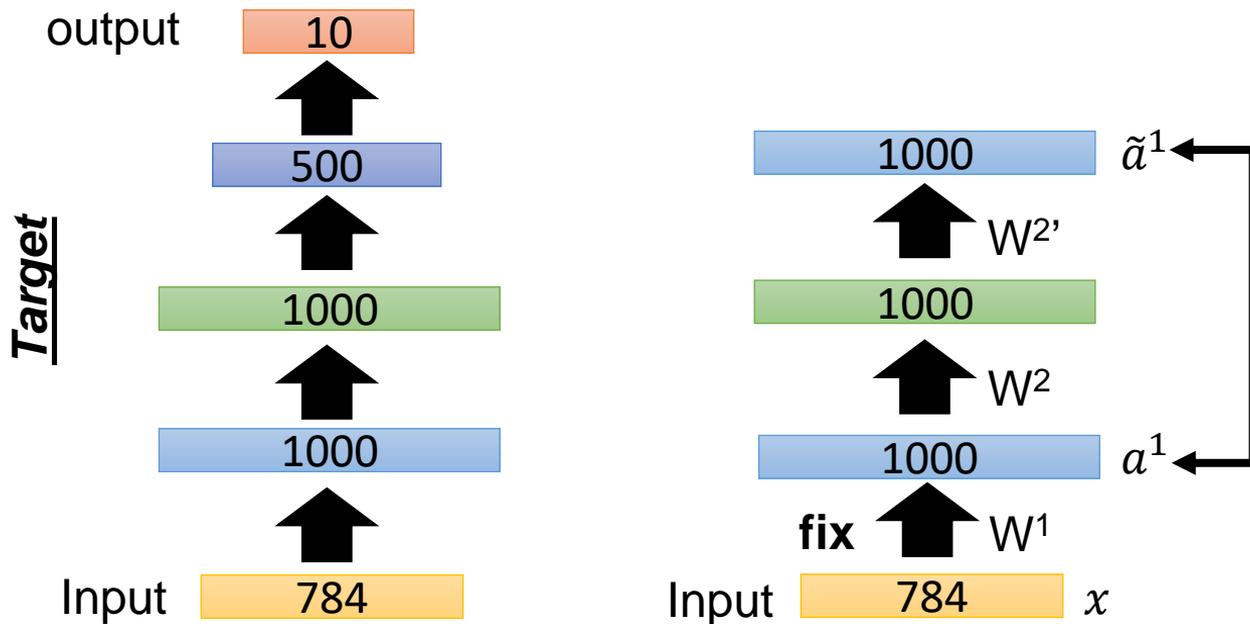
Randomly mask 15% of tokens



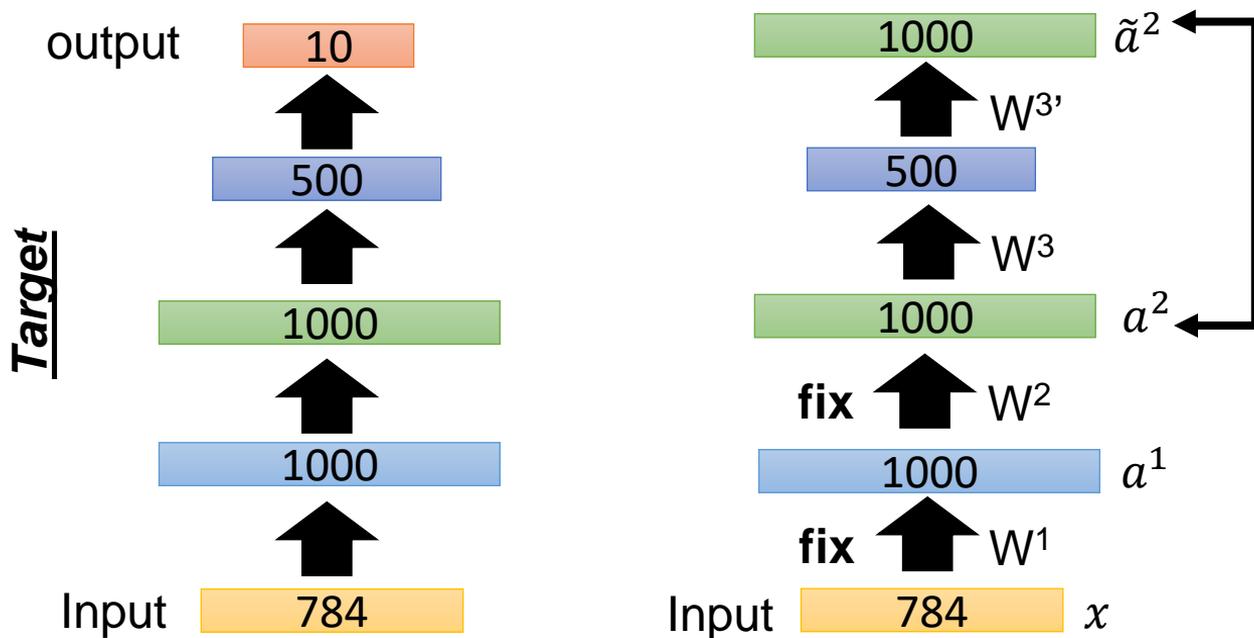
Auto-Encoder Layer-Wise Pre-Training



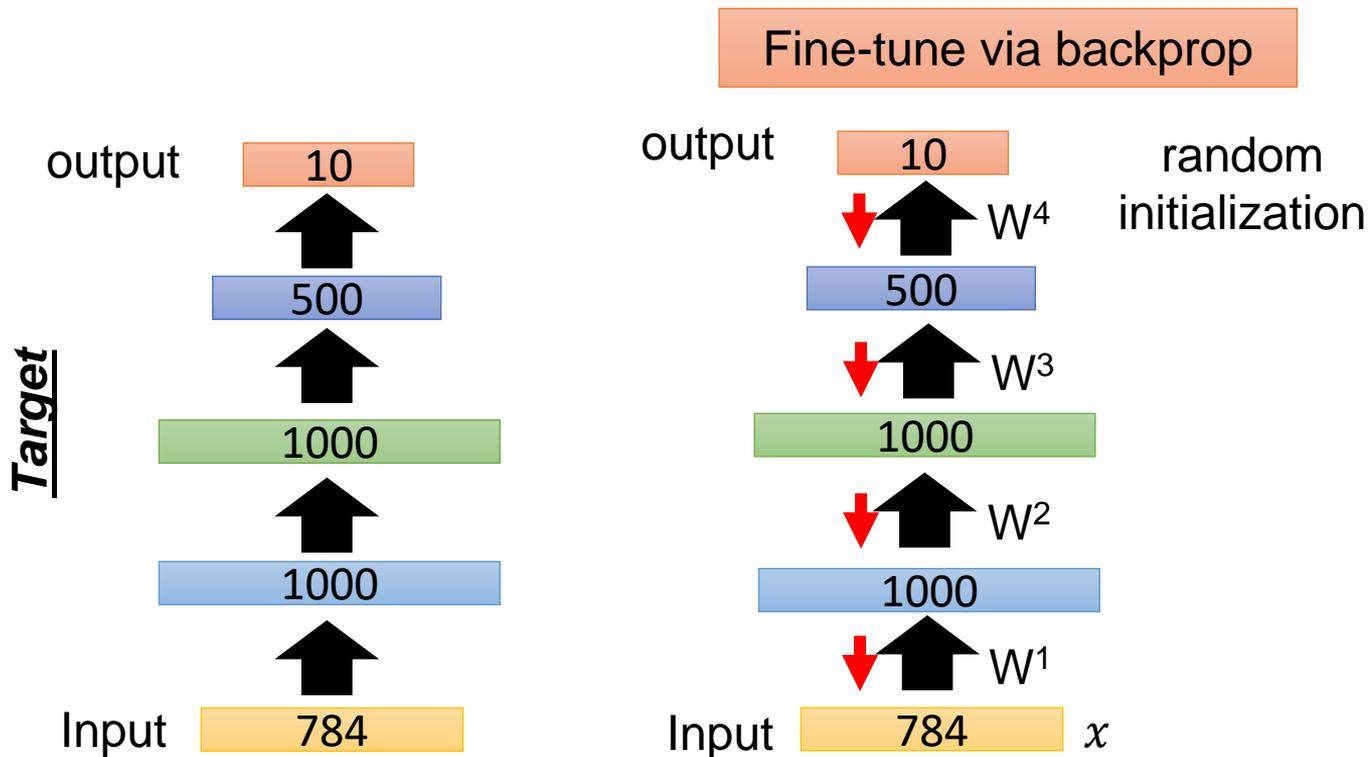
Auto-Encoder Layer-Wise Pre-Training



Auto-Encoder Layer-Wise Pre-Training

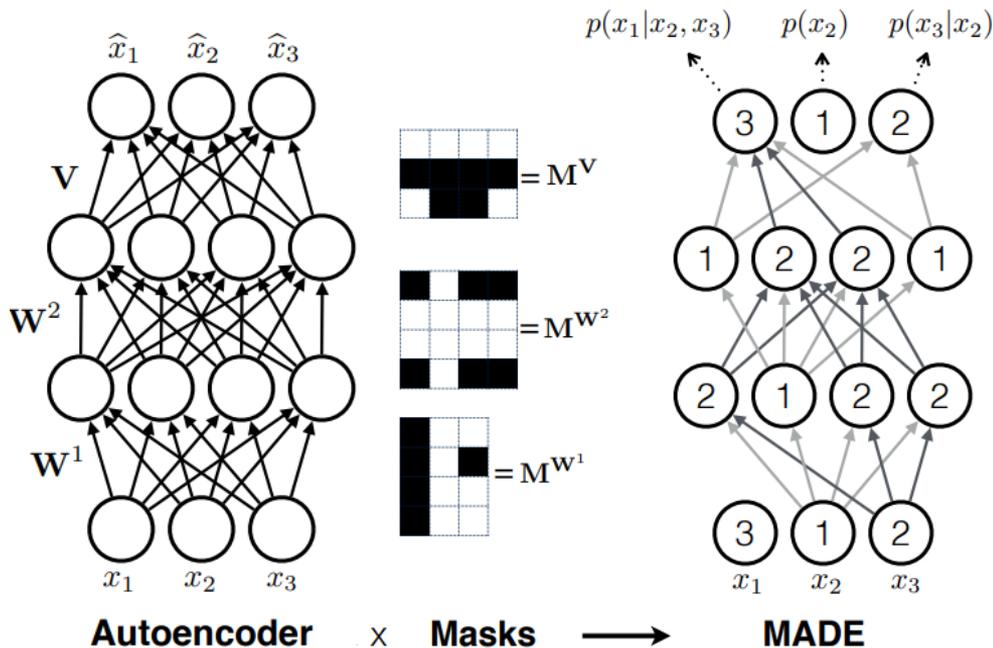


Auto-Encoder Layer-Wise Pre-Training



Masked Auto-Encoder (Germain et al., 2015)

- MADE: masked auto-encoder for distribution estimation
 - Reconstruction in a given ordering

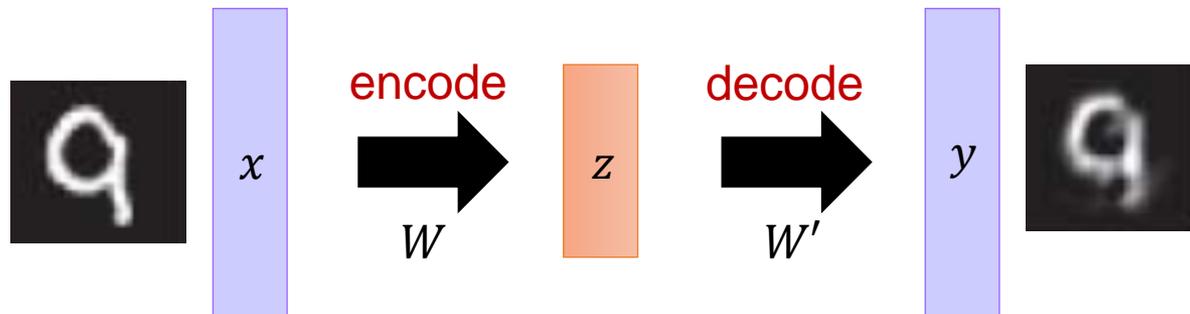


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Variational Auto-Encoder

Representation Learning and Generation

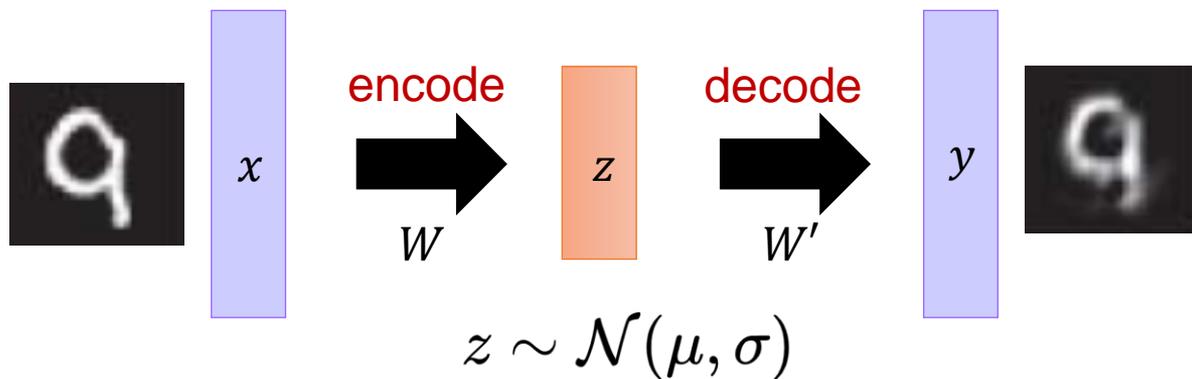
Generation from Latent Codes



How can we set a latent code for generation?

Latent Code Distribution Constraints

- Constrain the **data distribution** for learned latent codes
- Generate the latent code via a prior distribution

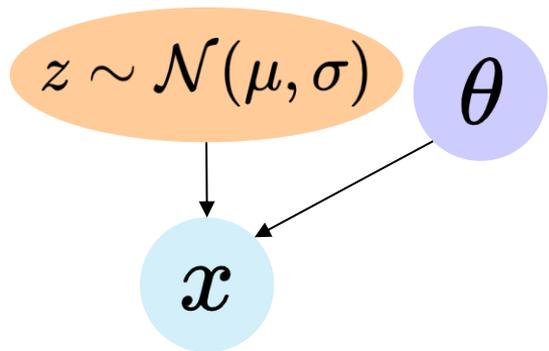


Variational Auto-Encoder

- An observed output x
- A latent variable z **generated from a Gaussian**
- A function (network) f parameterized by θ maps from z to x

$$\mathbf{x} = f(\mathbf{z}; \theta)$$

Observed Latent

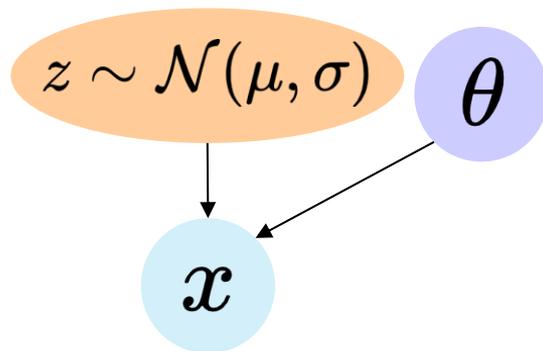


Idea: the compact representations follow a distribution

Variational Auto-Encoder

$$\underset{\text{Observed}}{\mathbf{x}} = f(\underset{\text{Latent}}{\mathbf{z}; \theta})$$

- For each datapoint i
 - Draw latent variables $z_i \sim p(z)$
 - Draw a datapoint $x_i \sim p_{\theta}(x | z)$



- Joint probability distribution over data and latent variables

$$p(x, z) = p(z) p_{\theta}(x | z)$$

prior posterior

- Learning objective: maximize the corpus log likelihood

$$\log P(\mathcal{X}) = \sum_{x \in \mathcal{X}} \log P(x; \theta)$$

Variational Auto-Encoder

- The marginal likelihood of a single datapoint x

$$P(x; \theta) = \int P(x | z; \theta) P(z) dz$$

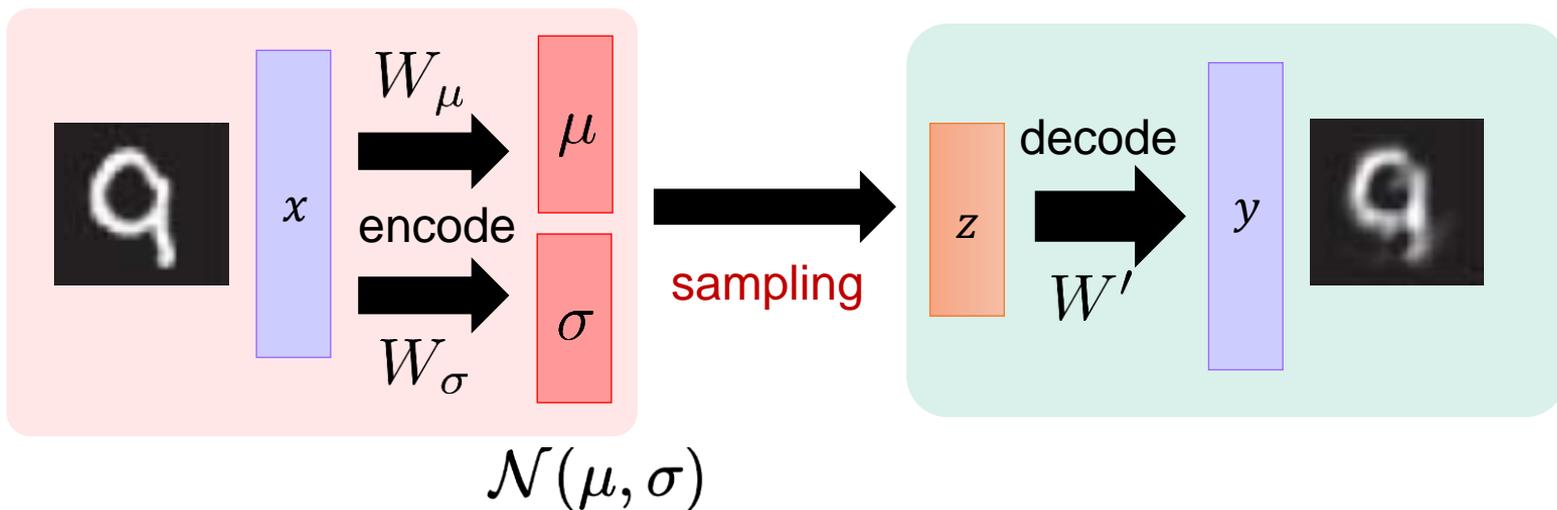
- Approximation by sampling z

$$P(x; \theta) \approx \sum_{z \sim P(z)} P(x | z; \theta)$$

Variational Auto-Encoder

Two tasks

- Learn to generate data from the latent code: $p_{\theta}(x | z)$
- Learn the distribution of latent factors: $p_{\theta}(z | x)$



Variational Auto-Encoder

Two tasks

- Learn to generate data from the latent code: $p_{\theta}(x | z)$
- Learn the distribution of latent factors: $p_{\theta}(z | x)$

$$p_{\theta}(z | x) = \frac{p_{\theta}(x | z)p(z)}{p(x)} = \int p(z)p_{\theta}(x | z)dz \quad \text{intractable}$$

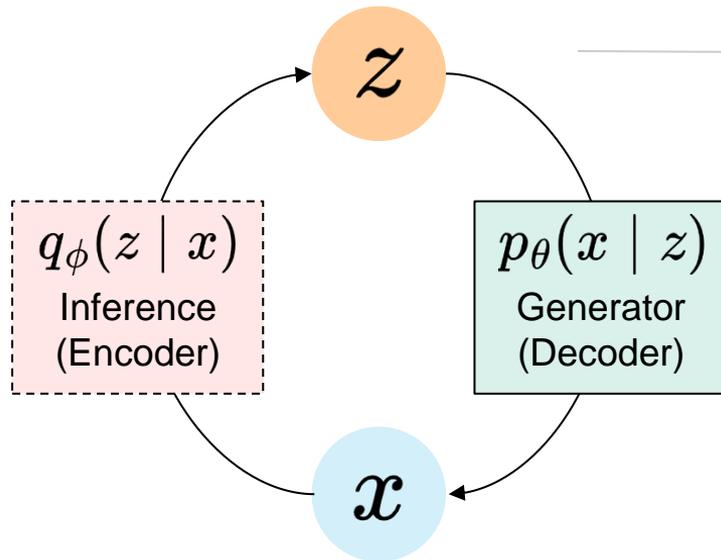
- Variational inference** approximates the true posterior $p_{\theta}(z | x)$ with a family of distributions $q_{\phi}(z | x)$

$$\text{minimize } \text{KL}(q_{\phi}(z | x) || p_{\theta}(z | x))$$

Variational Auto-Encoder

Two tasks

- Generator (Decoder): $p_{\theta}(x | z)$
- Inference (Encoder): $q_{\phi}(z | x)$

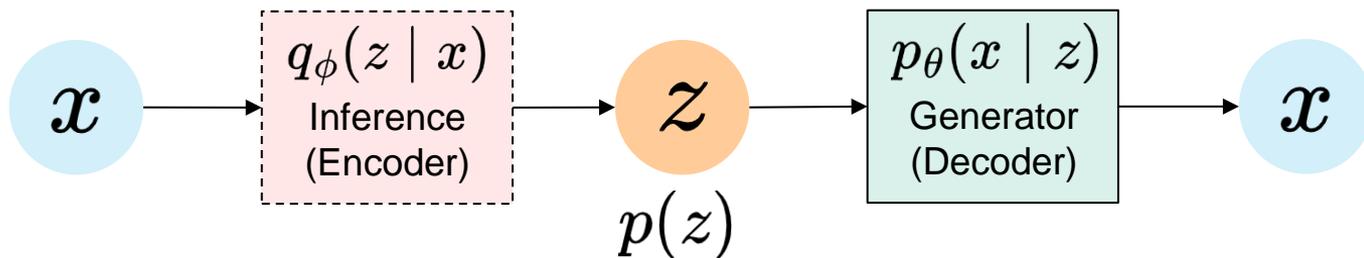


$$\underbrace{\mathbb{E}_{z \sim q_{\phi}(z|x)} [\log p_{\theta}(x | z)]}_{\text{reconstruction loss}} - \underbrace{D_{\text{KL}}(q_{\phi}(z | x) || p(z))}_{\text{KL regularizer}}$$

Regularized Auto-Encoder

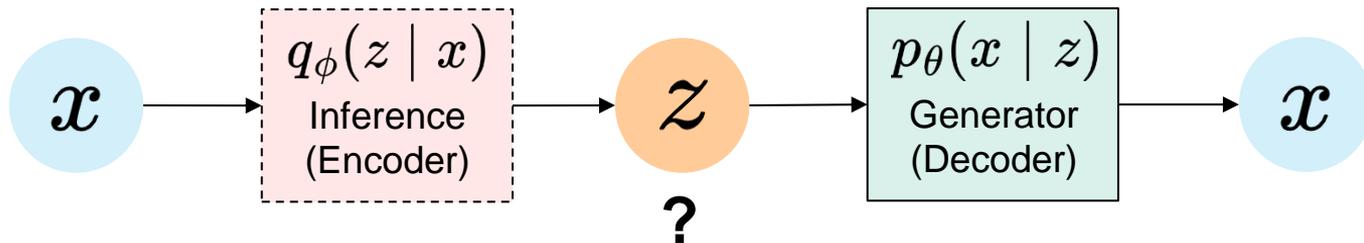
Variational Auto-Encoder

VAE



$$\mathbb{E}_{z \sim q_\phi(z|x)} [\log p_\theta(x | z)] - D_{\text{KL}}(q_\phi(z | x) \parallel p(z))$$

AE



AE is not generative model: (1) Can't sample new data from AE
 (2) Can't compute the log likelihood of data x

Image Reconstruction

AE



VAE



Text Reconstruction

○ AE: standard encoder-decoder

embedding interpolation

i went to the store to buy some groceries .
i store to buy some groceries .
i were to buy any groceries .
horses are to buy any groceries .
horses are to buy any animal .
horses the favorite any animal .
horses the favorite favorite animal .
horses are my favorite animal .

○ VAE

embedding interpolation

“ i want to talk to you . ”
“i want to be with you . ”
“i do n't want to be with you . ”
i do n't want to be with you .
she did n't want to be with him .

he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

VAE Training Tips

Posterior collapse issue

- KL divergence is easier to learn, so model learning relies solely on decoder and ignore latent variable

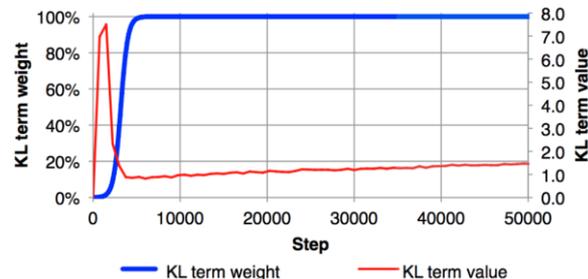
$$\mathbb{E}_{z \sim q_{\phi}(z|x)} [\log p_{\theta}(x | z)] - D_{\text{KL}}(q_{\phi}(z | x) || p(z))$$

requires good generative model

set the mean/variance of q to be the same as p

Solutions

- KL divergence annealing: an increasing constant to weight KL term
- KL thresholding $\sum_i \max[\lambda, D_{\text{KL}}(q_{\phi}(z_i|x) || p(z_i))]$



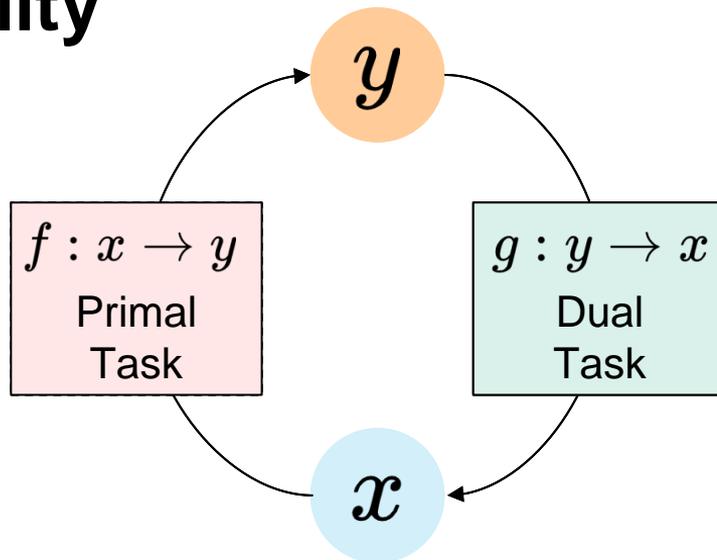
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Dual Learning

Learning Two Tasks via Duality

[Slides credited from ACML 2018 Tutorial](#)

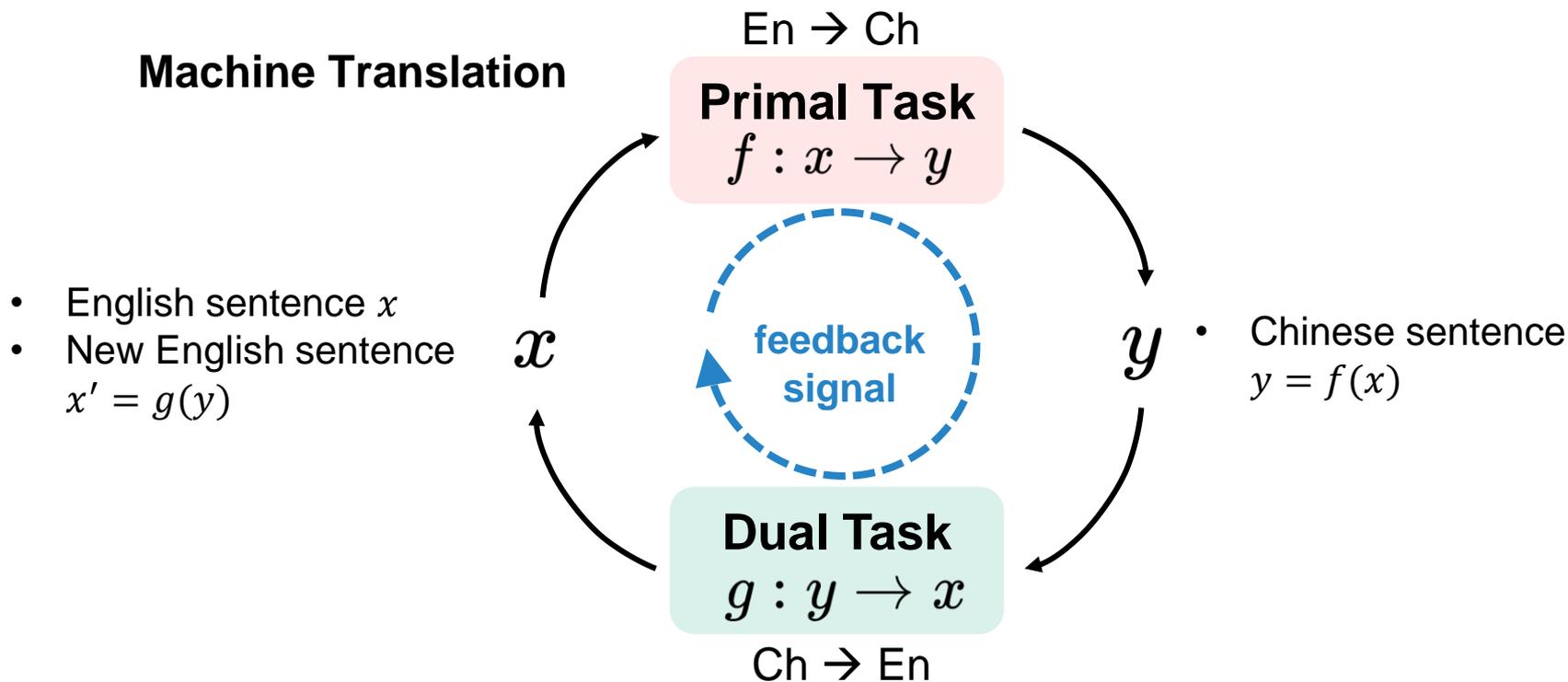
Task Duality



AI Tasks	$f: x \rightarrow y$	$g: y \rightarrow x$
Machine translation	EN \rightarrow CH	CH \rightarrow EN
Speech processing	ASR	TTS
Image understanding	captioning	Image generation
Language understanding	Language understanding	Language generation
Question answering	QA	Question generation

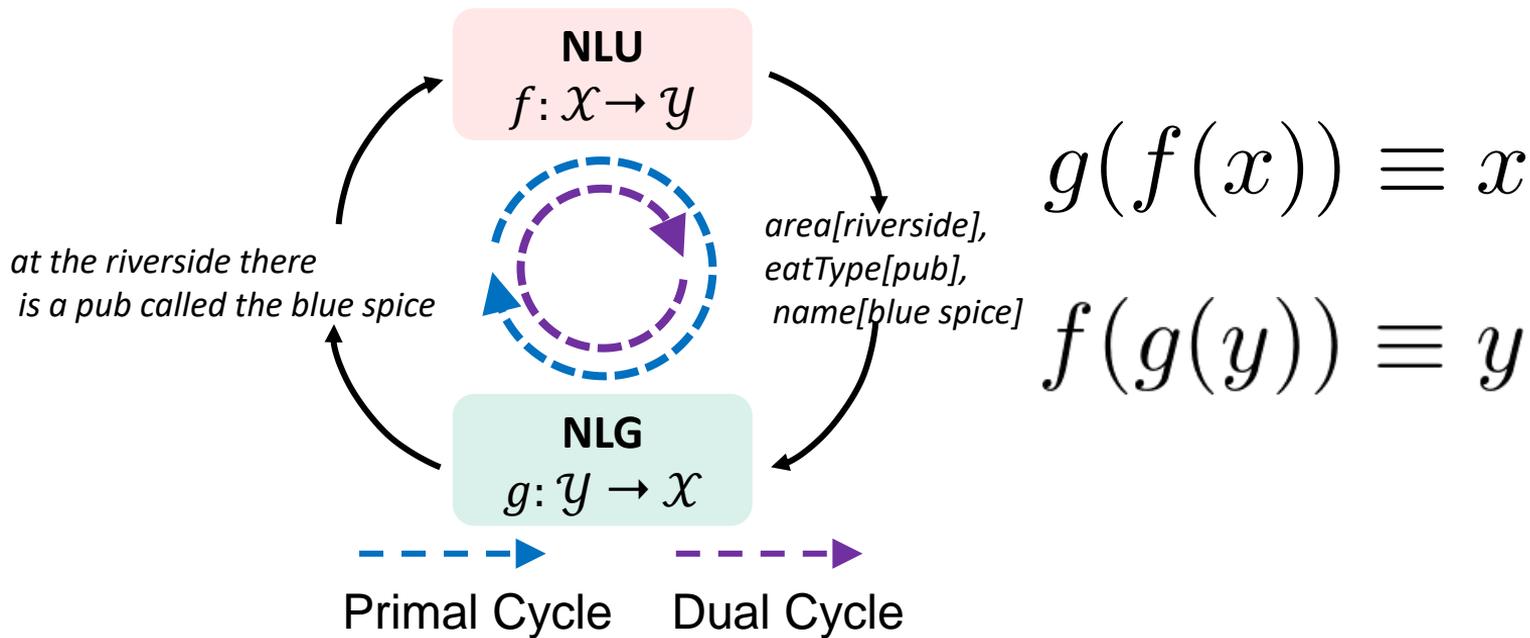
Dual Unsupervised Learning

- Idea: improve tasks by leveraging feedback signal via RL etc.



Joint Dual Learning

- Idea: perfectly *reconstructing* the input via two models



Joint Dual Learning Objective

Explicit

- Reconstruction Likelihood

$$\begin{cases} \log p(x | f(x_i; \theta_{x \rightarrow y}); \theta_{y \rightarrow x}) & \text{Primal} \\ \log p(y | g(y_i; \theta_{y \rightarrow x}); \theta_{x \rightarrow y}) & \text{Dual} \end{cases}$$

- Automatic Evaluation Score

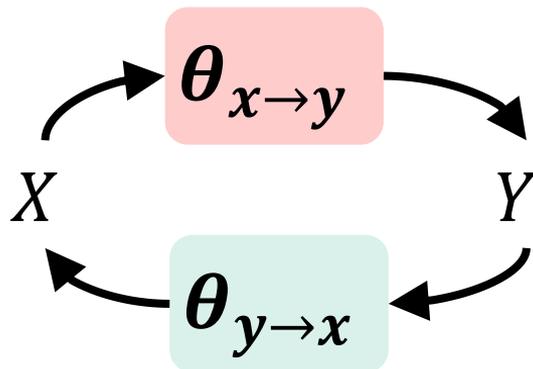
- BLEU and ROUGE for language (NLG)
- F-score for semantic (NLU)

Implicit

- Model-based methods estimating data distribution
 - Language modeling (LM) for language
 - Masked autoencoder (MADE) for semantics

Dual Supervised Learning (Xia et al., 2017)

- Proposed for machine translation
- Consider two domains X and Y , and two tasks $X \rightarrow Y$ and $Y \rightarrow X$



We have $P(x, y) = P(x | y)P(y) = P(y | x)P(x)$

Ideally $P(x, y) = P(x | y; \theta_{y \rightarrow x})P(y) = P(y | x; \theta_{x \rightarrow y})P(x)$

Dual Supervised Learning

- Exploit the duality by forcing models to follow the probabilistic constraint $P(x | y; \theta_{y \rightarrow x})P(y) = P(y | x; \theta_{x \rightarrow y})P(x)$

Objective function

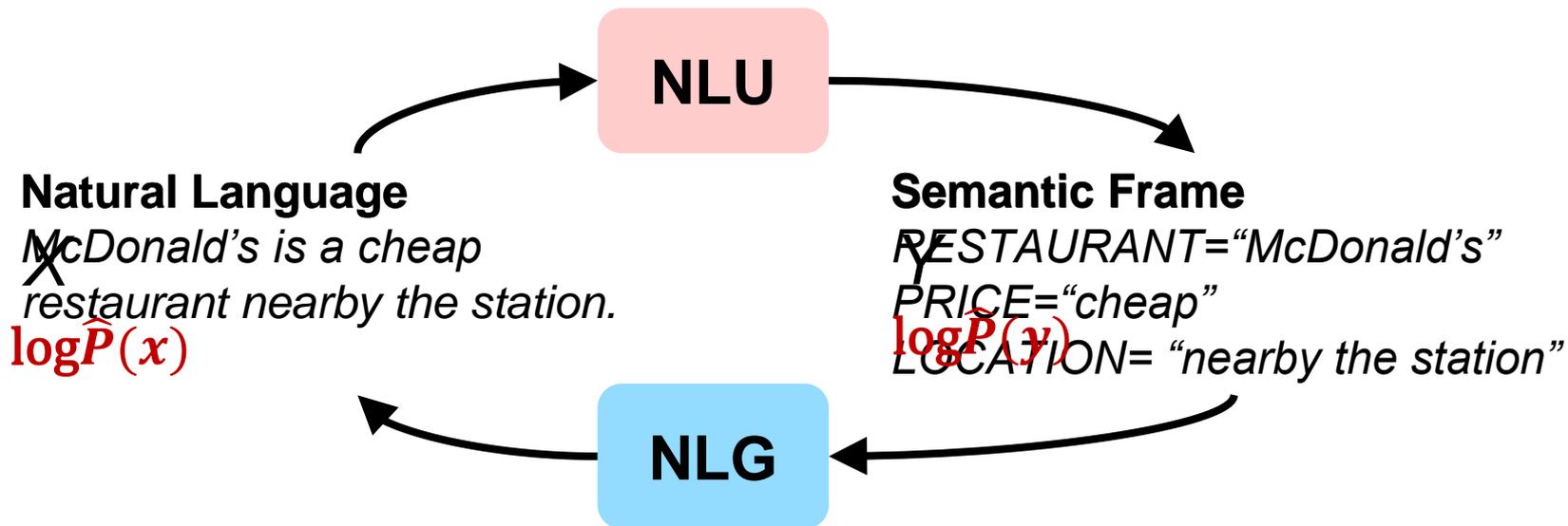
$$\begin{cases} \min_{\theta_{x \rightarrow y}} \mathbb{E}[l_1(f(x; \theta_{x \rightarrow y}), y)] + \lambda_{x \rightarrow y} l_{duality} \\ \min_{\theta_{y \rightarrow x}} \mathbb{E}[l_2(g(y; \theta_{y \rightarrow x}), x)] + \lambda_{y \rightarrow x} l_{duality} \end{cases}$$

$$l_{duality} = (\log \hat{P}(x) + \log P(y | x; \theta_{x \rightarrow y}) - \log \hat{P}(y) - \log P(x | y; \theta_{y \rightarrow x}))^2$$

How to model the marginal distributions of X and Y ?

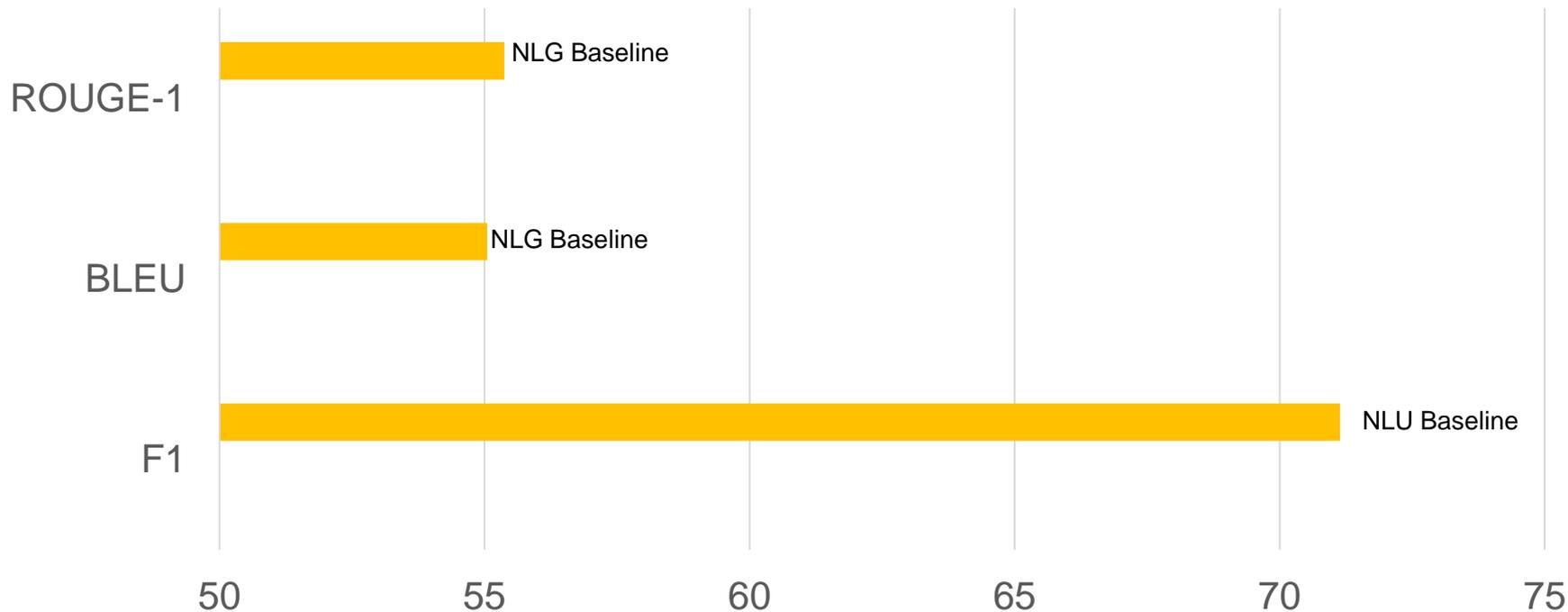
Dual Supervised Learning

- Considering NLU and NLG



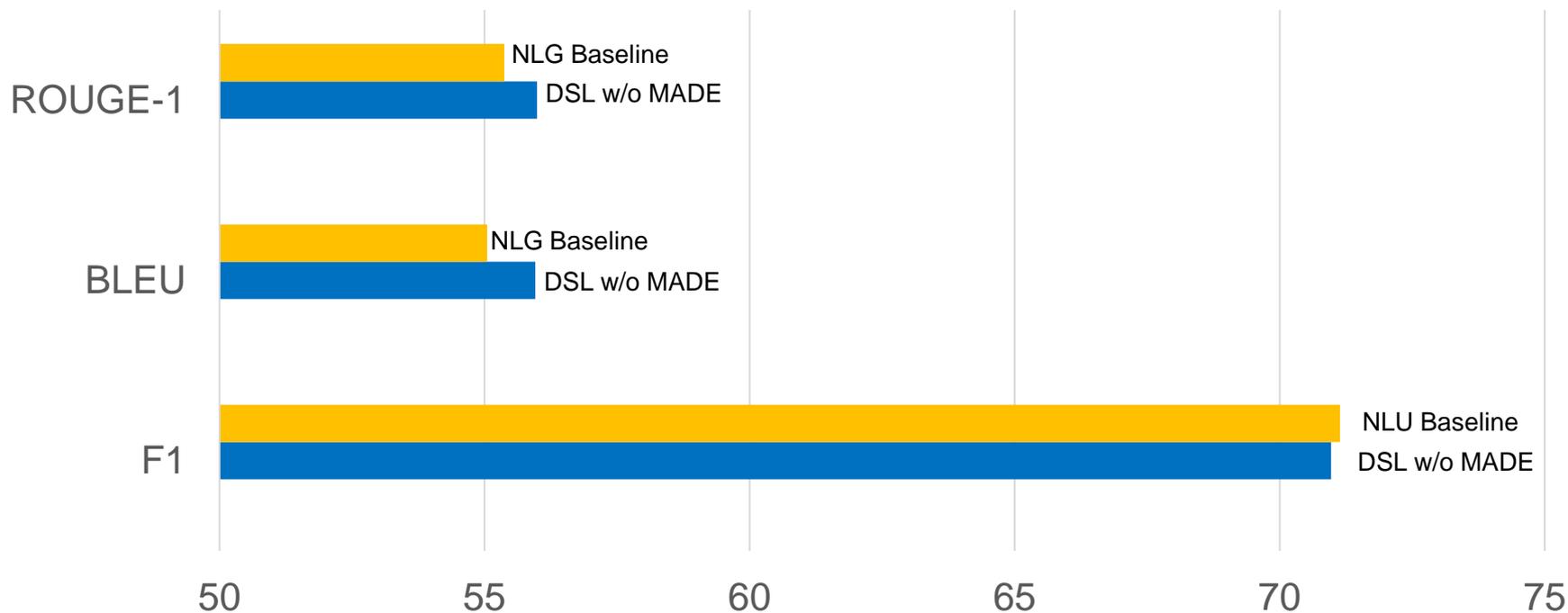
NLU/NLG Results

- E2E NLG data: 50k examples in the restaurant domain
- NLU: F-1 score; NLG: BLEU, ROUGE



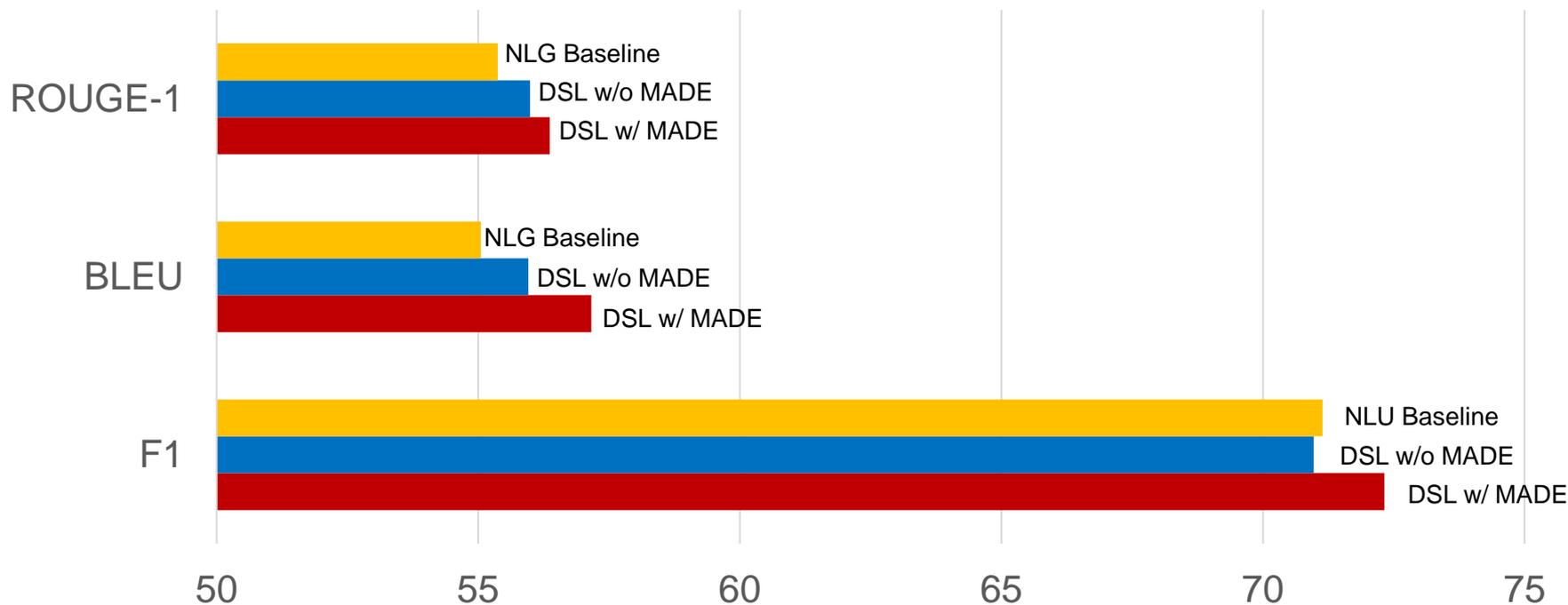
NLU/NLG Results

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NLU/NLG Results

- E2E NLG data: 50k examples in the restaurant domain
- NLU: F-1 score; NLG: BLEU, ROUGE



Comparison

Unsupervised/semi-supervised learning: only one task; no feedback signals for unlabeled data

Co-training: only one task; different feature sets provide complementary information about the instance

Multi-task learning: multiple tasks share the same representation

Transfer learning: use auxiliary tasks to boost the target task

Dual learning: multiple tasks involved; automatically generate reinforcement feedback for unlabeled data,

Dual learning: multiple tasks involved; no assumption on feature sets

Dual learning: don't need to share representations, only when the closed loop

Dual learning: all tasks are mutually and simultaneously boosted

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Self-Supervised Learning

Self-Prediction and Contrastive Learning

[Slides credited from NeurIPS 2021 Tutorial](#)

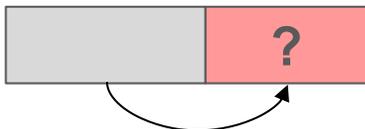
Self-Supervised Learning

- Self-supervised learning (SSL): a special type of representation learning via unlabeled data
- Idea: constructing supervised tasks out of unsupervised data
 - High cost of data annotation
 - Limited annotated data
 - Good representation makes it easier to transfer to diverse downstream tasks

Self-Supervised Learning

Self-Prediction

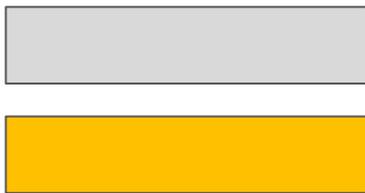
- Given **an individual** data sample, the task is to predict one missing part of the sample given the other part



“intra-sample” prediction

Contrastive Learning

- Given **multiple** data samples, the task is to predict their relationship



relationship?

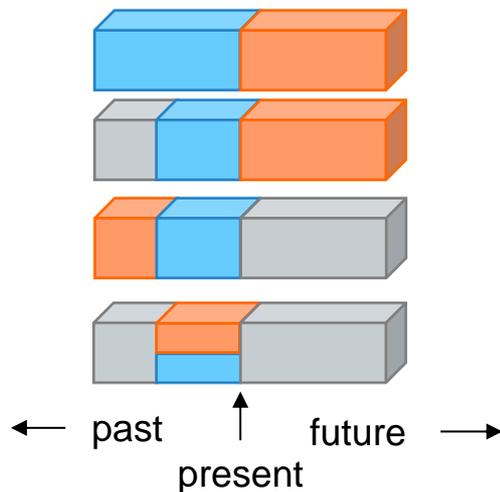
“inter-sample” prediction

Self-Prediction

(illustration from Yann LeCun)

○ Assume: a part of the input is unknown and predict it

- Predict the **future** from the **past**
- Predict the **future** from the **recent past**
- Predict the **past** from the **present**
- Predict the **top** from the **bottom**
- Predict the **occluded** from the **visible**



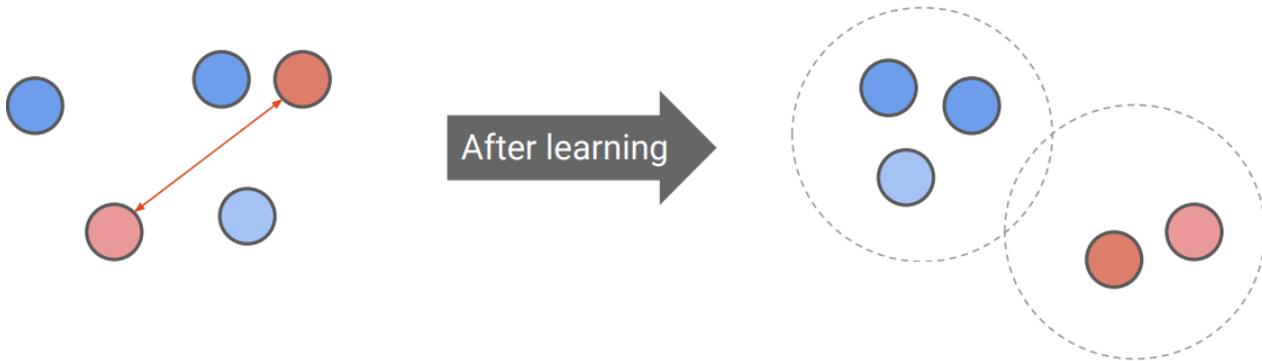
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Contrastive Learning

Adapting Embedding Spaces

Contrastive Learning

- Idea: learn an embedding space where *similar* sample pairs stay *close* to each other while *dissimilar* ones are *far apart*
 - Inter-sample classification
 - Feature clustering
 - Multi-view coding



Inter-Sample Classification

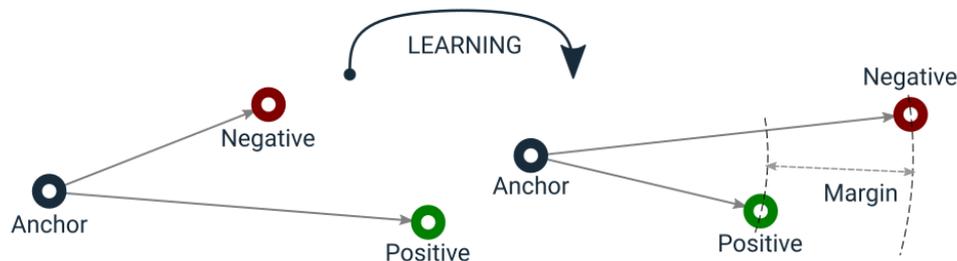
- Task: given both similar (“positive”) and dissimilar (“negative”) candidates, identifying which is similar to the anchor datapoint
- Datapoint candidates
 1. The original input and its **distorted version**
 2. Data capturing the same target from **different views**

Inter-Sample Classification

Triplet loss (Schroff et al., 2015)

- minimize the distance between the anchor x and positive x^+ and maximize the distance between the anchor x and negative x^- at the same time

$$\mathcal{L}_{\text{triplet}}(x, x^+, x^-) = \sum_x \max(0, \underbrace{\|f(x) - f(x^+)\|_2^2}_{\text{as close as possible}} - \underbrace{\|f(x) - f(x^-)\|_2^2}_{\text{as far as possible}} + \epsilon)$$



Inter-Sample Classification

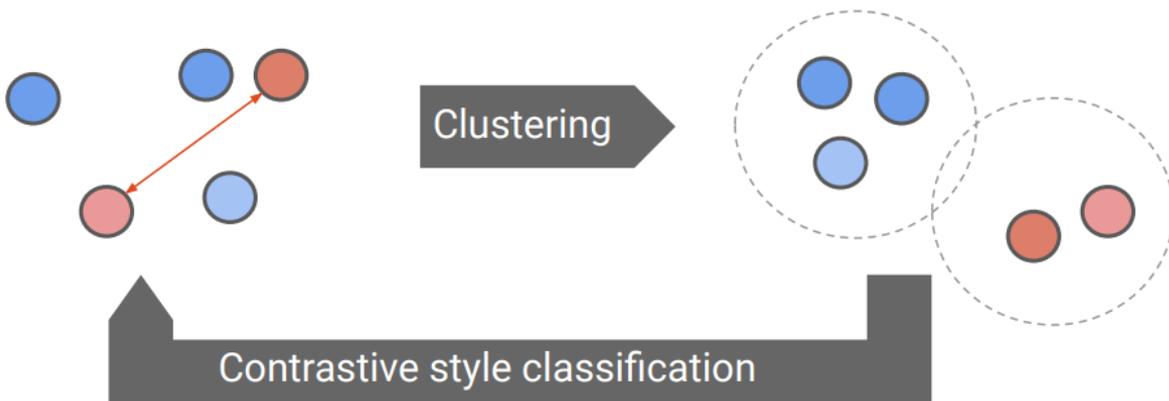
○ N-pair loss (Sohn, 2016)

- generalizes to include comparison with multiple negative samples

$$\mathcal{L}_{\text{N-pair}}(x, x^+, \{x_i^-\}) = \log \left(1 + \sum_i \exp(f(x)^T f(x_i^-) - f(x)^T f(x^+)) \right)$$

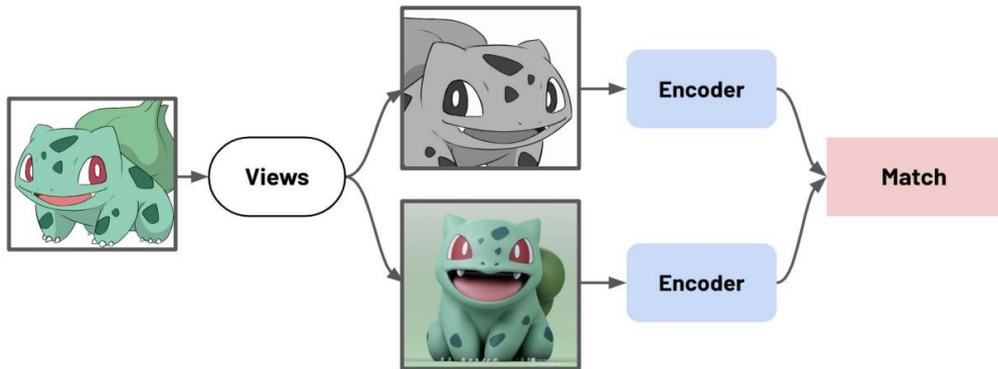
Feature Clustering

- Idea: cluster similar datapoints based on learned features
→ assign pseudo labels to samples for intra-sample classification



Multiview Coding

- Idea: apply the InfoNCE objective to different views of input
 - Data augmentation is adopted for generating different views
 - “views” can come from different modalities



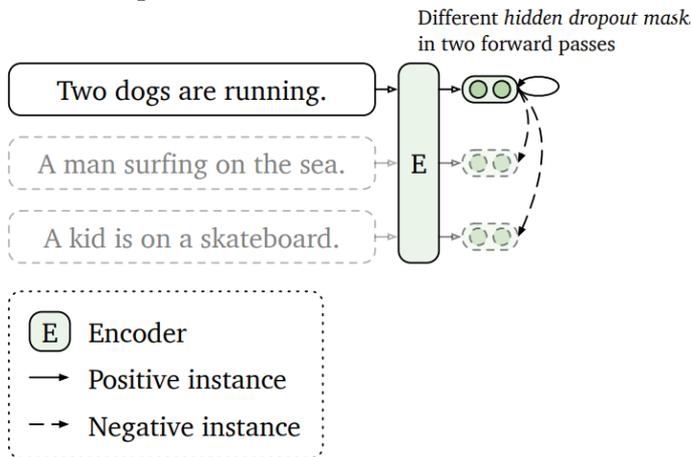
mainstream approaches for contrastive learning

Contrastive Learning in NLP

SimCSE (Gao et al., 2021): simple contrastive learning of sentence embeddings

- Unsupervised: predict a sentence from itself with only dropout noise

(a) Unsupervised SimCSE

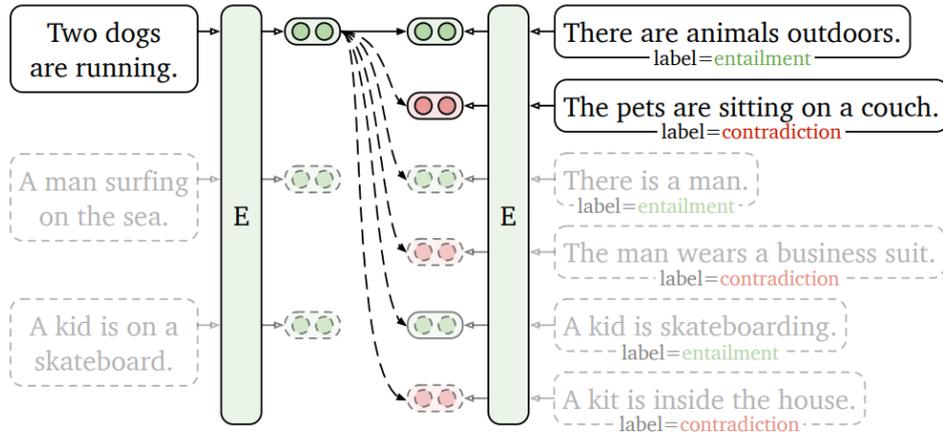


Model	STS12	STS13	STS14	STS15	STS16	STS-B	SICK-R	Avg.
<i>Unsupervised models</i>								
GloVe embeddings (avg.)*	55.14	70.66	59.73	68.25	63.66	58.02	53.76	61.32
BERT _{base} (first-last avg.)	39.70	59.38	49.67	66.03	66.19	53.87	62.06	56.70
BERT _{base} -flow	58.40	67.10	60.85	75.16	71.22	68.66	64.47	66.55
BERT _{base} -whitening	57.83	66.90	60.90	75.08	71.31	68.24	63.73	66.28
IS-BERT _{base} [♥]	56.77	69.24	61.21	75.23	70.16	69.21	64.25	66.58
CT-BERT _{base}	61.63	76.80	68.47	77.50	76.48	74.31	69.19	72.05
* SimCSE-BERT _{base}	68.40	82.41	74.38	80.91	78.56	76.85	72.23	76.25
RoBERTa _{base} (first-last avg.)	40.88	58.74	49.07	65.63	61.48	58.55	61.63	56.57
RoBERTa _{base} -whitening	46.99	63.24	57.23	71.36	68.99	61.36	62.91	61.73
DeCLUTR-RoBERTa _{base}	52.41	75.19	65.52	77.12	78.63	72.41	68.62	69.99
* SimCSE-RoBERTa _{base}	70.16	81.77	73.24	81.36	80.65	80.22	68.56	76.57
* SimCSE-RoBERTa _{large}	72.86	83.99	75.62	84.77	81.80	81.98	71.26	78.90

Contrastive Learning in NLP

- **SimCSE** (Gao et al., 2021): simple contrastive learning of sentence embeddings
 - *Supervised*: further adapt embeddings based on labels

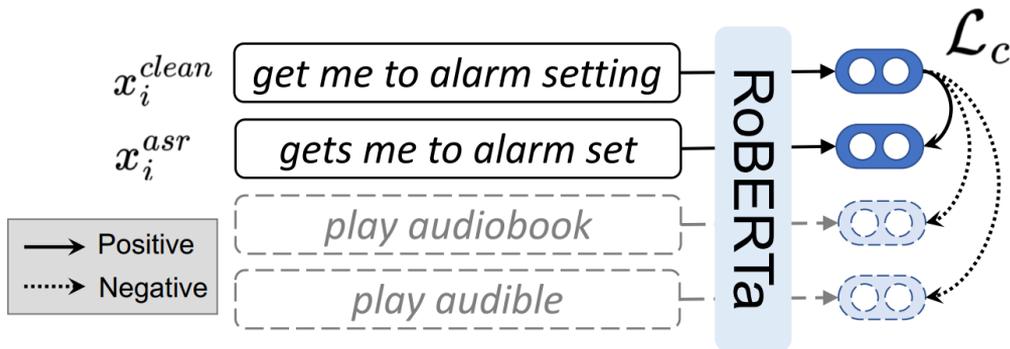
(b) Supervised SimCSE



	Supervised models								
InferSent-GloVe*	52.86	66.75	62.15	72.77	66.87	68.03	65.65	65.01	
Universal Sentence Encoder*	64.49	67.80	64.61	76.83	73.18	74.92	76.69	71.22	
SBERT _{base} *	70.97	76.53	73.19	79.09	74.30	77.03	72.91	74.89	
SBERT _{base-flow}	69.78	77.27	74.35	82.01	77.46	79.12	76.21	76.60	
SBERT _{base-whitening}	69.65	77.57	74.66	82.27	78.39	79.52	76.91	77.00	
CT-SBERT _{base}	74.84	83.20	78.07	83.84	77.93	81.46	76.42	79.39	
* SimCSE-BERT _{base}	75.30	84.67	80.19	85.40	80.82	84.25	80.39	81.57	
SRoBERTa _{base} *	71.54	72.49	70.80	78.74	73.69	77.77	74.46	74.21	
SRoBERTa _{base-whitening}	70.46	77.07	74.46	81.64	76.43	79.49	76.65	76.60	
* SimCSE-RoBERTa _{base}	76.53	85.21	80.95	86.03	82.57	85.83	80.50	82.52	
* SimCSE-RoBERTa _{large}	77.46	87.27	82.36	86.66	83.93	86.70	81.95	83.76	

Contrastive Learning in NLP

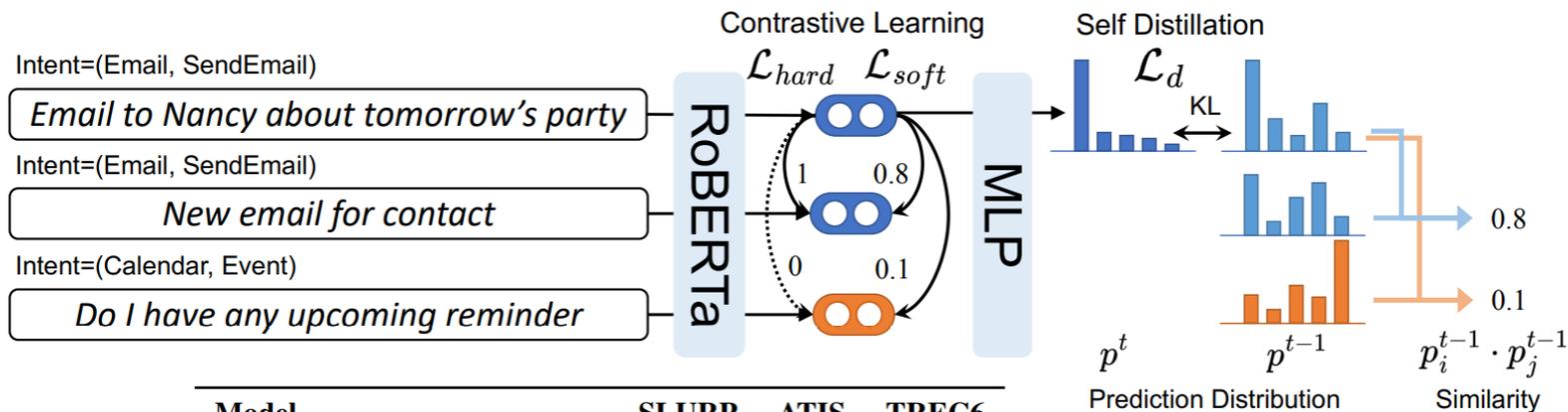
- **SpokenCSE** (Chang & Chen, 2022): improve ASR robustness
 - *Unsupervised*: learning with the paired clean/noisy sentences



Model	SLURP	ATIS	TREC6
RoBERTa	83.97	94.53	84.08
Phoneme-BERT [†]	83.78	94.83	85.96
SimCSE	84.47	94.07	84.92
Proposed (pre-train only)	84.51	95.02	85.20

Contrastive Learning in NLP

- SpokenCSE (Chang & Chen, 2022): improve ASR robustness
 - Supervised: learning with self-distillation



Language vs. Vision

Texts

- Self supervision (LM)
- Large training data
- Zero-shot transferability



Images

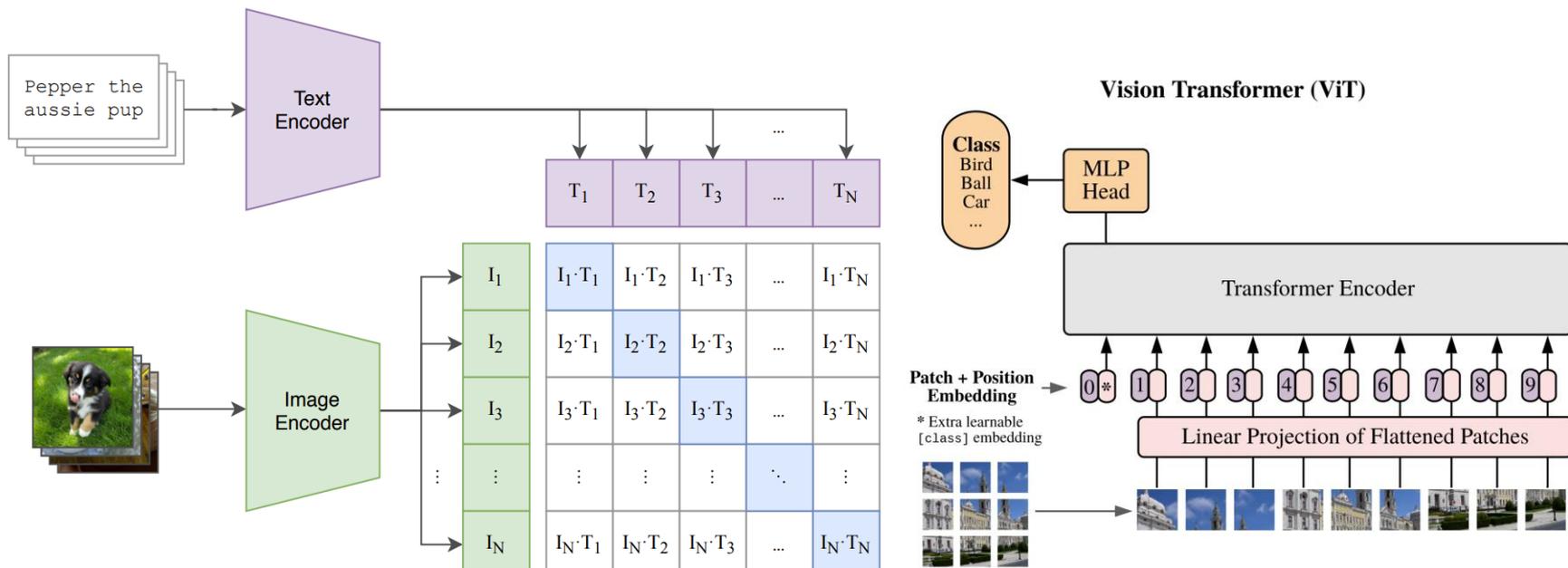
- Supervised learning
- Not that large training data (ImageNet)



Idea: enabling better transferability by connecting vision tasks with languages

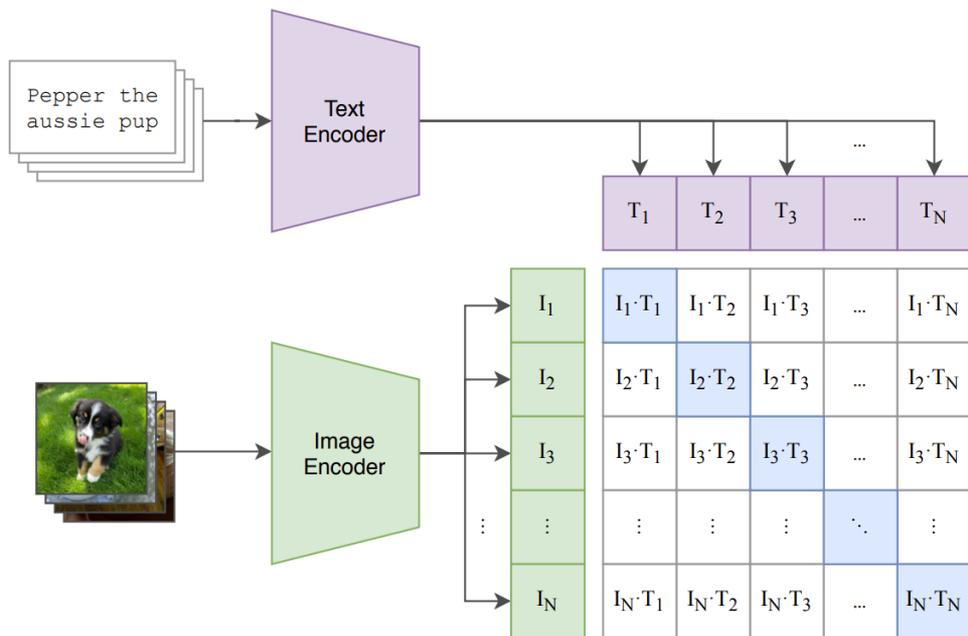
CLIP: Contrastive Language-Image Pretraining

- WebImageText (WIT): a newly constructed dataset of 400 million (image, text) pairs on the Internet



CLIP: Contrastive Language-Image Pretraining

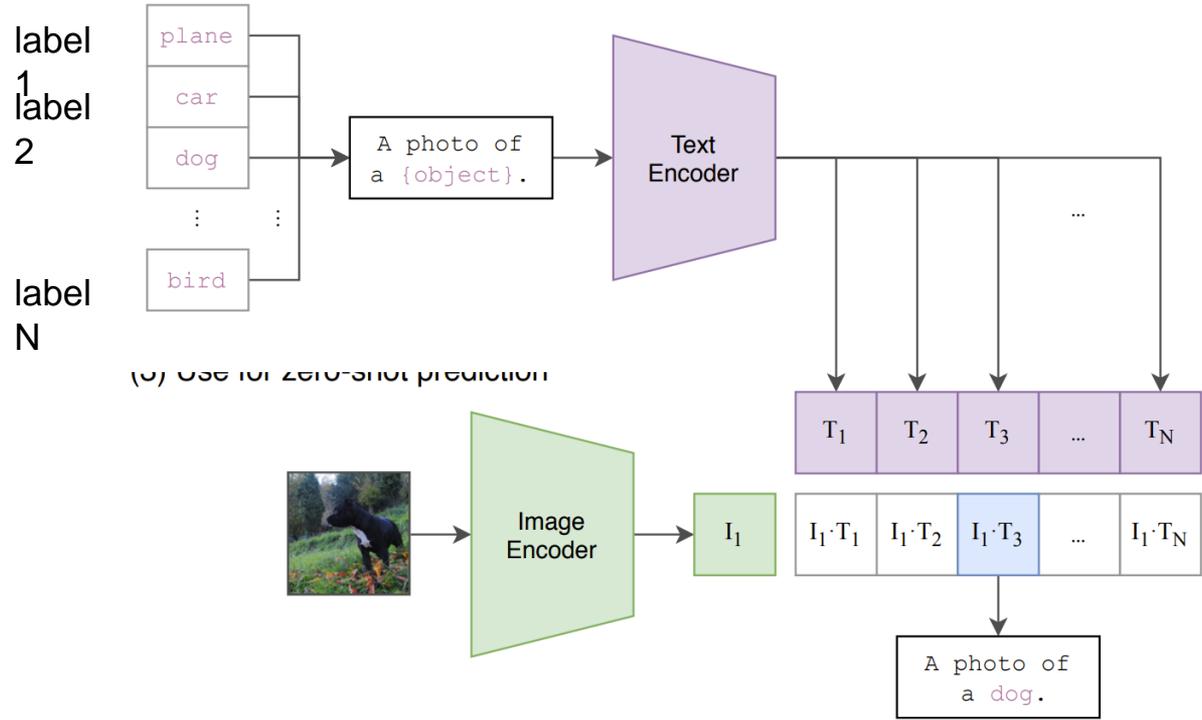
- WebImageText (WIT): a newly constructed dataset of 400 million (image, text) pairs on the Internet



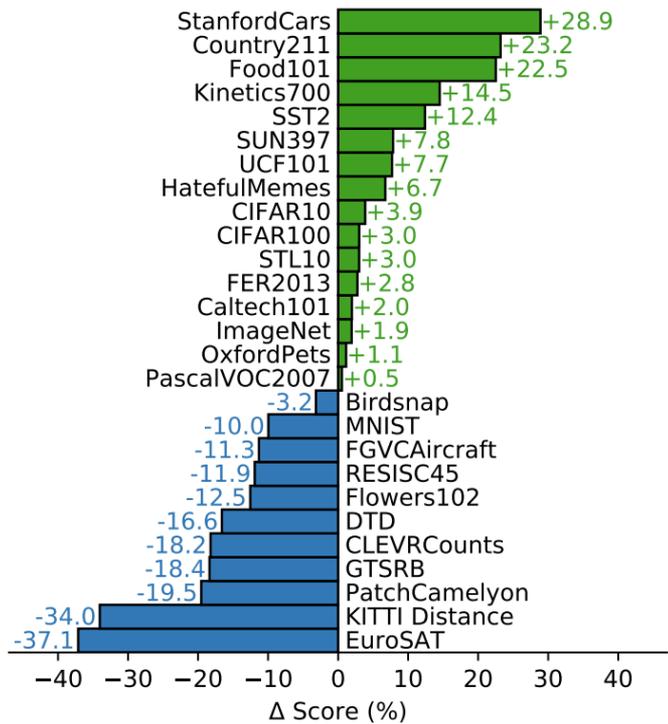
$$\min \left(\sum_{i=1}^N \sum_{j=1}^N (I_i \cdot T_j)_{i \neq j} - \sum_{i=1}^N (I_i \cdot T_i) \right)$$

batch-size=32,768

Zero-Shot Image Classification



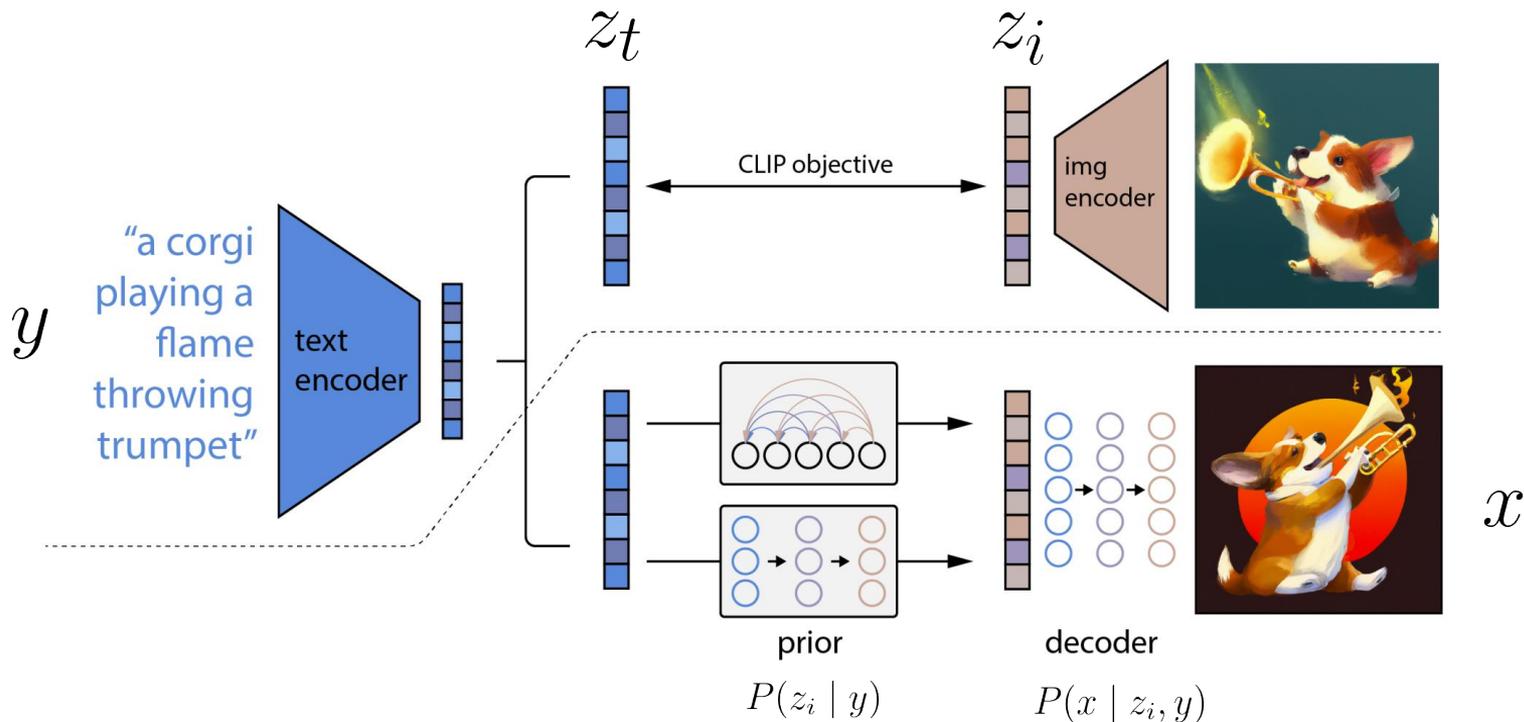
Zero-Shot Transferability



Zero-Shot CLIP vs. Linear Probe on ResNet50

	Dataset Examples	ImageNet ResNet101	Zero-Shot CLIP	Δ Score
ImageNet		76.2	76.2	0%
ImageNetV2		64.3	70.1	+5.8%
ImageNet-R		37.7	88.9	+51.2%
ObjectNet		32.6	72.3	+39.7%
ImageNet Sketch		25.2	60.2	+35.0%
ImageNet-A		2.7	77.1	+74.4%

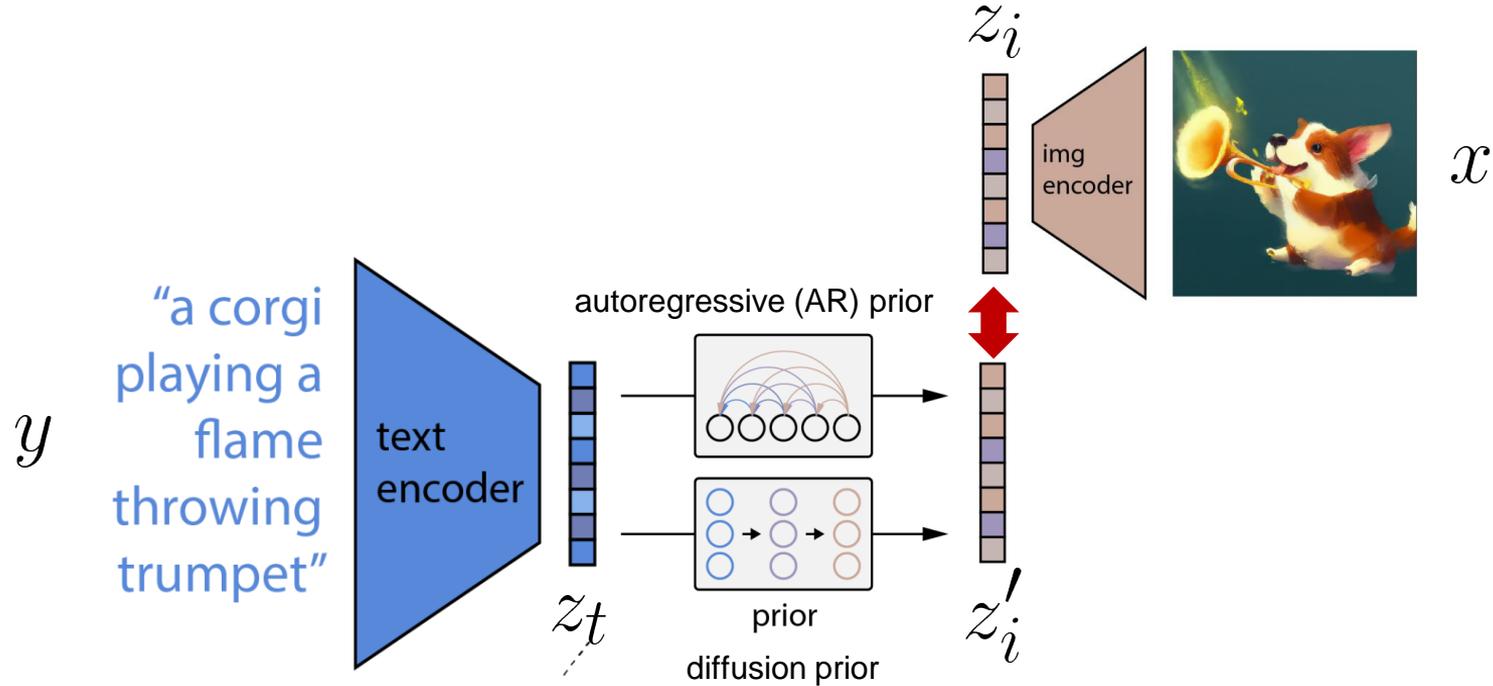
DALL-E 2: Image Generation with CLIP



$$P(x | y) = P(x, z_i | y) = P(x | z_i, y)P(z_i | y)$$

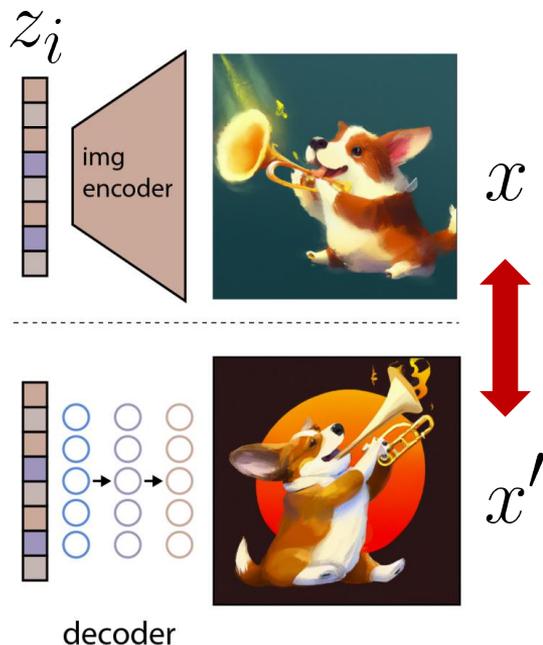
Prior Training

- Goal: $P(z_i | y)$ produces a CLIP image embedding given a caption



Decoder Training

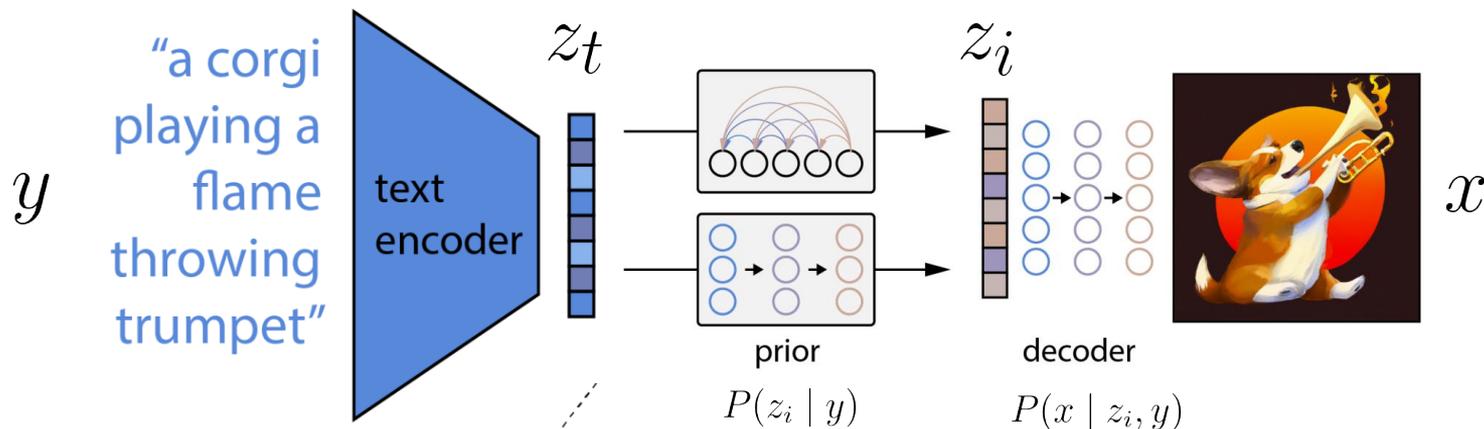
- Goal: $P(x \mid z_i, y)$ generate images similar to the given ones



GLIDE (text-guided image generation)

Inference for Image Generation

- Goal: $P(x | y)$ generates images given text captions



$$P(x | y) = P(x, z_i | y) = P(x | z_i, y)P(z_i | y)$$

Generated Images



“a green train is coming down the tracks”

“a group of skiers are preparing to ski down a mountain.”

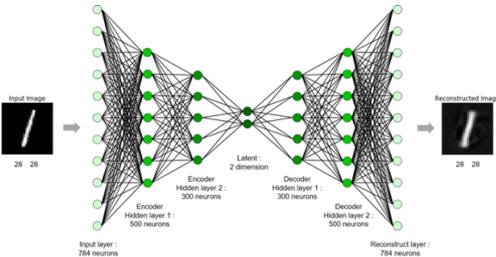
“a small kitchen with a low ceiling”

“a group of elephants walking in muddy water.”

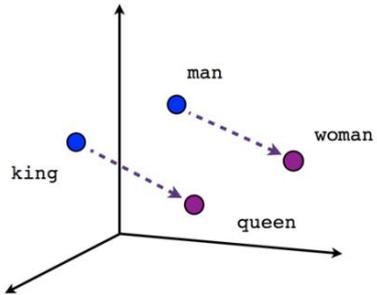
“a living area with a television and a table”

Diverse Approaches and Applications

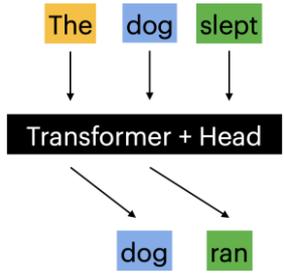
Auto-Encoders



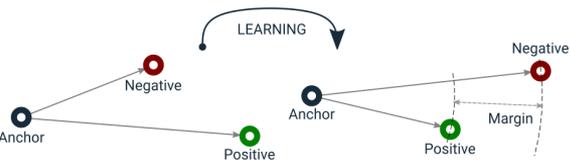
word2vec



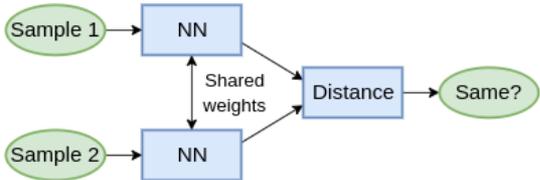
Autoregressive Language Modeling



Contrastive Learning



Siamese Networks



Concluding Remarks

- Labeling data is expensive, but we have large unlabeled data
- AE / VAE
 - exploits unlabeled data to learn latent factors as representations
 - learned representations can be transfer to other tasks
- Dual Learning
 - utilize the duality of two tasks
 - towards semi-supervised learning / unsupervised learning
- Self-Prediction
 - predict one missing part of the sample given the other part
- Contrastive Learning
 - positive pairs have similar embeddings