Unsupervised Learning & Generative AI

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Machine Learning

Outline

1. **Unsupervised Learning**
   - Text Models
   - Image Models
2. **ChatGPT**
3. **Autoencoders (AE)**
   - Manifold Learning*
4. **Variational Autoencoders (VAE)**
5. **Flow-based Models**
6. **Diffusion Models**
7. **Generative Adversarial Networks***
   - Basic Architecture
   - Challenges
   - More GANs

Outline

Unsupervised Learning

- Dataset: $\mathbb{X} = \{\boldsymbol{x}^{(i)}\}_i$, where $\boldsymbol{x}^{(i)}$'s are i.i.d. samples of $\mathbf{x}$
  - No supervision $\boldsymbol{y}^{(i)}$ (labels)
- What can we learn without labels?

Unsupervised Learning

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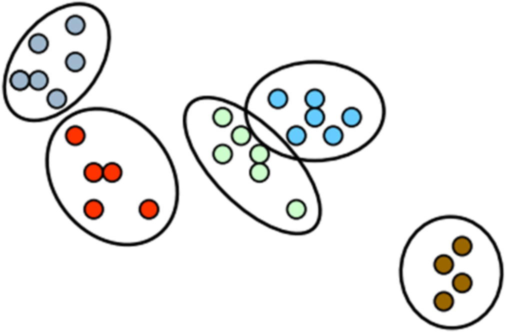
  - No supervision $\boldsymbol{y}^{(i)}$ (labels)
- What can we learn without labels? The ***structures*** in $\mathbb{X}$
  - Inter-sample structures
  - Intra-sample structures

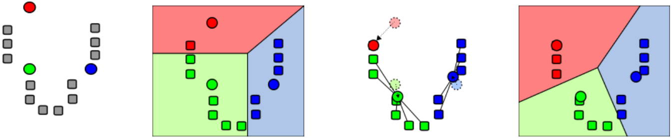
Clustering I

- Goal: to divide $\boldsymbol{x}^{(i)}$'s into K groups/***clusters***
  - Based on some similarity/distance measure between $\boldsymbol{x}^{(i)}$ and $\boldsymbol{x}^{(j)}$



Clustering II

- K-means algorithm (K fixed): iteratively move clusterheads until convergence



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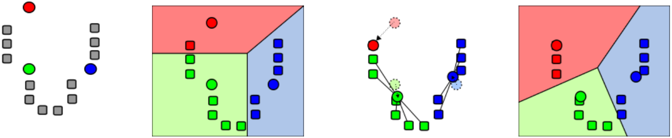
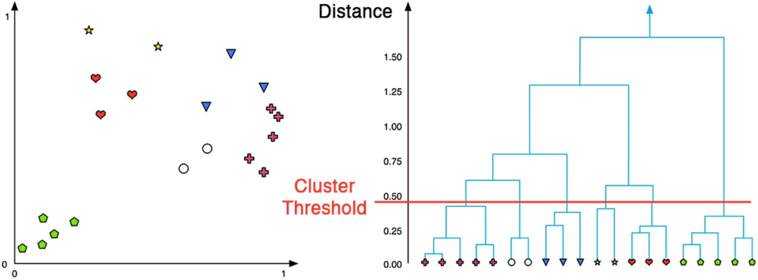


- Hierarchical clustering (variable K): iteratively merge two points/groups,then cut



Factorization for Tabular $\mathbb{X}$

- Let $\boldsymbol{X}$ be a rating matrix where $\boldsymbol{X}_{i,:} = \boldsymbol{x}^{(i)}$

Items

Users

User/Item	A	B	C	D
Ted		4		3
Carol	3		2	
Bob		5		2
Alice			4	

Factors

Ted	1.4	.9
Carol	1.2	1
Bob	1.5	.9
Alice	1.2	.8

*

A	B	C	D
1.4	1.3	.9	1.2
.8	1.1	2	.8

- Goal: to approximate $\boldsymbol{X}$ with a dense matrix $\hat{\boldsymbol{X}} = \boldsymbol{W}\boldsymbol{H}$
  - To make recommendations based on $\hat{\boldsymbol{X}}_{i,:}$ for user i, known as ***collaborative filtering***
- How?

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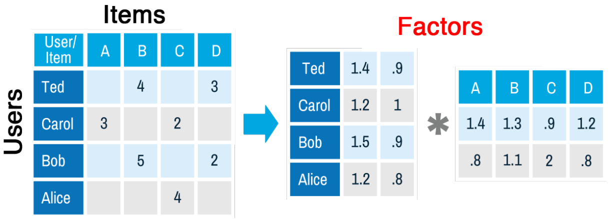


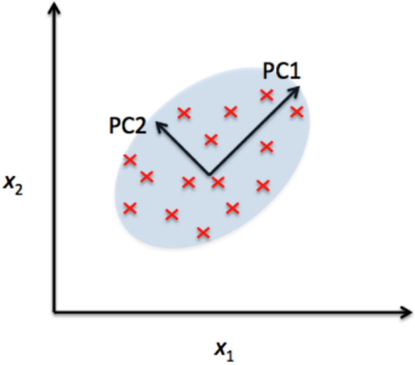
- Goal: to approximate $\boldsymbol{X}$ with a dense matrix $\hat{\boldsymbol{X}} = \boldsymbol{W}\boldsymbol{H}$
  - To make recommendations based on $\hat{\boldsymbol{X}}_{i,:}$ for user i, known as ***collaborative filtering***
- How? Non-negative matrix factorization (NMF) [19, 20]:

$$\arg \min_{\boldsymbol{W} \geq \boldsymbol{O}, \boldsymbol{H} \geq \boldsymbol{O}} \|\boldsymbol{X} - \boldsymbol{W}\boldsymbol{H}\|_F$$

  - So, positive elements in $\boldsymbol{W}$ and $\boldsymbol{H}$ can be seen as ***factor*** degrees

Dimension Reduction

- Goal: to learn a low dimensional representation $\mathbf{z}$ of $\mathbf{x}$
  - E.g., PCA



Self-Supervised Learning

- Goal: to learn a model that is able to "fill in the blanks"

$\boldsymbol{x}^{(i)}$  $\boldsymbol{y}^{(i)}$

Self-Supervised Learning

- Goal: to learn a model that is able to "fill in the blanks"
- Links unsupervised tasks with supervised models
  - Much more training data for models
  - Representation learning with deep networks

$\boldsymbol{x}^{(i)}$  $\boldsymbol{y}^{(i)}$

Example I: Word2Vec

- Goal: to learn a model for blank filling

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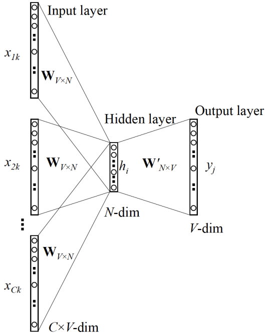
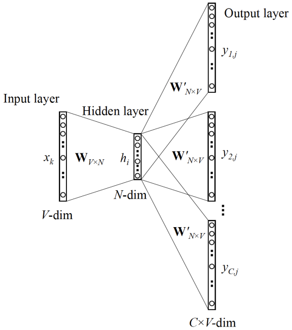
  - E.g., word2vec [26, 25]: "... *the cat sat* **on**..."



CBOW



Skip Gram

Example I: Word2Vec

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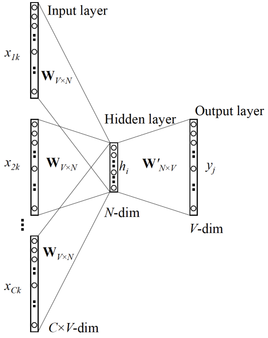

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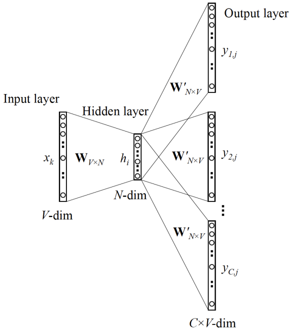

Skip Gram

- Latent representation $\mathbf{h}$ encodes the ***semantics*** of a word
  - No need for synonym dictionary; big data tell that already

Example II: Doc2Vec

- How to encode a document?

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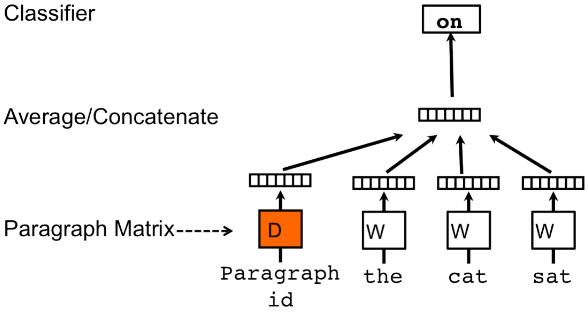
- How to encode a document?
- Bag of words (TF-IDF), average word2vec, etc.
  - Do ***not*** capture the semantics due to sentence/paragraph/doc structure
    - "*John likes* Mary" $\neq$ "*Mary likes* John"

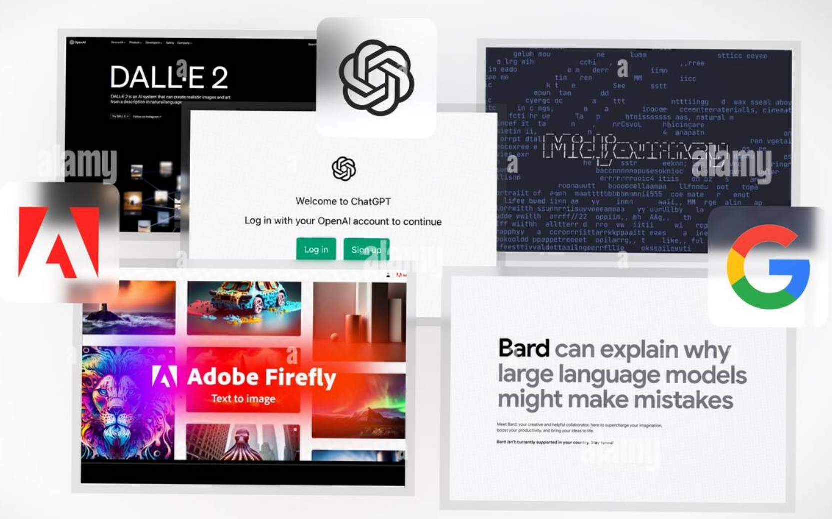
Example II: Doc2Vec

- How to encode a document?
- Bag of words (TF-IDF), average word2vec, etc.
  - Do ***not*** capture the semantics due to sentence/paragraph/doc structure
    - "*John likes* Mary" $\neq$ "*Mary likes* John"
- Why not apply self-supervised learning to docs?
  - Doc2vec [17]: to capture the ***context*** not explained by words
  - ***Transductive*** rather than inductive; does not work with unseen docs



Generative Models

- Goal: to generate new samples of $\mathbf{x}$
  - Can be conditioned on instructions (input)
- Largely based on self-supervised learning



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Generating Text

- With large (self-supervised) training data, ***transformers*** [46] have shown to perform better than RNNs and CNNs
  - Mainly due to the $O(1)$ point distance
- Two common text models based on transformer:
  - BERT [7]: non-autoregressive
  - GPT [31]: autoregressive

BERT [7]

- Massively trained ***encoder*** of the original transformer
  - Non-autoregressive
- Pre-training tasks:
  - Masked language model ("Cloze" task)
    - "A quick brown [MASK] jumps over the lazy dog" → "fox" 11%, "ant" 5%, ...
  - Next sentence prediction
    - "[MASK] go to store [SEP] to buy a [MASK] of milk"→ True 93%, False 7%

One Pre-training, Multiple Fine-tuning Tasks

- Special input to identify downstream task: [CLS] token

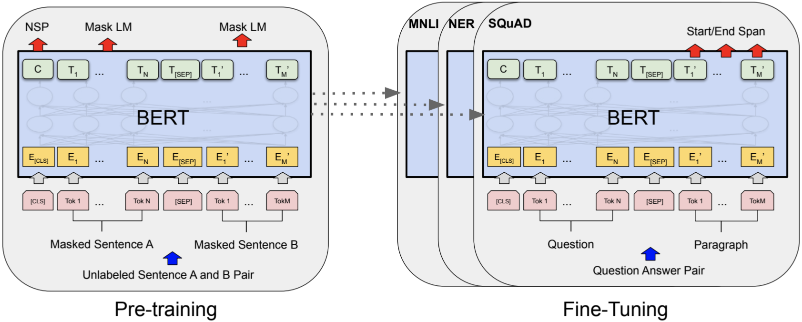
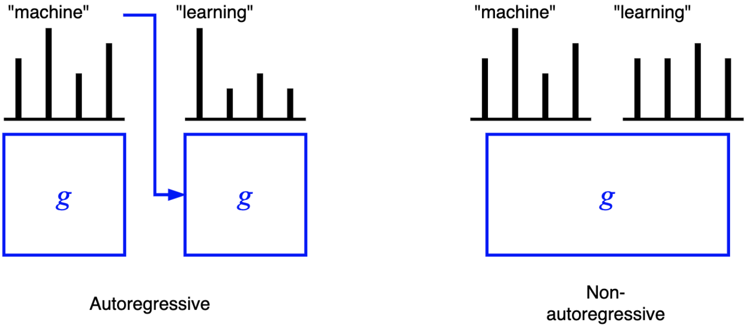


Figure 1: Overall pre-training and fine-tuning procedures for BERT. Apart from output layers, the same architectures are used in both pre-training and fine-tuning. The same pre-trained model parameters are used to initialize models for different down-stream tasks. During fine-tuning, all parameters are fine-tuned. `[CLS]` is a special symbol added in front of every input example, and `[SEP]` is a special separator token (e.g. separating questions/answers).

GPT [31]

- Massively trained ***decoder*** of the original transformer
  - Autoregressive
- Multitask pre-training by maximizing $\Pr(\text{output}|\text{input}, \text{task})$:
  - Translation: $\Pr(\text{french text}|\text{en text}, \text{translation})$
  - Question answering: $\Pr(\text{answer}|\text{question}, \text{qa})$
  - Reading comprehension: $\Pr(\text{answer}|\text{document}, \text{question}, \text{reading})$
- Usage for downstream task: fine-tuning or ***prompting***

Autoregressive or Not?

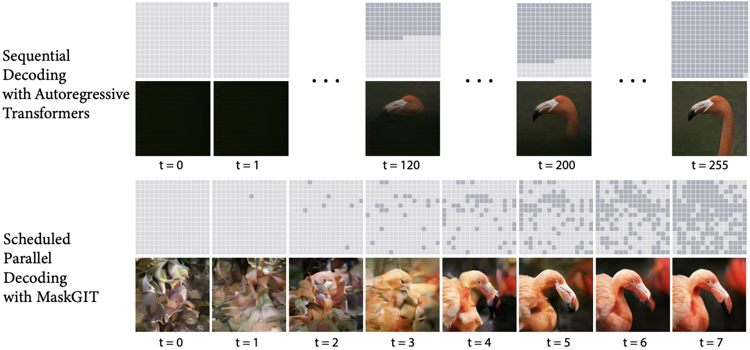


- It's easier for an autoregressive model to generate coherent text
- In this lecture, we focus on GPT and its variants

Outline

Autoregressive or Not?

- Autoregressive models can still give good (if not better) performance
  - E.g., PixelRNN [45], PixelCNN [44], or MaskGIT [5]
- But unlike in text domain, generating images pixel-by-pixel is ***very slow***
- Speed-up?
  - Scheduled ***parallel-pixel*** generation (e.g., MaskGIT)
  - ***Stepwise*** generation of ***whole*** images (e.g., flow-based and diffusion models)



Whole-Image Generation I

- Goal: given $\mathbb{X}$, to learn a ***generator function*** g such that $\hat{\boldsymbol{x}} = g(\boldsymbol{c};\Theta_g)$ looks like a real image in $\mathbb{X}$
  - $\boldsymbol{c}$ is a code or condition
  - Θ_g represents parameters of g
- Objective from Information Theory perspective:

$$\arg\min_g \mathrm{D}(\mathrm{P}_{\mathsf{data}} \| \mathrm{P}_g)$$

  - $\mathrm{P}_{\mathsf{data}}$ is the distribution of real data in the ground truth
  - P_g is the distribution of generated data
  - D is a divergence measure, e.g., D_{KL}

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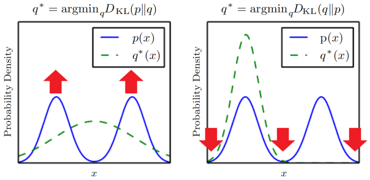
- Why not $\mathrm{D}_{\mathsf{KL}}(\mathrm{P}_g \| \mathrm{P}_{\mathsf{data}})$?



Whole-Image Generation II

- Minimizing $\mathrm{D_{KL}}(\mathrm{P_{data}} \| \mathrm{P}_g)$ amounts to maximizing $\mathrm{P}(\mathbb{X}|\Theta_g)$, the log likelihood of Θ_g:

$$
\begin{aligned}
g^* &= \arg\min_g \mathrm{D_{KL}}(\mathrm{P_{data}} \| \mathrm{P}_g) \\
&= \arg\max_g \mathrm{E}_{\mathbf{x}\sim \mathrm{P_{data}}}[\log \mathrm{P}_g(\mathbf{x})] + \mathrm{H}(\mathbf{x} \sim \mathrm{P_{data}}) \\
&= \arg\max_g \mathrm{E}_{\mathbf{x}\sim \mathrm{P_{data}}}[\log \mathrm{P}_g(\mathbf{x})] \\
&\approx \arg\max_g \textstyle\sum_{\boldsymbol{x}^{(i)} \in \mathbb{X}} \log \mathrm{P}_g(\boldsymbol{x}^{(i)}) \\
&= \arg\max_g \log \textstyle\prod_{\boldsymbol{x}^{(i)} \in \mathbb{X}} \mathrm{P}_g(\boldsymbol{x}^{(i)})
\end{aligned}
$$

$$
\begin{aligned}
\Theta_g^* &= \arg\max_{\Theta_g} \log \textstyle\prod_{\boldsymbol{x}^{(i)} \in \mathbb{X}} \mathrm{P}(\boldsymbol{x}^{(i)} | \Theta_g) \\
&= \arg\max_{\Theta_g} \log \mathrm{P}(\mathbb{X} | \Theta_g)
\end{aligned}
$$

- Other divergence measures can lead to similar results

Common Whole-Image Generation Methods

- Autoencoder (single-step: $\hat{\boldsymbol{x}} = g(\boldsymbol{c})$)
  - Pros: easy
  - Cons: but no creativity, blurry images
- Variational Autoencoder (single-step: $\hat{\boldsymbol{x}} = g(\boldsymbol{c})$)
  - Pros: creative
  - Cons: only maximizes a lower bound of $\mathrm{P}(\mathbb{X}|\Theta_g)$; blurry images
- Flow-based methods (multi-step: $\hat{\boldsymbol{x}} = g^{(T)}(\cdots g^{(2)}(g^{(1)}(\boldsymbol{c})))$)
  - Pros: maximizes $\mathrm{P}(\mathbb{X}|\Theta_g)$ directly
  - Cons: limited expressiveness of g for invertibility; slow training and inference
- GANs (single-step: $\hat{\boldsymbol{x}} = g(\boldsymbol{c})$)
  - Pros: good image quality (sharp and coherent)
  - Cons: difficult to train (convergence issue, mode collapse, vanishing gradients, etc.)
- Diffusion models (multi-step: $\hat{\boldsymbol{x}} = g^{(T)}(\cdots g^{(2)}(g^{(1)}(\boldsymbol{c})))$)
  - Pros: good image quality; efficient & stable to train, can be made conditional easily
  - Cons: slow inference

Outline

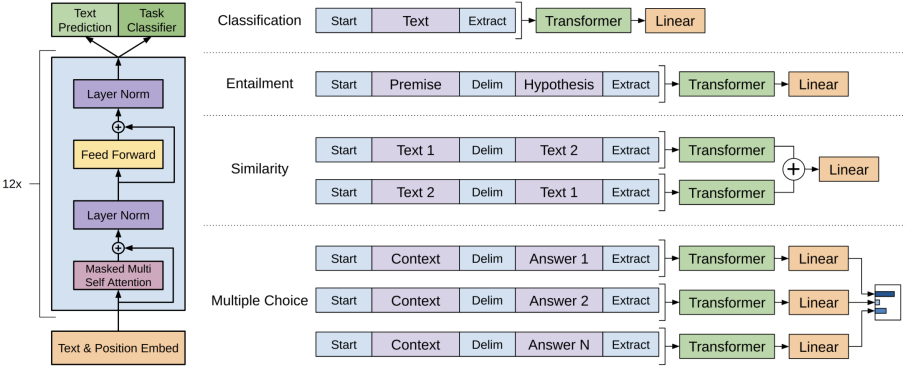
Evolutions

- 2018 GPTv1 [31]
  - Self-supervised pre-training
- 2019 GPTv2 [32]
  - ***Multitask*** pre-training
- 2020 GPTv3 [4]
  - ***Few-shot*** & ***in-context*** learning
- 2022 GPTv3.5 [29]
  - ***Alignment*** using (supervised) instruction tuning + reinforcement learning from human feedback (RLHF)
- 2023 GPT4: mixture of experts

GPTv1 [31]

- Aims at 2-step training process:
  1. Self-supervised pre-training on unlabeled data
     - To predict next word in a sentence (language model)
  2. Discriminative fine-tuning on labeled data in downstream tasks
     - Here, fine-tuning could also mean training a new model based on extracted features

Example Fine-tuning Tasks



Does Self-supervised Pre-training Help?

Table 5: Analysis of various model ablations on different tasks. Avg. score is a unweighted average of all the results. (*mc*= Mathews correlation, *acc*=Accuracy, *pc*=Pearson correlation)

Method	Avg. Score	CoLA (mc)	SST2 (acc)	MRPC (F1)	STSB (pc)	QQP (F1)	MNLI (acc)	QNLI (acc)	RTE (acc)
Transformer w/ aux LM (full)	74.7	45.4	91.3	82.3	82.0	**70.3**	**81.8**	**88.1**	**56.0**
Transformer w/o pre-training	59.9	18.9	84.0	79.4	30.9	65.5	75.7	71.2	53.8
Transformer w/o aux LM	**75.0**	**47.9**	**92.0**	**84.9**	**83.2**	69.8	81.1	86.9	54.4
LSTM w/ aux LM	69.1	30.3	90.5	83.2	71.8	68.1	73.7	81.1	54.6

GPTv2 [32]

- Many NLP tasks can be formulated as the problem of maximizing $\Pr(\text{output}|\text{input}, \text{task})$
  - Translation: $\Pr(\text{french text}|\text{en text}, \text{translation})$
  - Question answering: $\Pr(\text{answer}|\text{question}, \text{qa})$
  - Reading comprehension: $\Pr(\text{answer}|\text{document}, \text{question}, \text{reading})$
- GPTv3 [4]: ***few-shot*** & ***in-context*** learning
- GPTv3.5 [29]: ***alignment*** using (supervised) instruction tuning & reinforcement learning from human feedback (RLHF)
- GPT4: mixture of experts

GPTv3 [4]

- The model learns from few shots (examples), even ***in context***
  - Enables ***prompting*** techniques for downstream tasks
  - E.g.,few shots, chain of thought (CoT), or simply "Let's work this out step-by-step to ensure the answer is correct"

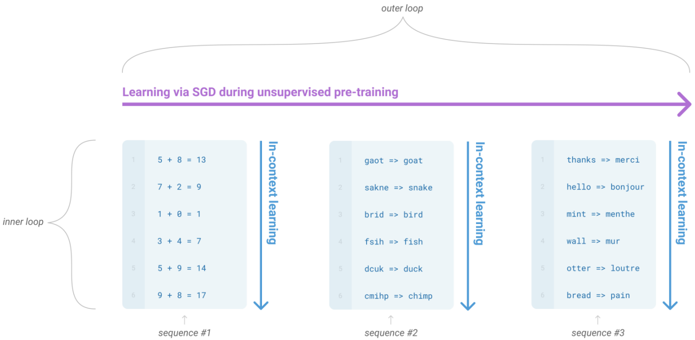
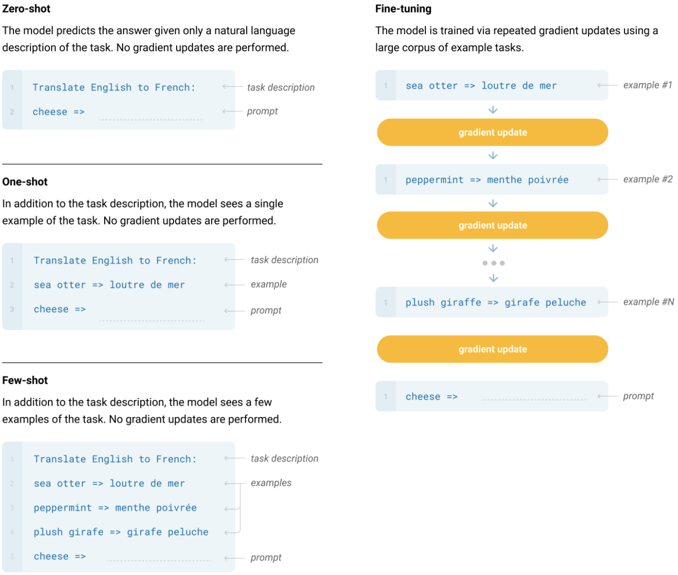


Figure 1.1: Language model meta-learning. During unsupervised pre-training, a language model develops a broad set of skills and pattern recognition abilities. It then uses these abilities at inference time to rapidly adapt to or recognize the desired task. We use the term "in-context learning" to describe the inner loop of this process, which occurs within the forward-pass upon each sequence. The sequences in this diagram are not intended to be representative of the data a model would see during pre-training, but are intended to show that there are sometimes repeated sub-tasks embedded within a single sequence.

Zero/Few Shot Prompting vs. Fine-tuning



Performance vs. Model Size

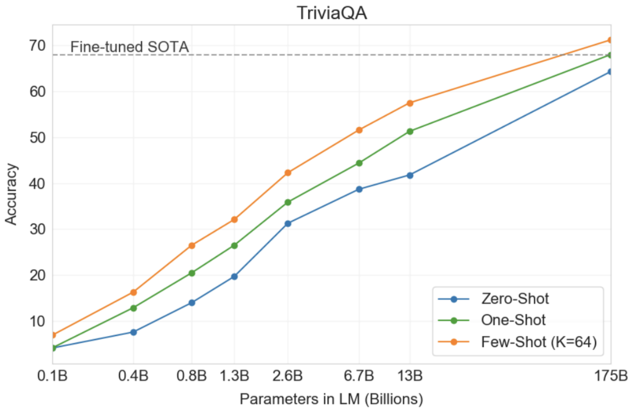
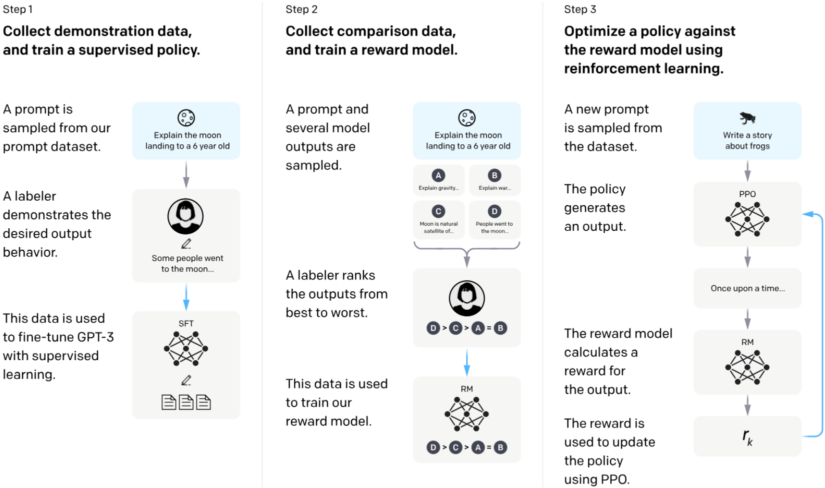


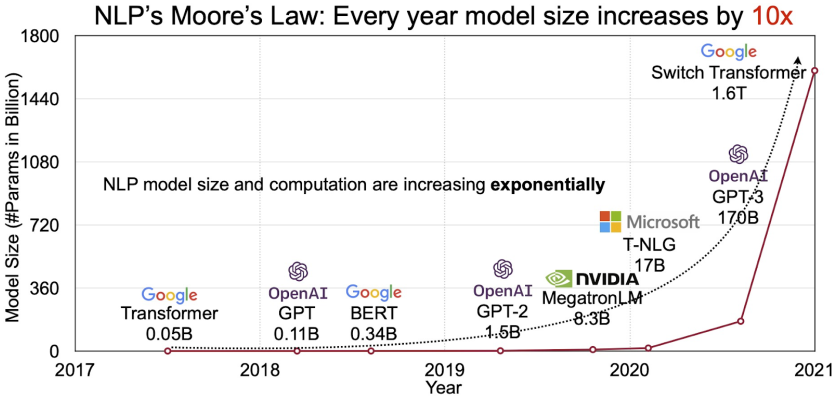
Figure 3.3: On TriviaQA GPT3's performance grows smoothly with model size, suggesting that language models continue to absorb knowledge as their capacity increases. One-shot and few-shot performance make significant gains over zero-shot behavior, matching and exceeding the performance of the SOTA fine-tuned open-domain model, RAG [LPP+20]

GPTv3.5 [29]

- From GPT to "ChatGPT" through ***alignment***
  - Supervised (multi-task) instruction tuning
  - Reinforcement learning from human feedback (RLHF)



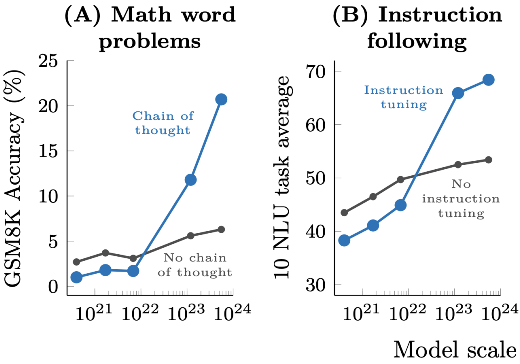
Sizes of Large Language Models (LLMs)



- Training costs [42]:
  - 110M params: \$2.5k–\$50k
  - 340M params: \$10k–\$200k
  - 1.5B param: \$80k–\$1.6m

Size Does Matter!

- Emerging abilities of LLMs [48]



- A balance: 70B parameters + 1.4T training tokens [11]

GPT Variants

- Low-rank adaptation (LoRA) [12]: to efficiently fine-tune LLMs
- WebGPT [28]: GPT that can search the web
- Retrieval-augmented generation (RAG) [21]: GPT to query external knowledge (vector) base
- GPTs that can reflect on their answers [2, 27]

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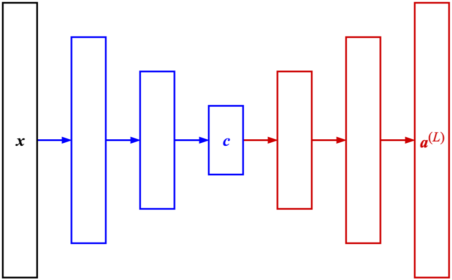
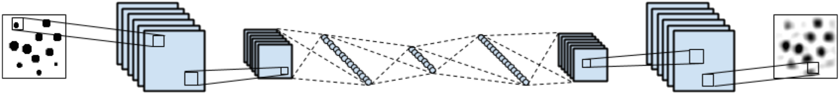
Autoencoders (AE)

- ***Encoder***: to learn a low dimensional representation $\mathbf{c}$ (called *code*) of input $\mathbf{x}$
- ***Decoder***: to reconstruct $\mathbf{x}$ from $\mathbf{c}$
- Objective: $\arg\max_{\Theta} \log \mathrm{P}(\mathbb{X} \,|\, \Theta) = \arg\max_{\Theta} \sum_i \log \mathrm{P}(\boldsymbol{x}^{(i)} \,|\, \Theta)$
- Assuming that $\mathbf{x} \sim \mathcal{N}(\mu, \cdot)$, we have linear output units $\boldsymbol{a}^{(L)} = \boldsymbol{z}^{(L)} = \hat{\mu}$
  - $\log \mathrm{P}(\boldsymbol{x}^{(i)} \,|\, \Theta) \propto -\|\boldsymbol{x}^{(i)} - \boldsymbol{a}^{(i,L)}\|^2$
  - $\arg\max_{\Theta} \sum_i \log \mathrm{P}(\boldsymbol{x}^{(i)} \,|\, \Theta) = \arg\min_{\Theta} \sum_i \|\boldsymbol{x}^{(i)} - \boldsymbol{a}^{(i,L)}\|^2$ (minimizing reconstruct error)



Convolutional Autoencoders

- Convolution + deconvolution layers:



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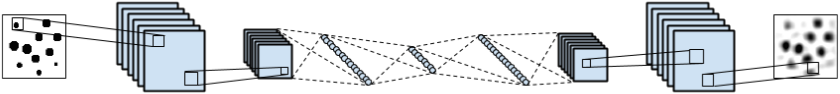

- Decoder is a simplified DeconvNet [49] trained from scratch:

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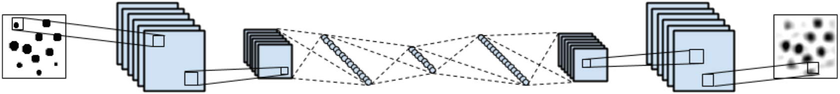

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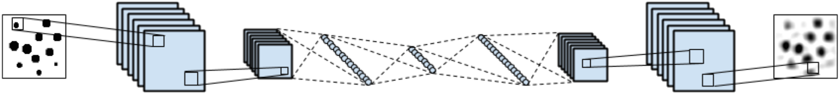
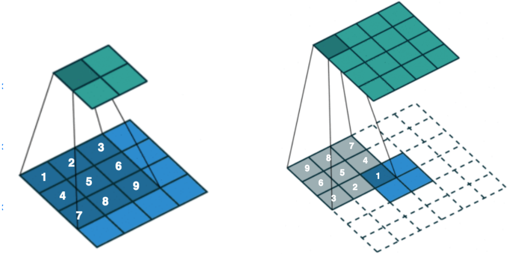
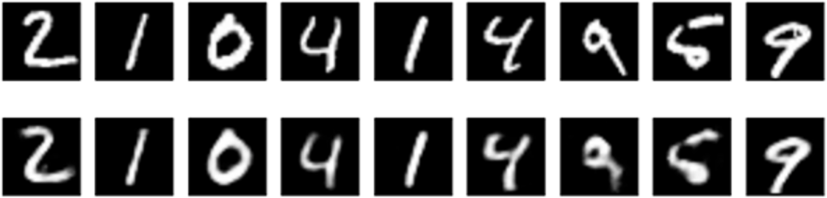


- Decoder is a simplified DeconvNet [49] trained from scratch:
  - Uppooling → upsampling (no need to remember max positions)
  - Deconvolution → convolution



Codes & Reconstructed $\mathbf{x}$

- A 32-bit code can roughly represents a 32×32 (1024 dimensional) MNIST image



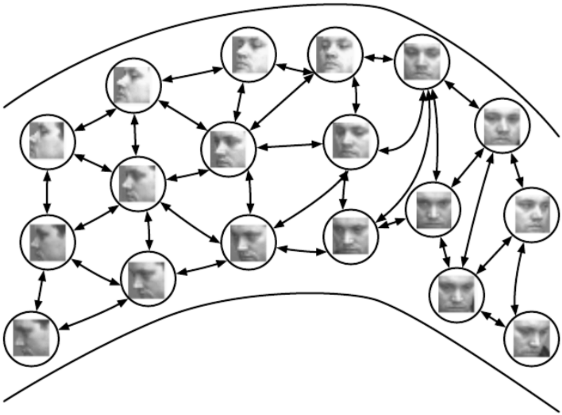
Outline

Manifolds I

- In many applications, data concentrate around one or more low-dimensional ***manifolds***

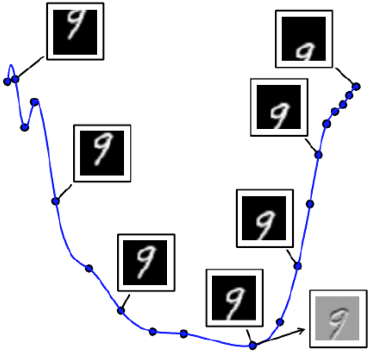
Manifolds I

- In many applications, data concentrate around one or more low-dimensional ***manifolds***
- A manifold is a topological space that are ***linear locally***



Manifolds II

- For each point $\boldsymbol{x}$ on a manifold, we have its ***tangent space*** spanned by ***tangent vectors***
  - Local directions specify how one can change $\boldsymbol{x}$ infinitesimally while staying on the manifold



Learning Manifolds I

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- Contractive autoencoder [35]: regularizes the code $\mathbf{c}$ such that it is invariant to local changes of $\mathbf{x}$:

$$\Omega(\mathbf{c}) = \sum_i \left\| \frac{\partial \boldsymbol{c}^{(i)}}{\partial \boldsymbol{x}^{(i)}} \right\|_F^2$$

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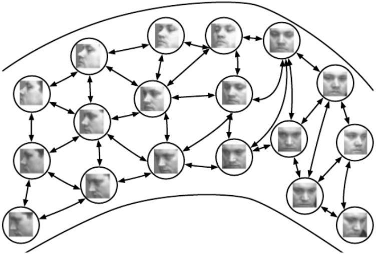
  - $\partial \boldsymbol{c}^{(i)} / \partial \boldsymbol{x}^{(i)}$ is a Jacobian matrix
- Hence, $\mathbf{c}$ represents only the variations needed to reconstruct $\mathbf{x}$
  - I.e., $\mathbf{c}$ changes most along tangent vectors



Learning Manifolds II

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Learning Manifolds II

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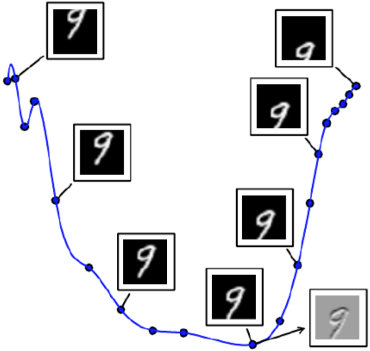
  - Encoder: to encode $\mathbf{x}$ ***with*** random noises
  - Decoder: to reconstruct $\mathbf{x}$ ***without*** noises

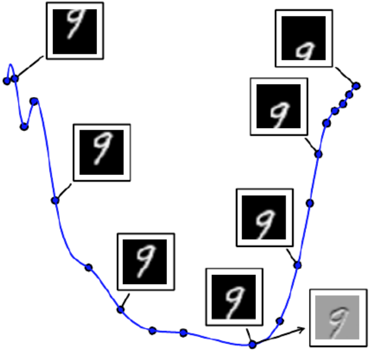
Getting Tangent Vectors I

- The code $\mathbf{c}$ represents a coordinate on a low dimensional manifold
  - E.g., the blue line
- How to get the tangent vectors of a given $\boldsymbol{c}$?



Getting Tangent Vectors II

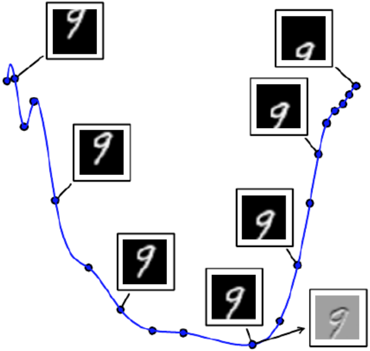
- Recall: directions in the input space that ***changes c most*** should be tangent vectors



Getting Tangent Vectors II

- Recall: directions in the input space that ***changes c most*** should be tangent vectors

- Given a point $\boldsymbol{x}$, let $\boldsymbol{c}$ be the code of $\boldsymbol{x}$ and $\boldsymbol{J}(\boldsymbol{x}) = \frac{\partial \boldsymbol{c}}{\partial \boldsymbol{x}}$ be the Jacobian matrix of $\boldsymbol{c}$ at $\boldsymbol{x}$



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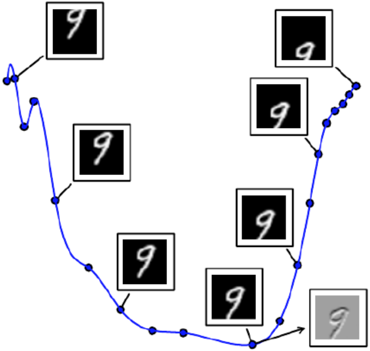

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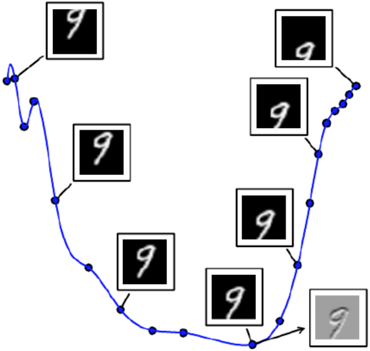
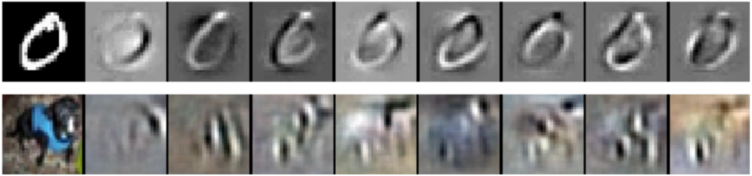
1. Decompose $\boldsymbol{J}(\boldsymbol{x})$ using SVD such that $\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^\top$
2. Let tangent vectors be ***rows of $\boldsymbol{V}$ corresponding to the largest singular values in $\boldsymbol{D}$***



Getting Tangent Vectors III

- In practice, $\boldsymbol{J}(\boldsymbol{x})$ usually has few large singular values
- Tangent vectors found by contractive/denoising autoencoders:



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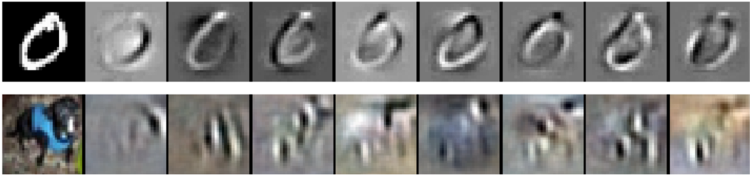
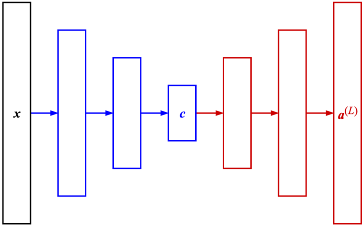


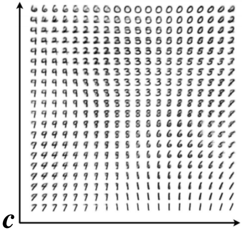
- Can be used by Tangent Prop [43]:
- Let $\{\boldsymbol{v}^{(i,j)}\}_j$ be tangent vectors of each example $\boldsymbol{x}^{(i)}$
- Trains an NN classifier f with cost penalty: $\Omega[f] = \sum_{i,j} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^{(i)})^\top \boldsymbol{v}^{(i,j)}$
  - Points in the same manifold share the same label

Outline

Problems of Autoencoder I

- Ideally, the decoder of an autoencoder can be used to generate images even with ***synthetic codes***





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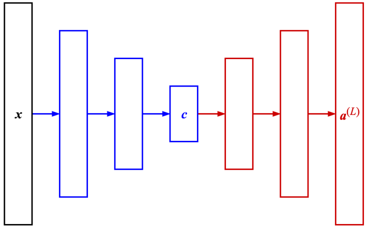
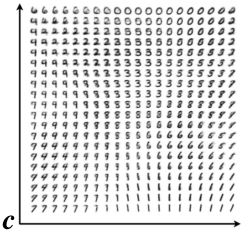




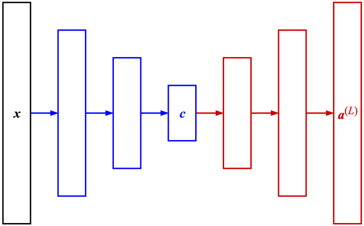
- In reality, the learnt $\mathbf{c}$ in code space has many "holes" that fail to map to images
  - More complex image patterns
  - Training data are never enough

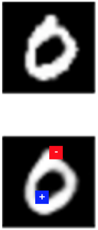
Problems of Autoencoder II

- Blurry images: the objective

$$\arg\max_{\Theta} \sum_i \log \mathrm{P}(\boldsymbol{x}^{(i)} \mid \Theta) = \arg\min_{\Theta} \sum_i \|\boldsymbol{x}^{(i)} - \boldsymbol{a}^{(i,L)}\|^2$$

does not panelize Gaussian pixel noises in $\boldsymbol{a}^{(i,L)}$





Variational Autoencoders (VAE) [15]

- Encoder $f(\cdot;\Theta_f)$: maps each sample of $\mathbf{x}$ (i.e., $\boldsymbol{x}^{(i)} \in \mathbb{X}$) to an ***axis-aligned normal distribution*** $\mathcal{N}(\mu, \sigma)$
  - Each code dimension is independent with each other
  - $f(\boldsymbol{x}) = (\mu, \sigma)$
- Decoder $g(\cdot;\Theta_g)$: same as that of AE
- How to minimize the objective $\arg\max_{\Theta_f,\Theta_g} \log \mathrm{P}(\mathbb{X} \mid \Theta_f, \Theta_g))$?

VAE Objective

- Objective:
  $\arg\max_{\Theta_f,\Theta_g} \log \mathrm{P}(\mathbb{X} \mid \Theta_f, \Theta_g) = \arg\max_{\Theta_f,\Theta_g} \sum_i \log \mathrm{P}(\boldsymbol{x}^{(i)} \mid \Theta_f, \Theta_g)$
- Considering $\log \mathrm{P}(\boldsymbol{x})$ for any sample $\boldsymbol{x}$, we have

$$
\begin{aligned}
\log \mathrm{P}(\boldsymbol{x}) &= \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \mathrm{P}(\boldsymbol{x})\, d\boldsymbol{c} \quad \text{// Q can be any distribution} \\
&= \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{c},\boldsymbol{x})}{\mathrm{P}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} = \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{c},\boldsymbol{x})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})} \frac{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})}{\mathrm{P}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} \\
&= \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{c},\boldsymbol{x})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} + \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})}{\mathrm{P}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} \\
&= \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{c},\boldsymbol{x})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} + \mathrm{D}_{\mathrm{KL}} \left(\mathrm{Q}(\mathbf{c}|\boldsymbol{x}) \| \mathrm{P}(\mathbf{c}|\boldsymbol{x}) \right) \\
&\geq \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{c},\boldsymbol{x})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c} \quad \text{// lower bound} \\
&= \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \left(\frac{\mathrm{P}(\boldsymbol{x}|\boldsymbol{c})\mathrm{P}(\boldsymbol{c})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})} \right) d\boldsymbol{c}
\end{aligned}
$$

- VAE lets $\mathrm{Q}(\cdot|\boldsymbol{x}) = \mathcal{N}(f(\boldsymbol{x};\Theta_f))$ and $\mathrm{P}(\cdot|\boldsymbol{c}) = \mathcal{N}(g(\boldsymbol{c};\Theta_g))$
  - So $\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) = \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x},\Theta_f)$ and $\mathrm{P}(\boldsymbol{x}|\boldsymbol{c}) = \mathrm{P}(\boldsymbol{x}|\boldsymbol{c},\Theta_g)$
- New objective: finds Θ_f and Θ_g that maximize the lower bound
  - Not necessarily maximize $\log \mathrm{P}(\boldsymbol{x} \mid \Theta_f, \Theta_g)$

Maximizing Lower Bound

$$
\begin{aligned}
&\int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log\left(\frac{\mathrm{P}(\boldsymbol{x}|\boldsymbol{c})\mathrm{P}(\boldsymbol{c})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})}\right) d\boldsymbol{c} \\
&\quad = \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x},\Theta_f) \log\left(\frac{\mathrm{P}(\boldsymbol{x}|\boldsymbol{c},\Theta_g)\mathrm{P}(\boldsymbol{c})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x},\Theta_f)}\right) d\boldsymbol{c} \\
&\quad = \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x},\Theta_f) \log\left(\frac{\mathrm{P}(\boldsymbol{c})}{Q(\boldsymbol{c}|\boldsymbol{x},\Theta_f)}\right) d\boldsymbol{c} + \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x},\Theta_f) \log \mathrm{P}(\boldsymbol{x}|\boldsymbol{c},\Theta_g) d\boldsymbol{c} \\
&\quad = -\mathrm{D}_{\mathrm{KL}}\left(\mathrm{Q}(\mathbf{c}|\boldsymbol{x},\Theta_f)\|\mathrm{P}(\mathbf{c})\right) + \mathrm{E}_{(\mathbf{c}|\boldsymbol{x},\Theta_f)\sim\mathrm{Q}}\left[\log \mathrm{P}(\boldsymbol{x}|\mathbf{c},\Theta_g)\right]
\end{aligned}
$$

- For $\mathrm{P}(\mathbf{c}) = \mathcal{N}(\mathbf{0},\boldsymbol{I})$:
- To minimize the first term, the encoder $f(\boldsymbol{x};\Theta_f) = (\mu,\sigma)$ has a loss term [15]

$$\exp(\sigma) - (\mathbf{1}+\sigma) + \|\mu\|^2$$

- To maximize the second term, the decoder
  1. Samples $\boldsymbol{c}$ from $\mathcal{N}(\mu,\sigma)$ to get $g(\boldsymbol{c};\Theta_g)$, the mean of output $\mathcal{N}$
  2. Minimizes a loss term $\|\boldsymbol{x}-\boldsymbol{a}^{(L)}\|^2$ as in AE

Outline

1. Unsupervised Learning
   - Text Models
   - Image Models
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3. Autoencoders (AE)
   - Manifold Learning*
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Problems of VAE

- Only maximize a lower bound of the likelihood $\mathrm{P}(\mathbb{X}|\Theta_f, \Theta_g)$
  - Θ_f and Θ_g are encoder and decoder weights, respectively
- Still blurry images
  - The decoder's loss is the same with that of AE

Flow-based Models

- Idea: let the decoder $g(\cdot;\Theta_g)$ be a ***deterministic invertible*** function
  - Given $\mathbf{c} \sim \mathcal{N}(\mathbf{0},\boldsymbol{I})$, we have $\mathbf{x} = g(\mathbf{c};\Theta_g)$ of complex distribution
  - Conversely, given $\mathbf{x}$, we have $\mathbf{c} = g^{-1}(\mathbf{x};\Theta_g)$
- The likelihood can be maximize directly:

$$\begin{aligned}
&\arg\max_g \log \mathrm{P}_g(\mathbb{X}) \\
&\quad = \arg\max_g \textstyle\sum_i \log \mathrm{P}_{\mathbf{x}}(g(\boldsymbol{c}^{(i)})) \\
&\quad = \arg\max_g \textstyle\sum_i \log \left[\mathrm{P}_{\mathbf{c}}(g^{-1}(\boldsymbol{x}^{(i)}))\,|\det\left(\boldsymbol{J}(g^{-1})(\boldsymbol{x}^{(i)})\right)|\right] \\
&\quad = \arg\max_g \textstyle\sum_i \log \mathrm{P}_{\mathbf{c}}(g^{-1}(\boldsymbol{x}^{(i)})) + \log|\det\left(\boldsymbol{J}(g^{-1})(\boldsymbol{x}^{(i)})\right)|
\end{aligned}$$

- First term: finds g (Θ_g) that maps all $\boldsymbol{x}^{(i)}$ to 0
- Second term: prevents g (Θ_g) from mapping all $\boldsymbol{x}^{(i)}$ to 0
  - $\log|\det(\boldsymbol{O})| = -\inf$

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- Second term: prevents g (Θ_g) from mapping all $\boldsymbol{x}^{(i)}$ to 0
  - $\log|\det(\boldsymbol{O})| = -\inf$
- But how to ensure the followings during training?
  - g is invertible
  - $\det\left(\boldsymbol{J}(g^{-1})(\cdot)\right)$ can be easily computed

Ensuring Invertibility

- Glow [16]: make g^{-1} an 1×1 convolution layer
  - $\mathbf{x}_{i,j,:} = \begin{bmatrix} \mathrm{x}_{i,j,1} \\ \mathrm{x}_{i,j,2} \\ \mathrm{x}_{i,j,3} \end{bmatrix}, \quad g^{-1} = \boldsymbol{W}_{3\times 3},$
$$g^{-1}(\mathbf{x}_{i,j,:}) = \boldsymbol{W}_{3\times 3} \begin{bmatrix} \mathrm{x}_{i,j,1} \\ \mathrm{x}_{i,j,2} \\ \mathrm{x}_{i,j,3} \end{bmatrix} = \begin{bmatrix} \mathrm{c}_{i,j,1} \\ \mathrm{c}_{i,j,2} \\ \mathrm{c}_{i,j,3} \end{bmatrix}$$
- At training time, initialize $\boldsymbol{W}_{3\times 3}$ as an invertible matrix
  - $g^{-1} = \boldsymbol{W}_{3\times 3}$ is likely to be invertible after SGD updates
  - Determinant is easy to compute: $\det\left(\boldsymbol{J}(g^{-1})(\boldsymbol{x}^{(i)})\right) = \det(\boldsymbol{W}_{3\times 3})^{W\times H}$
- At inference time, use $g = \boldsymbol{W}_{3\times 3}^{-1}$ to generate images

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- At inference time, use $g = \boldsymbol{W}_{3\times 3}^{-1}$ to generate images
- Problem: g has limited expressiveness

Step-wise Generation

- Cascade multiple invertible g to have a more complex one:

$$\mathbf{x} = g^{(T)}(\cdots g^{(2)}(g^{(1)}(\mathbf{c})))$$

Step-wise Generation

- Cascade multiple invertible g to have a more complex one:

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- Result: sharp images

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Problems of Flow-based Models

- Limited model expressiveness
- Slow training and inference
    - #steps can be large

Denoising Diffusion Probabilistic Models (DDPM) [10]

- Borrow some good ideas from previous works
  - Probabilistic formulation of VAE that models encoder in the objective
  - Step-wise encoding/decoding in generative flows
- But, unlike flows, the encoding steps
  - Are ***predefined***; no parameter to learn
  - Can be simplified to ***one encoding step***

Encoding

- Predefined encoding functions $f^{(t)}(\cdot;\beta^{(t)})$, $t=1,\cdots,T$:
  - $\beta^{(t)}$, $\forall t$, are hyperparameters; no learning needed
- Let each sample $\boldsymbol{x}=\boldsymbol{x}^{(0)}$
- $\mathbf{x}^{(1)}=f^{(1)}(\boldsymbol{x}^{(0)};\beta^{(1)})=\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)}+\sqrt{\beta^{(1)}}\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})$
  - So, $(\mathbf{x}^{(1)}|\mathbf{x}^{(0)}=\boldsymbol{x}^{(0)})\sim\mathcal{N}(\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)},\beta^{(1)}\boldsymbol{I})$

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  - So, $(\mathbf{x}^{(1)}|\mathbf{x}^{(0)} = \boldsymbol{x}^{(0)}) \sim \mathcal{N}(\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)}, \beta^{(1)}\boldsymbol{I})$
- $$\begin{aligned} \mathbf{x}^{(2)} &= f^{(2)}(\boldsymbol{x}^{(1)};\beta^{(t)}) = \sqrt{1-\beta^{(2)}}\boldsymbol{x}^{(1)} + \sqrt{\beta^{(2)}}\varepsilon \\ &= \sqrt{1-\beta^{(2)}}\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)} + \sqrt{1-(1-\beta^{(2)})(1-\beta^{(1)})}\varepsilon \\ &= \sqrt{\alpha^{(2)}\alpha^{(1)}}\boldsymbol{x}^{(0)} + \sqrt{1-\alpha^{(2)}\alpha^{(1)}}\varepsilon \end{aligned}$$
  - $\sqrt{1-\beta^{(1)}}\sqrt{\beta^{(2)}}\varepsilon + \sqrt{\beta^{(2)}}\varepsilon \sim \mathcal{N}(\mathbf{0},((1-\beta^{(1)})\beta^{(2)}+\beta^{(2)})\boldsymbol{I})$
  - Let $\alpha^{(t)} = 1-\beta^{(t)}$ (derived hyperparameter)
  - Only one ε is added

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  - So, $(\mathbf{x}^{(1)}|\mathbf{x}^{(0)}=\boldsymbol{x}^{(0)})\sim\mathcal{N}(\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)},\beta^{(1)}\boldsymbol{I})$
- $$\begin{aligned}\mathbf{x}^{(2)} &= f^{(2)}(\boldsymbol{x}^{(1)};\beta^{(t)})=\sqrt{1-\beta^{(2)}}\boldsymbol{x}^{(1)}+\sqrt{\beta^{(2)}}\boldsymbol{\varepsilon}\\ &= \sqrt{1-\beta^{(2)}}\sqrt{1-\beta^{(1)}}\boldsymbol{x}^{(0)}+\sqrt{1-(1-\beta^{(2)})(1-\beta^{(1)})}\boldsymbol{\varepsilon}\\ &= \sqrt{\alpha^{(2)}\alpha^{(1)}}\boldsymbol{x}^{(0)}+\sqrt{1-\alpha^{(2)}\alpha^{(1)}}\boldsymbol{\varepsilon}\end{aligned}$$
  - $\sqrt{1-\beta^{(1)}}\sqrt{\beta^{(2)}}\boldsymbol{\varepsilon}+\sqrt{\beta^{(2)}}\boldsymbol{\varepsilon}\sim\mathcal{N}(\mathbf{0},((1-\beta^{(1)})\beta^{(2)}+\beta^{(2)})\boldsymbol{I})$
  - Let $\alpha^{(t)}=1-\beta^{(t)}$ (derived hyperparameter)
  - Only one $\boldsymbol{\varepsilon}$ is added
- $\mathbf{x}^{(t)}=\sqrt{\bar{\alpha}^{(t)}}\boldsymbol{x}^{(t-1)}+\sqrt{1-\bar{\alpha}^{(t)}}\boldsymbol{\varepsilon}$
  - Let $\bar{\alpha}^{(t)}=\alpha^{(t)}\alpha^{(t-1)}\cdots\alpha^{(1)}$ (derived hyperparameter)

Objective

- As VAE, DDPM maximizes a lower bound of $\mathrm{P}(\mathbb{X})$
- VAE: for each $\boldsymbol{x}$, where $\mathrm{P}(\boldsymbol{x}) = \int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log \mathrm{P}(\boldsymbol{x})\, d\boldsymbol{c}$, maximize:

$$\int_{\boldsymbol{c}} \mathrm{Q}(\boldsymbol{c}|\boldsymbol{x}) \log\left(\frac{\mathrm{P}(\boldsymbol{x},\boldsymbol{c})}{\mathrm{Q}(\boldsymbol{c}|\boldsymbol{x})}\right) d\boldsymbol{c} = \mathrm{E}_{\mathbf{c}|\boldsymbol{x}\sim\mathrm{Q}}\left[\log\left(\frac{\mathrm{P}(\boldsymbol{x},\mathbf{c})}{\mathrm{Q}(\mathbf{c}|\boldsymbol{x})}\right)\right] \leq \mathrm{P}(\boldsymbol{x})$$

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- DDPM: for each $\boldsymbol{x}$ where $\mathrm{P}(\boldsymbol{x}^{(0)}) = \int_{\boldsymbol{x}^{(1)},\cdots,\boldsymbol{x}^{(T)}} \mathrm{Q}(\boldsymbol{x}^{(1)},\cdots,\boldsymbol{x}^{(T)}|\boldsymbol{x}^{(0)}) \log \mathrm{P}(\boldsymbol{x}^{(0)})\, d\boldsymbol{x}^{(1)}\cdots d\boldsymbol{x}^{(T)}$, maximize:

$$\mathrm{E}_{(\mathbf{x}^{(1)},\cdots,\mathbf{x}^{(T)}|\boldsymbol{x}^{(0)})\sim\mathrm{Q}}\left[\log\left(\frac{\mathrm{P}(\boldsymbol{x}^{(0)},\mathbf{x}^{(1)},\cdots,\mathbf{x}^{(T)})}{\mathrm{Q}(\mathbf{x}^{(1)},\cdots,\mathbf{x}^{(T)}|\boldsymbol{x}^{(0)})}\right)\right],$$

  which can be simplified to [23]:

$$-\mathrm{D}_{\mathrm{KL}}\left(\mathrm{Q}(\mathbf{x}^{(T)}|\boldsymbol{x}^{(0)})\|\mathrm{P}(\mathbf{x}^{(T)})\right) + \mathrm{E}_{\mathbf{x}^{(1)}|\boldsymbol{x}^{(0)}\sim\mathrm{Q}}\left[\log \mathrm{P}(\boldsymbol{x}^{(0)}|\mathbf{x}^{(1)})\right] + \\ -\sum_{t=2}^{T} \mathrm{E}_{\mathbf{x}^{(t)}|\boldsymbol{x}^{(0)}\sim\mathrm{Q}}\left[\mathrm{D}_{\mathrm{KL}}\left(\mathrm{Q}(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)},\boldsymbol{x}^{(0)})\|\mathrm{P}(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)})\right)\right]$$

  - First term controlled by encoding process (predefined)
  - Second & third term controlled by denoising process (learnable)

Denoising I

- For simplicity, we focus on maximizing the third term:

$$-\sum_{t=2}^{T} \mathrm{E}_{\mathbf{x}^{(t)}|\boldsymbol{x}^{(0)}\sim \mathrm{Q}}\left[\mathrm{D}_{\mathrm{KL}}\left(\mathrm{Q}(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)},\boldsymbol{x}^{(0)})\|\mathrm{P}(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)})\right)\right]$$

- Goal: for each observed $\boldsymbol{x}^{(t)}$, minimize

$$\mathrm{D}_{\mathrm{KL}}\left(\mathrm{Q}(\mathbf{x}^{(t-1)}|\color{red}{\boldsymbol{x}^{(t)}},\boldsymbol{x}^{(0)})\|\mathrm{P}(\mathbf{x}^{(t-1)}|\color{red}{\boldsymbol{x}^{(t)}})\right)$$

- Note that

$$\begin{aligned}
\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)},\boldsymbol{x}^{(0)}) &= \frac{\mathrm{Q}(\mathbf{x}^{(t-1)},\boldsymbol{x}^{(t)},\boldsymbol{x}^{(0)})}{\mathrm{Q}(\boldsymbol{x}^{(t)},\boldsymbol{x}^{(0)})} \\
&= \frac{\mathrm{Q}(\boldsymbol{x}^{(t)}|\mathbf{x}^{(t-1)})\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(0)})\mathrm{Q}(\boldsymbol{x}^{(0)})}{\mathrm{Q}(\boldsymbol{x}^{(t)}|\boldsymbol{x}^{(0)})\mathrm{Q}(\boldsymbol{x}^{(0)})} \\
&= \frac{\mathrm{Q}(\boldsymbol{x}^{(t)}|\mathbf{x}^{(t-1)})\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(0)})}{\mathrm{Q}(\boldsymbol{x}^{(t)}|\boldsymbol{x}^{(0)})}
\end{aligned}$$

- Since $\mathrm{Q}(\boldsymbol{x}^{(t)}|\mathbf{x}^{(t-1)})$ & $\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(0)})$ are Gaussian, we have [23]:
$\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)},\boldsymbol{x}^{(0)}) = \mathcal{N}\left(\frac{\sqrt{\alpha^{(t)}}(1-\alpha^{(t-1)})\boldsymbol{x}^{(t)}+\sqrt{\bar{\alpha}^{(t-1)}}\beta^{(t)}\boldsymbol{x}^{(0)}}{1-\bar{\alpha}^{(t)}}, \frac{1-\bar{\alpha}^{(t-1)}}{1-\bar{\alpha}^{(t)}}\beta^{(t)}\boldsymbol{I}\right)$

Denoising II

- Goal: for each observed $\boldsymbol{x}^{(t)}$, minimize

$$\mathrm{D_{KL}}\left(\mathrm{Q}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)},\boldsymbol{x}^{(0)})\|\mathrm{P}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)})\right),$$

  where $\mathrm{Q}(\cdots) = \mathscr{N}\left(\frac{\sqrt{\alpha^{(t)}}(1-\alpha^{(t-1)})\boldsymbol{x}^{(t)}+\sqrt{\bar{\alpha}^{(t-1)}}\beta^{(t)}\boldsymbol{x}^{(0)}}{1-\bar{\alpha}^{(t)}},\cdots\right)$ is ***fixed***
- DDPM finds Θ that move the mean of $\mathrm{P}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)},\Theta)$ (also Gaussian) toward $\mathrm{Q}(\cdots)$'s mean:

$$\frac{\sqrt{\alpha^{(t)}}(1-\alpha^{(t-1)})\boldsymbol{x}^{(t)}+\sqrt{\bar{\alpha}^{(t-1)}}\beta^{(t)}\boldsymbol{x}^{(0)}}{1-\bar{\alpha}^{(t)}}$$

Noise Predictor

- Θ moves $\mathrm{P}(\mathbf{x}^{(t-1)}|\boldsymbol{x}^{(t)},\Theta)$'s mean toward

$$
\begin{aligned}
&\frac{\sqrt{\alpha^{(t)}}(1-\alpha^{(t-1)})\boldsymbol{x}^{(t)}+\sqrt{\bar{\alpha}^{(t-1)}}\beta^{(t)}\boldsymbol{x}^{(0)}}{1-\bar{\alpha}^{(t)}} \\
&= \frac{\sqrt{\alpha^{(t)}}(1-\alpha^{(t-1)})\boldsymbol{x}^{(t)}+\sqrt{\bar{\alpha}^{(t-1)}}\beta^{(t)}\frac{\boldsymbol{x}^{(t)}-\sqrt{1-\bar{\alpha}^{(t)}}\varepsilon}{\sqrt{\bar{\alpha}^{(t)}}}}{1-\bar{\alpha}^{(t)}} \\
&= \frac{1}{\sqrt{\alpha^{(t)}}}\left(\boldsymbol{x}^{(t)}-\frac{1-\alpha^{(t)}}{\sqrt{1-\bar{\alpha}^{(t)}}}\varepsilon\right)
\end{aligned}
$$

- What's its corresponding network?

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- What's its corresponding network?
- By definition: let Θ parametrize a network outputting $\boldsymbol{x}^{(t-1)}$ given $\boldsymbol{x}^{(t)}$
  - But the input $\boldsymbol{x}^{(t)}$ also resides in the output target
- DDPM: let Θ parametrize a ***noise predictor*** outputting ε given $\boldsymbol{x}^{(t)}$
  - Objective: $\arg\min_{\Theta}\|\varepsilon-e(\boldsymbol{x}^{(t)},t;\Theta)\|^2$
  - Of U-Net [37] architecture
  - Shared between all t

Training & Inference Algorithms

- One-step encoding during training time
- Muti-step inference (sampling), with each intermediate decoding step t, $t > 1$, comes with extra noise $\sigma^{(t)}z$
  - Similar to output token sampling in GPT
  - Improves performance empirically

Algorithm 1 Training

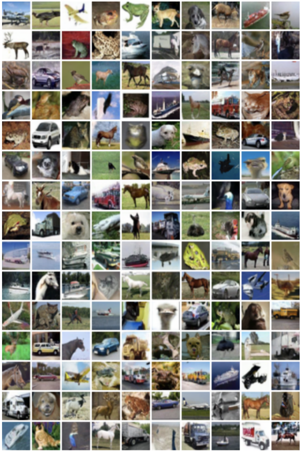
repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

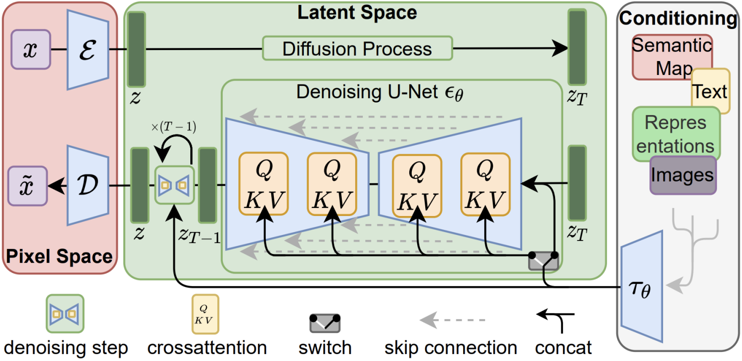
Results

- Sharp and coherent



Conditioning & Scaling

- Stable Diffusion [36]: separately train 3 networks
  - Text/condition embedding: only needs text data
  - Diffusion: needs paired (text-image) data but works at ***latent*** (low dimensional) space
  - Image encoder/decoder: only needs image data
- Text embedding as extra input for denoising net
- Other models like DALL-E [33] also use similar strategies



Results

Text-to-Image Synthesis on LAION. 1.45B Model.

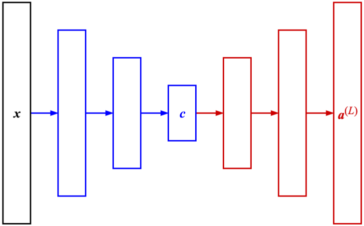
'A street sign that reads "Latent Diffusion" '	'A zombie in the style of Picasso'	'An image of an animal half mouse half octopus'	'An illustration of a slightly conscious neural network'	'A painting of a squirrel eating a burger'	'A watercolor painting of a chair that looks like an octopus'	'A shirt with the inscription: "I love generative models!" '

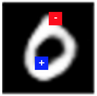
- Even the smallest text-image training set (LAION [41, 40]) has >400M samples!
  - MS COCO [22] "only" has 328K images

Outline

Why Do AE and VAE Give Blurry Images?

- Objective $\arg\max_{\Theta} \log \mathrm{P}(\mathbb{X}|\Theta) = \arg\min_{\Theta} \sum_n \|\boldsymbol{x}^{(n)} - \boldsymbol{a}^{(n,L)}\|^2$ does not panelize Gaussian pixel noises in $\boldsymbol{a}^{(i,L)}$
  - Root cause: assumption that $\mathbf{x} \sim \mathcal{N}$





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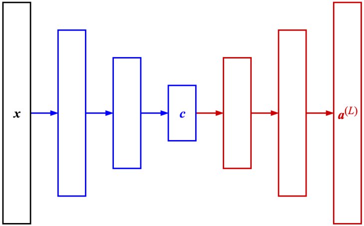

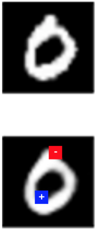

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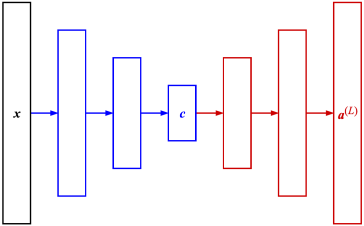

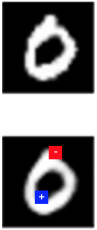

- Fix 1: maximizing the likelihood $\mathrm{P}(\mathbb{X}|\Theta)$ without assuming $\mathbf{x} \sim \mathcal{N}$
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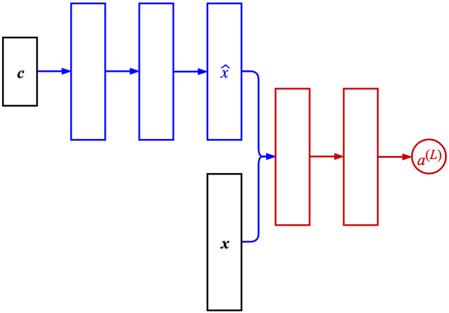
- Fix 2: maximizing the chance that $a^{(L)}$ ***is a true image from another NN point of view***

Outline

Network Design

- ***Generative adversarial networks*** (***GAN***) [8] consist of:



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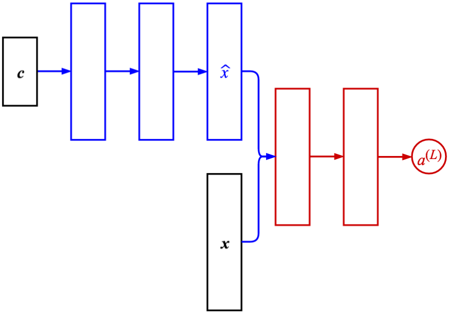

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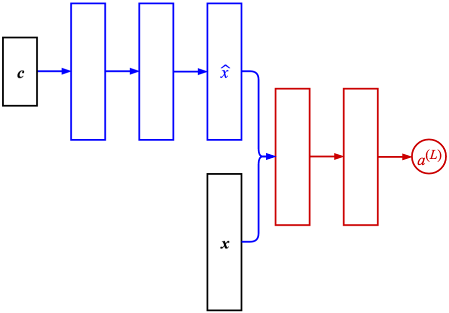
  - Weights for $\boldsymbol{x}$ and $\hat{\boldsymbol{x}}$ are tied
  - A binary classifier with Sigmoid output unit $a^{(L)} = \hat{\rho}$ for $\mathrm{P}(\mathrm{y} = \text{true point} \,|\, \mathbf{x}) \sim \mathrm{Bernoulli}(\rho)$



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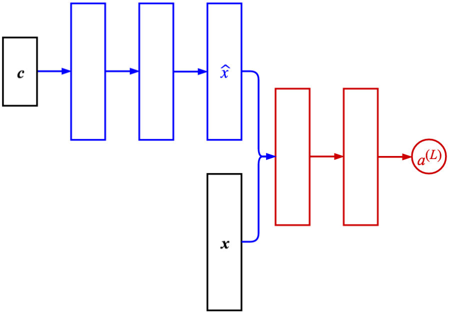
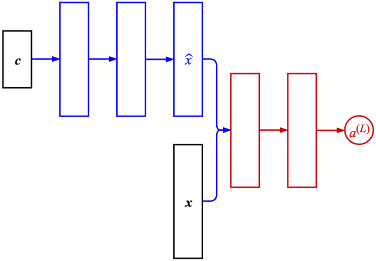
- Goal: to train a g that tricks f into believing $g(\boldsymbol{c})$ is real



Cost Function

- Given N real training points and N generated points:

$$\arg\min_{\Theta_g}\max_{\Theta_f}\log\mathrm{P}(\mathbb{X}\,|\,\Theta_g,\Theta_f)$$
$$=\arg\min_{\Theta_g}\max_{\Theta_f}\sum_n\log f(\boldsymbol{x}^{(n)})+\sum_m\log(1-f(g(\boldsymbol{c}^{(m)})))$$



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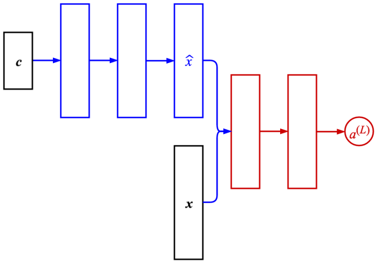
\end{aligned}
$$

- Recall that f maximizes the log likelihood
$\log \mathrm{P}(\mathbb{X}\,|\,\Theta)\propto\sum_n \log \mathrm{P}(y^{(n)}\,|\,\boldsymbol{x}^{(n)},\Theta)=\sum_n \log\left[(\hat{\rho}^{(n)})^{y^{(n)}}(1-\hat{\rho}^{(n)})^{(1-y^{(n)})}\right]$



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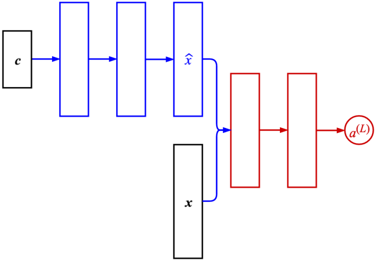

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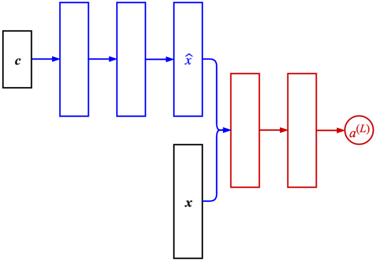
- Inner max first, then outer min
- $\hat{\rho}^{(n)}$ depends on Θ_f only
- $\hat{\rho}^{(m)}$ depends on both Θ_f and Θ_g



Training: Alternative SGD

$$\arg\min_{\Theta_g}\max_{\Theta_f}\sum_n \log f(\boldsymbol{x}^{(n)}) + \sum_m \log(1 - f(g(\boldsymbol{c}^{(m)})))$$

- Initialize Θ_g for g and Θ_f for f
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- Why limiting the steps (K) when updating Θ_f?

Training: Alternative SGD

$$\arg\min_{\Theta_g}\max_{\Theta_f}\sum_n \log f(\boldsymbol{x}^{(n)})+\sum_m \log(1-f(g(\boldsymbol{c}^{(m)})))$$

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1. ***Repeat K times (with fixed Θ_g):***
   1. Sample N real points $\{\boldsymbol{x}^{(n)}\}_n$ from $\mathbb{X}$ and N codes from $\mathbf{c}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})$
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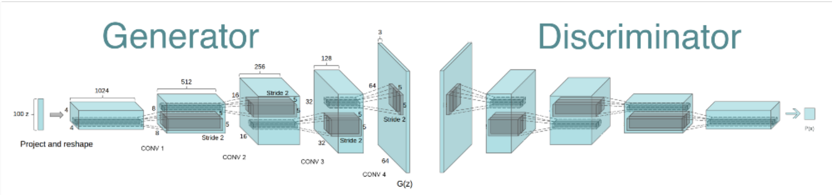
  - Limiting K so to prevent g from being updated for "wrong" target

Results

- Domain-specific architecture, e.g., DC-GAN [30]



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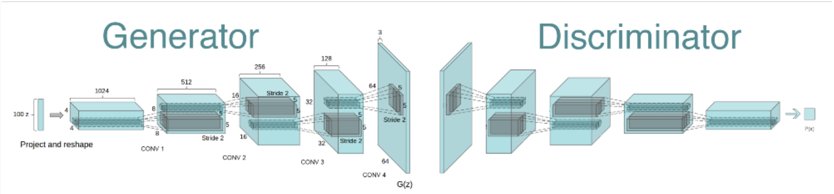

GANs Are Hard to Train!

- Tips for Training Stable GANs
- Keep Calm and train a GAN. Pitfalls and Tips...
- 10 Lessons I Learned Training GANs for one Year
- GAN hacks on GitHub

Outline

Challenge: Non-Convergence

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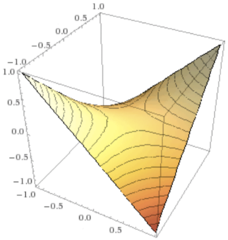

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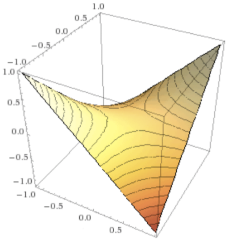

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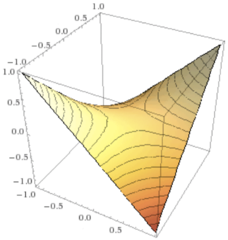
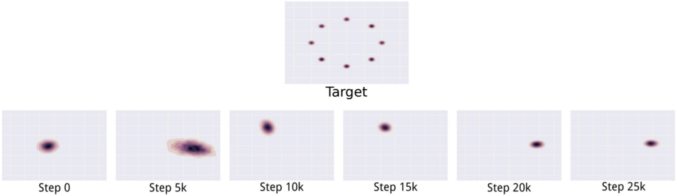


- The updated Θ_f and Θ_g may cancel each other's progress
- Requires human monitoring and termination

Mode Collapsing

- Even worse: ***mode collapsing***
  - g may oscillate from generating one kind of points to generating another kind of points



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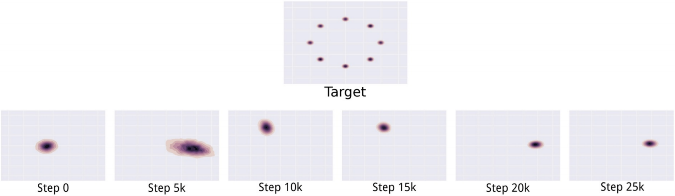

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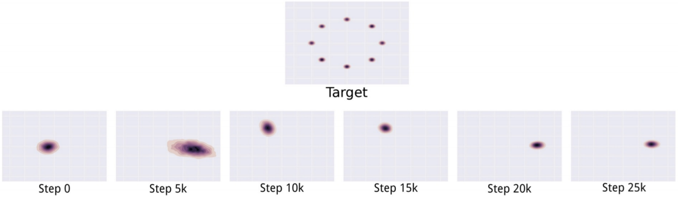

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- $\max_{\Theta_f}\min_{\Theta_g}$? g is encouraged to map every code to the "mode" that f believes is most likely to be real

Solutions

- Minibatch discrimination [39]
  - In $\max_{\Theta_f} \min_{\Theta_g}$ case, g collapses because $\nabla_{\Theta_f} C$ are computed independently for each point
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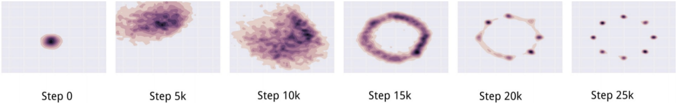
- Unrolled GANs [24]: to back-propagate through ***several*** max ***steps*** when computing $\nabla_{\Theta_g} C$



Challenge: Balance between g and f

$$\arg\min_{\Theta_g}\max_{\Theta_f}\sum_n \log f(\boldsymbol{x}^{(n)}) + \sum_m \log(1-f(g(\boldsymbol{c}^{(m)})))$$

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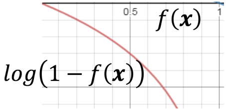

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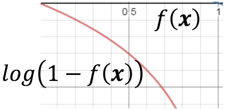

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Solution: Wasserstein GAN [1]

- Let f be a regressor ***without*** the sigmoid output layer
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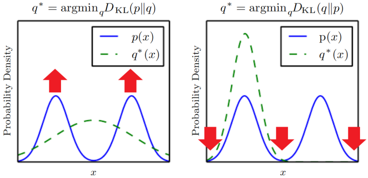

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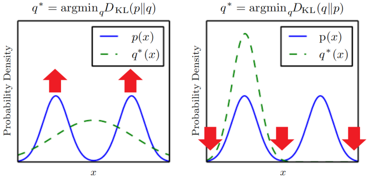

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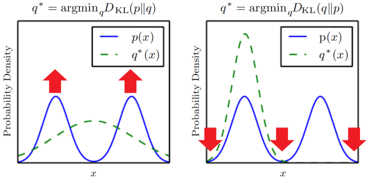

- GAN: $\arg\min_{\Theta_g} \max_{\Theta_f} \sum_n \log f(\boldsymbol{x}^{(n)}) + \sum_m \log(1 - f(g(\boldsymbol{c}^{(m)})))$
- Actually, the max term measures Jensen-Shannon divergence (a.k.a. symmetric KL divergence):

$$\mathrm{D}_{\mathrm{JS}}(\mathrm{P}_{\text{data}} \| \mathrm{P}_g) = \frac{1}{2}\mathrm{D}_{\mathrm{KL}}(\mathrm{P}_{\text{data}} \| \mathrm{Q}) + \frac{1}{2}\mathrm{D}_{\mathrm{KL}}(\mathrm{P}_g \| \mathrm{Q}), \text{ where } \mathrm{Q} = \frac{1}{2}(\mathrm{P}_g + \mathrm{P}_{\text{data}})$$

Why Jensen-Shannon Divergence? I

- Given a fixed g, we have

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- To have C^*, we can find f maximizing

$$
\mathrm{P}_{\mathsf{data}}(\boldsymbol{x}) \log f(\boldsymbol{x}) + \mathrm{P}_g(\boldsymbol{x}) \log(1 - f(\boldsymbol{x}))
$$

  for each $\boldsymbol{x}$
  - Assuming that f has infinite capacity

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C^* &= \max_{\Theta_f} \int_{\boldsymbol{x}} [\mathrm{P}_{\text{data}}(\boldsymbol{x})\log f(\boldsymbol{x}) + \mathrm{P}_g(\boldsymbol{x})\log(1-f(\boldsymbol{x}))] d\boldsymbol{x} \\
&= \int_{\boldsymbol{x}} \mathrm{P}_{\text{data}}(\boldsymbol{x}) \log \frac{\mathrm{P}_{\text{data}}(\boldsymbol{x})}{\mathrm{P}_{\text{data}}(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x})} d\boldsymbol{x} \\
&\qquad + \int_{\boldsymbol{x}} \mathrm{P}_g(\boldsymbol{x}) \log(\frac{\mathrm{P}_g(\boldsymbol{x})}{\mathrm{P}_{\text{data}}(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x})}) d\boldsymbol{x} \\
&= -2\log 2 + \int_{\boldsymbol{x}} \mathrm{P}_{\text{data}}(\boldsymbol{x}) \log \frac{\mathrm{P}_{\text{data}}(\boldsymbol{x})}{(\mathrm{P}_{\text{data}}(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x}))/2} d\boldsymbol{x} \\
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\end{aligned}$$

Why Jensen-Shannon Divergence? II

- Given P_{data}, P_g, and $\boldsymbol{x}$, what is the $f(\boldsymbol{x})$ that maximizes

$$\mathrm{P}_{\text{data}}(\boldsymbol{x})\log f(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x})\log(1-f(\boldsymbol{x}))?$$

- $f^*(\boldsymbol{x})=\frac{\mathrm{P}_{\text{data}}(\boldsymbol{x})}{\mathrm{P}_{\text{data}}(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x})}\in[0,1]$ [Proof]
- That is,

$$\begin{aligned}
C^* &= \max_{\Theta_f}\int_{\boldsymbol{x}}[\mathrm{P}_{\text{data}}(\boldsymbol{x})\log f(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x})\log(1-f(\boldsymbol{x}))]d\boldsymbol{x}\\
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&\qquad+\int_{\boldsymbol{x}}\mathrm{P}_g(\boldsymbol{x})\log(\frac{\mathrm{P}_g(\boldsymbol{x})}{(\mathrm{P}_{\text{data}}(\boldsymbol{x})+\mathrm{P}_g(\boldsymbol{x}))/2})d\boldsymbol{x}\\
&= -2\log 2+2\mathrm{D}_{\text{JS}}(\mathrm{P}_{\text{data}}\|\mathrm{P}_g)
\end{aligned}$$

Balance between g and f, Revisited I

- Cost function of GAN:

$$\arg\min_{\Theta_g} \max_{\Theta_f} \sum_n \log f(\boldsymbol{x}^{(n)}) + \sum_m \log(1 - f(g(\boldsymbol{c}^{(m)})))$$
$$= \arg\min_{\Theta_g} -2\log 2 + 2\mathrm{D}_{\mathsf{JS}}(\mathrm{P}_{\mathsf{data}} \| \mathrm{P}_g)$$

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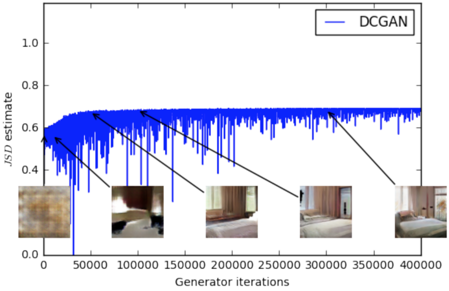
- However, no mater how g changes, $\mathrm{D}_{\mathsf{JS}}(\mathrm{P}_{\mathsf{data}} \| \mathrm{P}_g)$ remains high during the GAN training process



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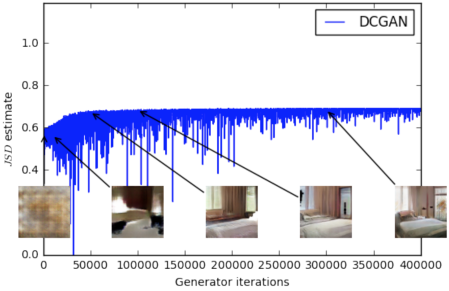
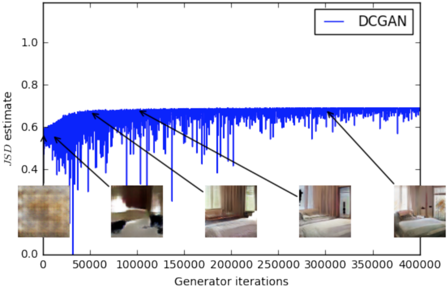


- There's something wrong with the design of the inner max problem!

Balance between g and f, Revisited II

- GAN: $\arg\min_{\Theta_g} D_{JS}(P_{data} \| P_g)$



Balance between g and f, Revisited II

- GAN: $\arg\min_{\Theta_g} \mathrm{D}_{\mathrm{JS}}(\mathrm{P}_{\mathrm{data}} \| \mathrm{P}_g)$
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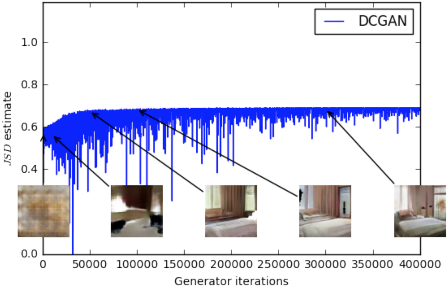

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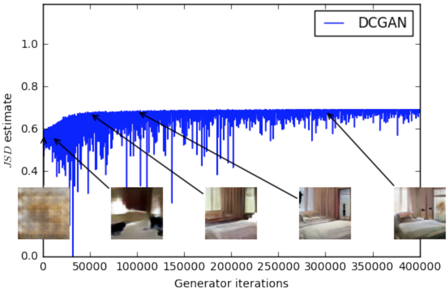

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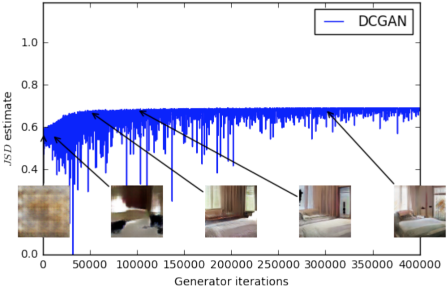

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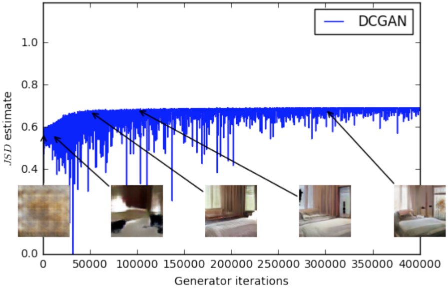

- Suppose $\mathrm{P}_g(\boldsymbol{x}) \neq 0 \Leftrightarrow \mathrm{P}_{\mathrm{data}}(\boldsymbol{x}) = 0$ and $\mathrm{P}_g(\boldsymbol{x}) = 0 \Leftrightarrow \mathrm{P}_{\mathrm{data}}(\boldsymbol{x}) \neq 0$, we have

$$\mathrm{D}_{\mathrm{JS}}(\mathrm{P}_g \| \mathrm{P}_{\mathrm{data}}) = \frac{1}{2}\mathrm{D}_{\mathrm{KL}}\left(\mathrm{P}_g \middle\| \frac{\mathrm{P}_g + \mathrm{P}_{\mathrm{data}}}{2}\right) + \frac{1}{2}\mathrm{D}_{\mathrm{KL}}\left(\mathrm{P}_{\mathrm{data}} \middle\| \frac{\mathrm{P}_g + \mathrm{P}_{\mathrm{data}}}{2}\right)$$

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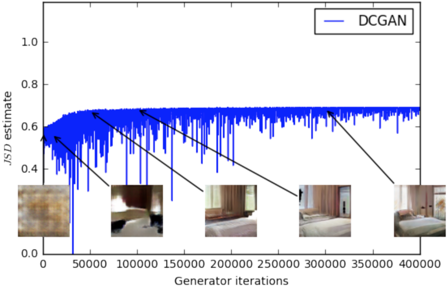

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\begin{aligned}
\mathrm{D}_{\mathrm{JS}}(\mathrm{P}_g \| \mathrm{P}_{\mathrm{data}}) &= \tfrac{1}{2}\mathrm{D}_{\mathrm{KL}}(\mathrm{P}_g \| \tfrac{\mathrm{P}_g + \mathrm{P}_{\mathrm{data}}}{2}) + \tfrac{1}{2}\mathrm{D}_{\mathrm{KL}}(\mathrm{P}_{\mathrm{data}} \| \tfrac{\mathrm{P}_g + \mathrm{P}_{\mathrm{data}}}{2}) \\
&= \tfrac{1}{2}\int_{\boldsymbol{x}} \mathrm{P}_g(\boldsymbol{x}) \log \frac{2\mathrm{P}_g(\boldsymbol{x})}{\mathrm{P}_g(\boldsymbol{x}) + \mathrm{P}_{\mathrm{data}}(\boldsymbol{x})} d\boldsymbol{x} \\
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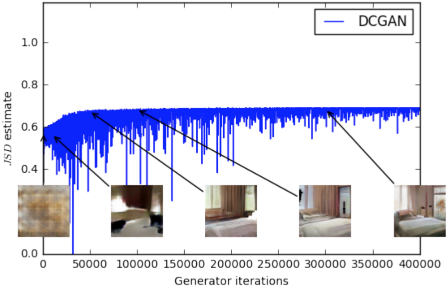

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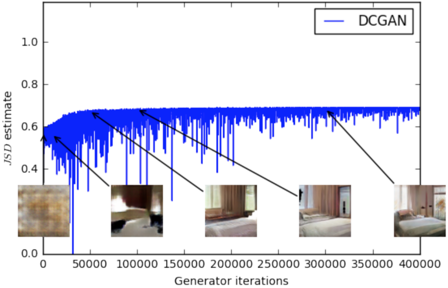

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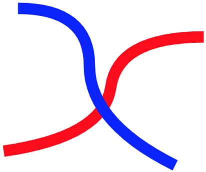
\end{aligned}$$

- Are P_g and P_{data} really disjointed during the GAN training?

Disjoining $\mathbf{P}_g$ and $\mathbf{P}_{\text{data}}$

- In a high dimensional space, $\mathbf{x}$ and $g(\mathbf{z})$ may resides in low dimensional manifolds
  - P_g and P_{data} may have values only on the manifolds



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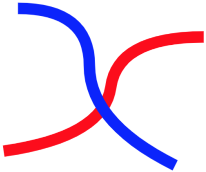

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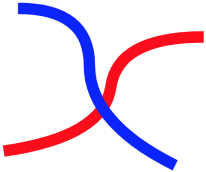

- P_g and P_{data} can be very different initially during GAN training
- The intersections where $\mathrm{P}_g(\boldsymbol{x}) \neq 0$ and $\mathrm{P}_{\text{data}}(\boldsymbol{x}) \neq 0$ can be neglected
  - $\mathrm{P}_g(\boldsymbol{x}) \neq 0 \Leftrightarrow \mathrm{P}_{\text{data}}(\boldsymbol{x}) = 0$ and $\mathrm{P}_g(\boldsymbol{x}) = 0 \Leftrightarrow \mathrm{P}_{\text{data}}(\boldsymbol{x}) \neq 0$ almost surely
  - Maximum JS divergence at all time

Better Divergence Measure?

- GAN: $\arg\min_{\Theta_g} \mathrm{D}_{\mathsf{JS}}(\mathrm{P}_{\mathsf{data}} \| \mathrm{P}_g)$
  - $\mathrm{D}_{\mathsf{JS}}(\mathrm{P}_{\mathsf{data}} \| \mathrm{P}_g)$ does ***not*** bring P_g and $\mathrm{P}_{\mathsf{data}}$ closer during GAN training

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- Wasserstein (or earth-mover) distance:

$$
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\mathrm{W}(\mathrm{P}_{\mathrm{data}}, \mathrm{P}_g) &= \inf_{\mathrm{Q} \in \Gamma(\mathrm{P}_{\mathrm{data}}, \mathrm{P}_g)} \mathrm{E}_{(\mathbf{x}, \hat{\mathbf{x}}) \sim \mathrm{Q}}[\|\mathbf{x} - \hat{\mathbf{x}}\|] \\
&= \inf_{\mathrm{Q} \in \Gamma(\mathrm{P}_{\mathrm{data}}, \mathrm{P}_g)} \int_{(\boldsymbol{x}, \hat{\boldsymbol{x}})} \mathrm{Q}(\boldsymbol{x}, \hat{\boldsymbol{x}}) \|\boldsymbol{x} - \hat{\boldsymbol{x}}\| d(\boldsymbol{x}, \hat{\boldsymbol{x}})
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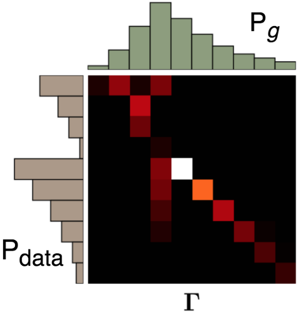
$$



Better Divergence Measure?

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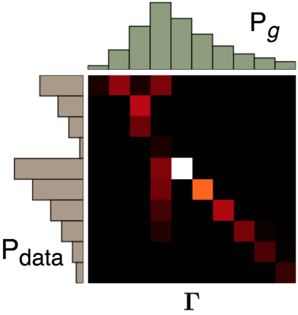
$$\begin{aligned} W(P_{\text{data}}, P_g) &= \inf_{Q \in \Gamma(P_{\text{data}}, P_g)} E_{(\mathbf{x}, \hat{\mathbf{x}}) \sim Q}[\|\mathbf{x} - \hat{\mathbf{x}}\|] \\ &= \inf_{Q \in \Gamma(P_{\text{data}}, P_g)} \int_{(\boldsymbol{x}, \hat{\boldsymbol{x}})} Q(\boldsymbol{x}, \hat{\boldsymbol{x}}) \|\boldsymbol{x} - \hat{\boldsymbol{x}}\| d(\boldsymbol{x}, \hat{\boldsymbol{x}}) \end{aligned}$$

- Intuitively, the minimal "cost" to change P_{data} into P_g



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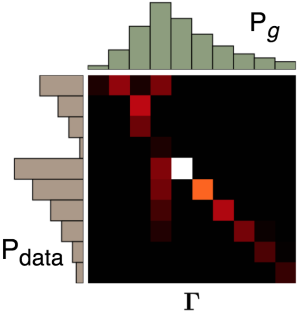
  - Intuitively, the minimal "cost" to change P_{data} into P_g
  - $\mathrm{W}(\mathrm{P}_{\text{data}}, \mathrm{P}_g)$ measures the "divergence" between P_g and P_{data} ***even when they are disjointed***



Wasserstein GAN I

- W-GAN: $\arg\min_{\Theta_g} \mathrm{W}(\mathrm{P}_{\mathsf{data}}, \mathrm{P}_g)$
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- Unfortunately, $\mathrm{W}(\mathrm{P}_{\mathsf{data}}, \mathrm{P}_g)$ is hard to solve directly

Wasserstein GAN II

Theorem

Consider f's that are Lipschitz continuous with constant 1, i.e.,

$$|f(\boldsymbol{x}) - f(\hat{\boldsymbol{x}})| \leq 1 \cdot \|\boldsymbol{x} - \hat{\boldsymbol{x}}\|, \forall \boldsymbol{x}, \hat{\boldsymbol{x}},$$

we have [a]

$$W(P_{\text{data}}, P_g) \quad = \sup_f E_{\mathbf{x} \sim P_{\text{data}}}[f(\mathbf{x})] - E_{\mathbf{x} \sim P_g}[f(\mathbf{x})]$$

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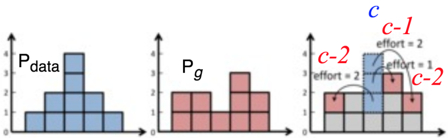
[a] https://vincentherrmann.github.io/blog/wasserstein/



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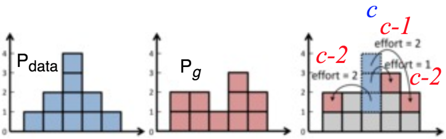

- W-GAN [1]: $\arg\min_{\Theta_g} \max_{\Theta_f} \mathrm{E}_{\mathbf{x} \sim \mathrm{P}_{\text{data}}}[f(\mathbf{x})] - \mathrm{E}_{\mathbf{x} \sim \mathrm{P}_g}[f(\mathbf{x})]$

Alternate SGD for W-GAN

$$\arg\min_{\Theta_g}\max_{\Theta_f} \mathrm{E}_{\mathbf{x}\sim \mathrm{P}_{\mathsf{data}}}[f(\mathbf{x})] - \mathrm{E}_{\mathbf{x}\sim \mathrm{P}_g}[f(\mathbf{x})]$$
$$= \arg\min_{\Theta_g}\max_{\Theta_f} \sum_n f(\boldsymbol{x}^{(n)}) - \sum_m f(g(\boldsymbol{c}^{(m)}))$$

- f a regressor ***without*** the sigmoid output layer

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- f a regressor ***without*** the sigmoid output layer
- Initialize Θ_g for g and Θ_f for f
- At each SGD step/iteration:

1. Repeat K times (with fixed Θ_g):
    1. Sample N real points $\{\boldsymbol{x}^{(n)}\}_n$ from $\mathbb{X}$ and N codes from $\mathbf{c} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
    2. $\Theta_f \leftarrow \Theta_f + \eta\, \mathit{clip}(\nabla_{\Theta_f}[\sum_n f(\boldsymbol{x}^{(n)}) - \sum_m f(g(\boldsymbol{c}^{(m)}))])$
2. Execute once (with fixed Θ_f):
    1. Sample N codes from $\mathbf{c} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
    2. $\Theta_g \leftarrow \Theta_g - \eta \nabla_{\Theta_g}[-\sum_m f(g(\boldsymbol{c}^{(m)}))]$

Why Gradient Clipping?

- Update rule for Θ_f:

$$\Theta_f \leftarrow \Theta_f + \eta\, clip(\nabla_{\Theta_f}[\sum_n f(\boldsymbol{x}^{(n)}) - \sum_m f(g(\boldsymbol{c}^{(m)}))])$$

- Gradient clipping: $\forall w \in \Theta_f$, $clip(w) = \max(\min(w, \tau), -\tau)$ for some threshold $\tau > 0$
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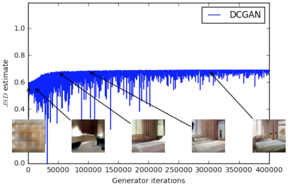
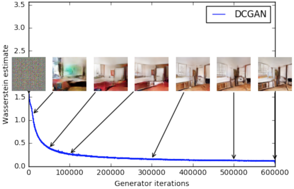
only if f is 1-Lipschitz continuous

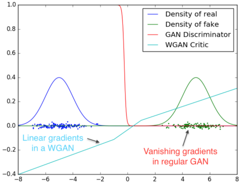
- Heuristics for making f 1-Lipchitz

Advantages of W-GAN

- "Corrects" the inner max problem
  - Wasserstein distance guides g even when P_g and P_{data} "disjointed"
  - Training less sensitive to K (balance between g and f)
- The max value can be used as a "stop" indicator
- f a regressor, avoids vanishing gradients for g







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- W-GAN use a small τ to make f 1-Lipschitz continuous
- However, too small a τ severely limits the capacity of f such it cannot actually maximize

$$\max_{\Theta_f} \mathrm{E}_{\mathbf{x}\sim \mathrm{P}_{\mathsf{data}}}[f(\mathbf{x})] - \mathrm{E}_{\mathbf{x}\sim \mathrm{P}_g}[f(\mathbf{x})]$$

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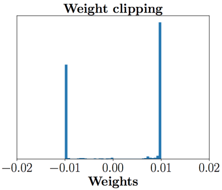
- Distribution of weight values of f $(\tau = 0.01)$:



- Exploding and vanishing gradients

Improved W-GAN II

- If f is 1-Lipschitz, then $\|\nabla f(\boldsymbol{x})\| \leq 1$ for all $\boldsymbol{x}$
- Why not just panelize $\|\nabla f(\boldsymbol{x})\| > 1$ for all $\boldsymbol{x}$?
- Cost function:

$$\arg\min_{\Theta_g} \max_{\Theta_f} \mathrm{E}_{\mathbf{x} \sim \mathrm{P}_{\mathsf{data}}}[f(\mathbf{x})] - \mathrm{E}_{\mathbf{x} \sim \mathrm{P}_g}[f(\mathbf{x})]$$
$$-\lambda \mathrm{E}_{\mathbf{x} \sim \mathrm{P}_{\mathsf{penalty}}}[\max(0, \|\nabla f(\mathbf{x})\| - 1)]$$

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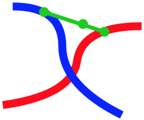

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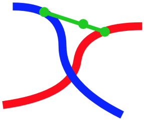
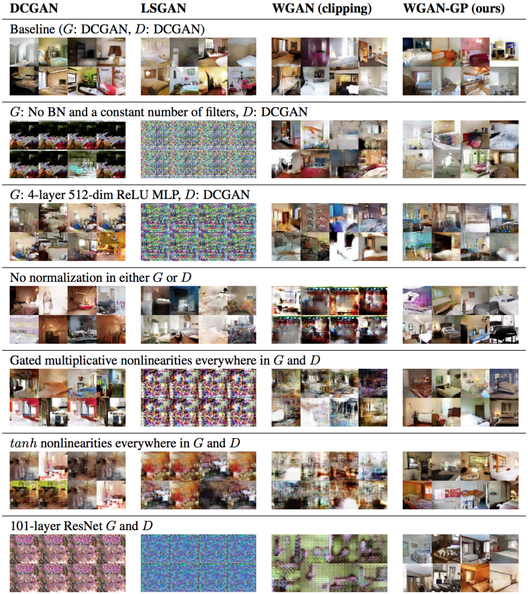


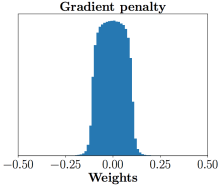
- W-GAN-GP [9]:

$$\arg\min_{\Theta_g}\max_{\Theta_f} \sum_n f(\boldsymbol{x}^{(n)}) - \sum_m f(g(\boldsymbol{c}^{(m)})) - \lambda \sum_p (\|\nabla f(\boldsymbol{x}^{(p)})\| - 1)^2$$

  - The larger $f(\boldsymbol{x}^{(p)})$ the better (subject to $\|\nabla f(\boldsymbol{x}^{(p)})\| \leq 1$)
  - Faster convergence

Results


DCGAN
LSGAN
WGAN (clipping)
WGAN-GP (ours)
Baseline (G: DCGAN, D: DCGAN)
G: No BN and a constant number of filters, D: DCGAN
G: 4-layer 512-dim ReLU MLP, D: DCGAN
No normalization in either G or D
Gated multiplicative nonlinearities everywhere in G and D
tanh nonlinearities everywhere in G and D
101-layer ResNet G and D


Gradient penalty
−0.50
−0.25
0.00
0.25
0.50
Weights

Challenge: Global Coherence

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- Large images generated by GANs usually lack global coherency

Counting

Perspective

Shape

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Shape

- A CNN, when used as f, detects ***existence*** of patterns more than their ***relative positions***
    - f loses track of the position of a pattern after several pooling layers
    - Relative position of patterns in $\mathbb{X}$ may change due to different view angels
- Solutions?

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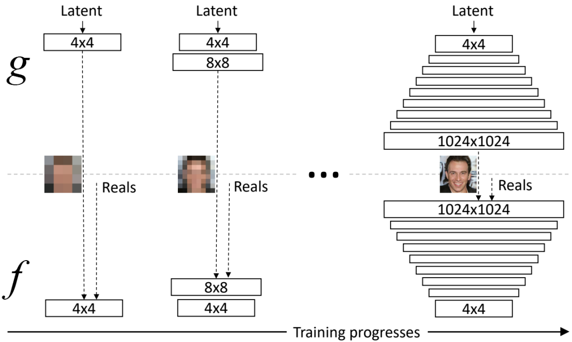
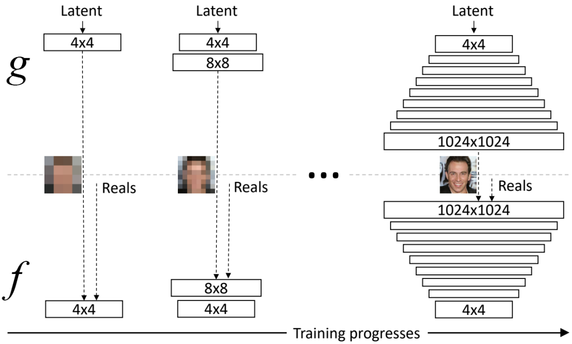
- A CNN, when used as f, detects ***existence*** of patterns more than their ***relative positions***
  - f loses track of the position of a pattern after several pooling layers
  - Relative position of patterns in $\mathbb{X}$ may change due to different view angels
- Solutions? A better f, such as the CapsuleNet [38]?

Progressive Growing of GANs [14]



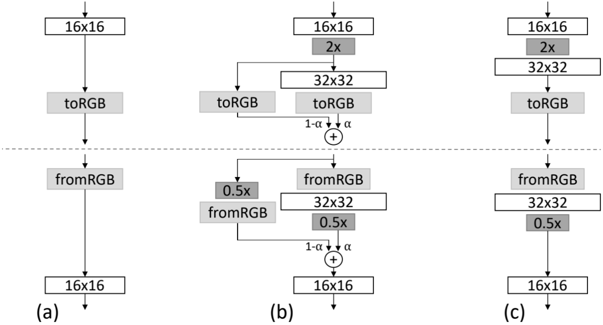
- Incrementally adds new layers in sequential GAN trainings
  - Convolution + upsampling for g each time
  - Convolution + downpooling for f each time
- Real images are downscaled to match the current resolution of g

Progressive Growing of GANs [14]



- Incrementally adds new layers in sequential GAN trainings
  - Convolution + upsampling for g each time
  - Convolution + downpooling for f each time
- Real images are downscaled to match the current resolution of g
- Goal: to let new layers ***add details without ruining the context***

Transition when Adding a New Layer



- Gradually increases α
  - New convolution layer in g/f learns to generate/detect details first
  - Then learns the "context"

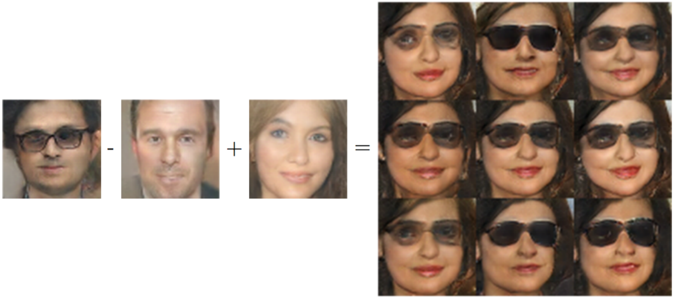
Results

- Minibatch discrimination [39] + W-GAN-GP [9] + progressive growing [14] + other tricks
- $2 \sim 6$ times faster

Outline

Code Space Arithmetics

- DC-GAN [30] can learn to use codes in meaningful ways:



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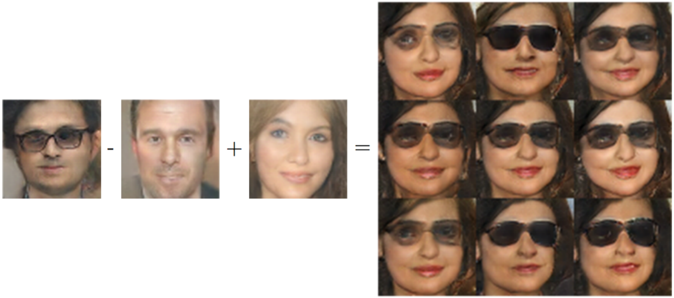


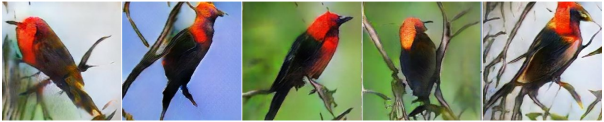
- Finding codes for images with constraints [50, 3] ‣ Demo 1 ‣ Demo 2

$$\arg\min_{\boldsymbol{c}} \|mask(g(\boldsymbol{c})) - \text{constraint}\|_F$$

Conditional GAN I

- Text to image synthesis [34]: $\mathbb{X} = \{(\boldsymbol{x}^{(n)}, \boldsymbol{\phi}^{(n)})\}_n$

  "*This bird is completely red with black wings and pointy beak.*"



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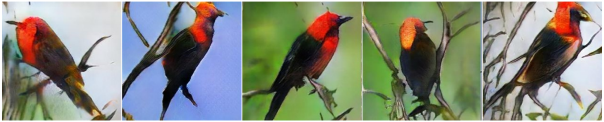
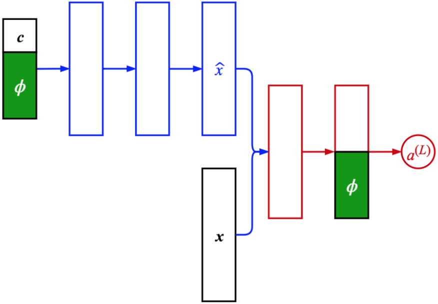
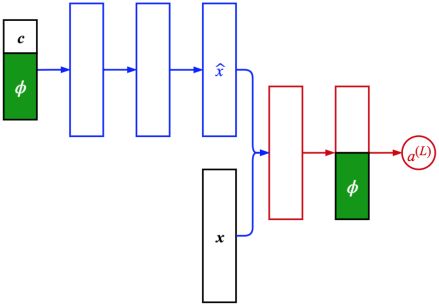


- How?



Conditional GAN II

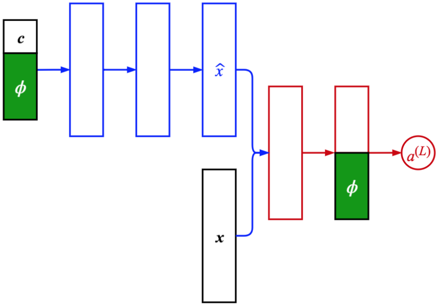
- Pitfall: g and f can choose to ignore the condition ϕ altogether
- Solution?



Conditional GAN II

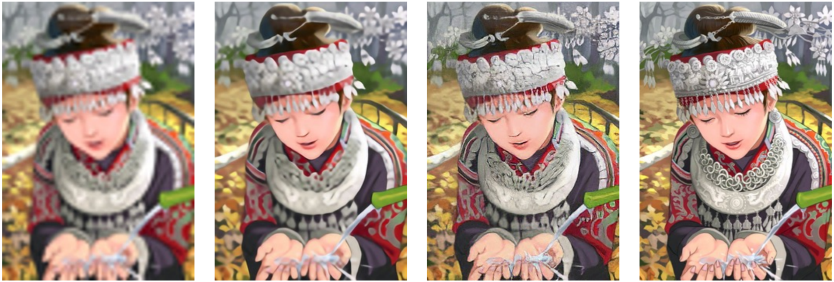
- Pitfall: g and f can choose to ignore the condition ϕ altogether
- Solution? Conditioned labeling

$$
\begin{aligned}
&(\boldsymbol{x}^{(n)}, \phi^{(n)}) \Rightarrow \text{true} \\
&(\boldsymbol{x}^{(n)}, \phi') \Rightarrow \text{false}, \forall \phi' \neq \phi^{(n)} \\
&(\hat{\boldsymbol{x}}^{(m)}, \phi^{(m)}) \Rightarrow \text{false}
\end{aligned}
$$



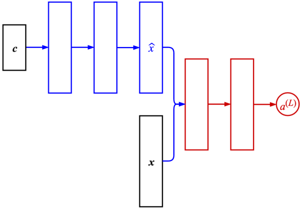
Super Resolution [18]

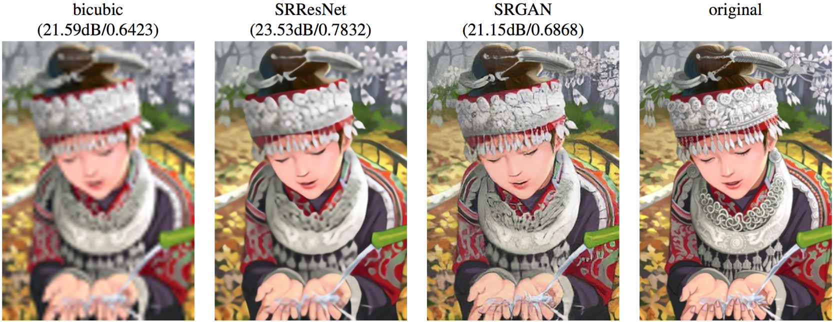
bicubic (21.59dB/0.6423) | SRResNet (23.53dB/0.7832) | SRGAN (21.15dB/0.6868) | original



Super Resolution [18]

- g : low res img $\to$ high res img
  - Training: $\boldsymbol{c}$'s are downscaled images





Super Resolution [18]

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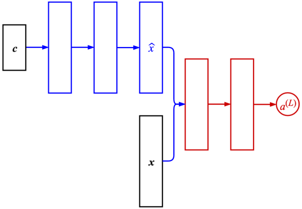
  - Training: $\boldsymbol{c}$'s are downscaled images
- No "creativity," f acts as a better lose metric



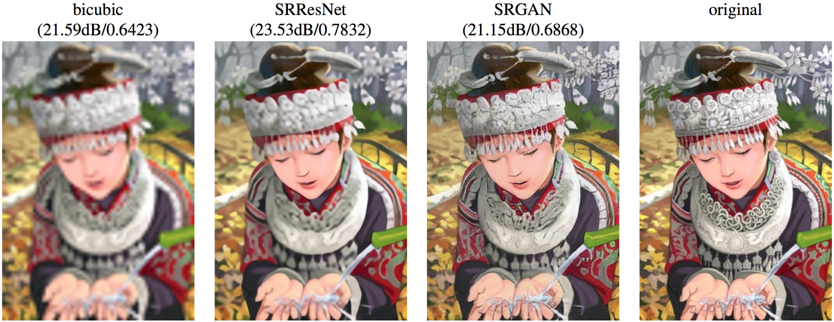


Image-to-Image Translation [13] I

- Given an image $\boldsymbol{x}_{\text{src}}$ in source domain, generate image(s) $\boldsymbol{x}_{\text{target}}$ in target domain
  - $\boldsymbol{x}_{\text{src}}$ and $\boldsymbol{x}_{\text{target}}$ are semantically aligned

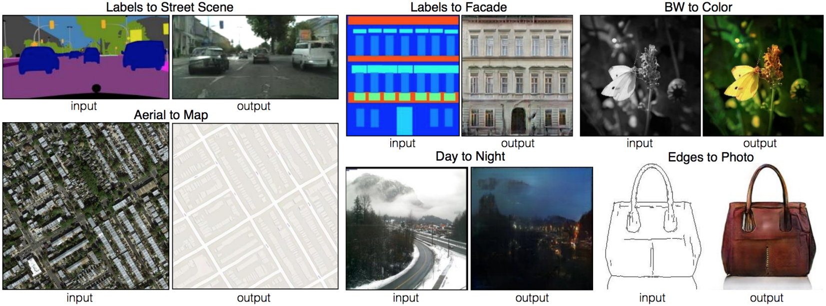
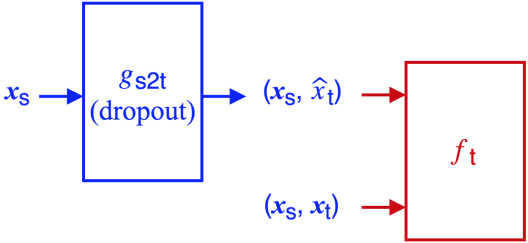


Image-to-Image Translation [13] II

- Based on conditional GAN:
  - $\boldsymbol{c} = \boldsymbol{x}_{\text{src}}$; $g(\boldsymbol{c}) = \boldsymbol{x}_{\text{target}}$
  - Conditioned labels
  - Uses dropout layers to create diversity (if needed)



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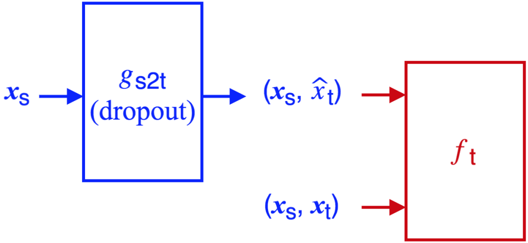
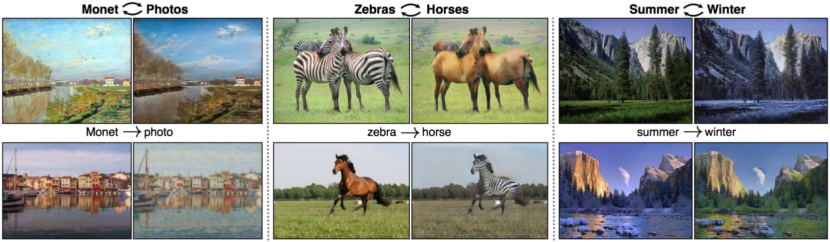
  - Conditioned labels
  - Uses dropout layers to create diversity (if needed)
- Requires ***paired*** examples $\mathbb{X} = \{(\boldsymbol{x}_{\text{src}}^{(n)}, \boldsymbol{x}_{\text{target}}^{(n)})\}_n$



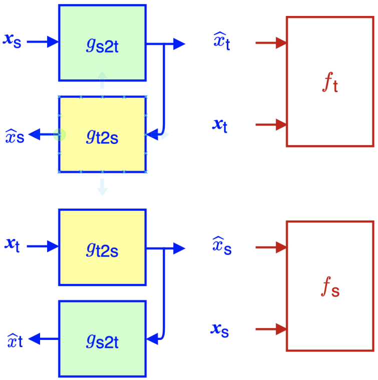
Unpaired Image-to-Image Translation I

- What if the images in different domains are ***unpaired***?
  - $\mathbb{X} = \{\boldsymbol{x}_{\text{src}}^{(n)}\}_n \cup \{\boldsymbol{x}_{\text{target}}^{(n)}\}_n$



Unpaired Image-to-Image Translation II

- Cycle GAN [51]: to train two generators $g_{\text{src2target}}$ and $g_{\text{target2src}}$ simultaneously in two GANs



Unpaired Image-to-Image Translation II

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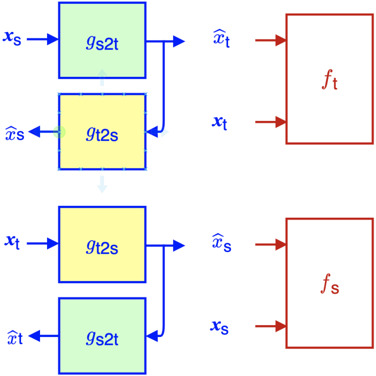
- Add a loss term $\sum_n \|\boldsymbol{x}^{(n)}_{\text{src}} - g_{\text{target2src}}(g_{\text{src2target}}(\boldsymbol{x}^{(n)}_{\text{src}}))\|_F$ and $\sum_n \|\boldsymbol{x}^{(n)}_{\text{target}} - g_{\text{src2target}}(g_{\text{target2src}}(\boldsymbol{x}^{(n)}_{\text{target}}))\|_F$ for $g_{\text{src2target}}$ and $g_{\text{target2src}}$



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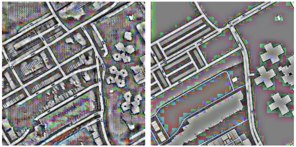
- Reality: $g_{\text{src2target}}$ and $g_{\text{target2src}}$ learns to hide inoformation [6]



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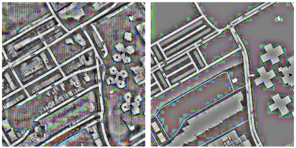

- *Unsupervised DNN models, including GANs, may not work as one may expect* quality?

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