Unsupervised Learning

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Machine Learning

Outline

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Unsupervised Learning

- Dataset: $\mathbb{X} = \{\boldsymbol{x}^{(i)}\}_i$
  - No supervision

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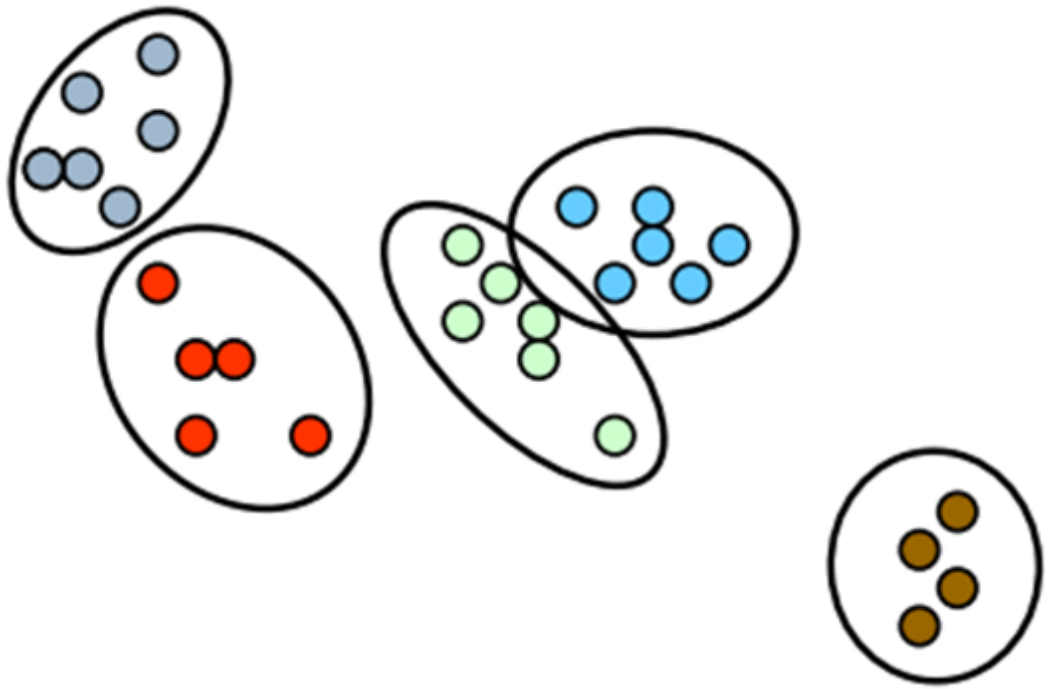
  - No supervision
- What can we learn?

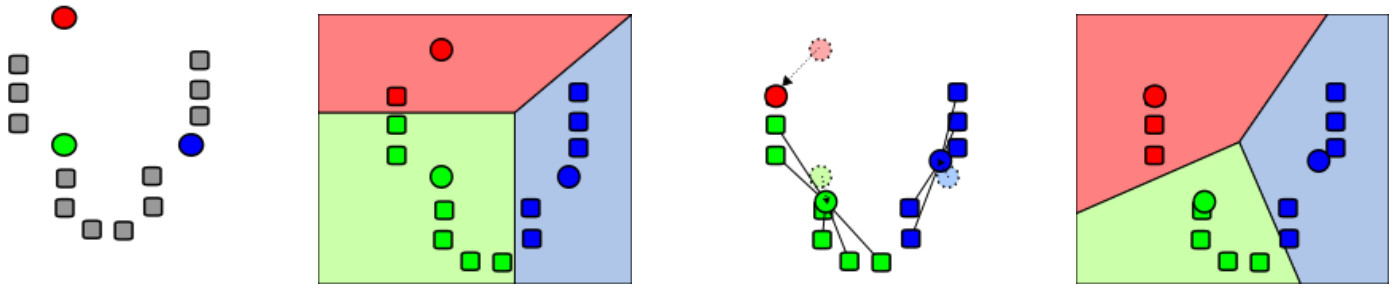
Clustering I

- Goal: to group similar $\boldsymbol{x}^{(i)}$'s



Clustering II

- K-means algorithm:



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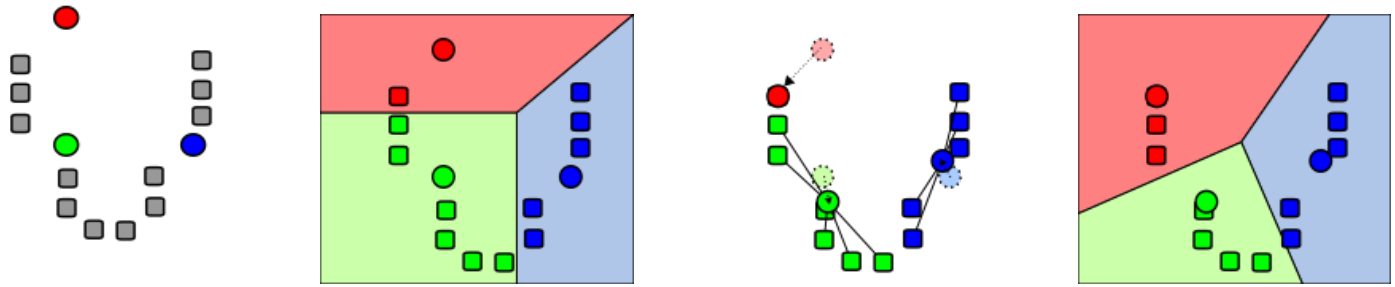
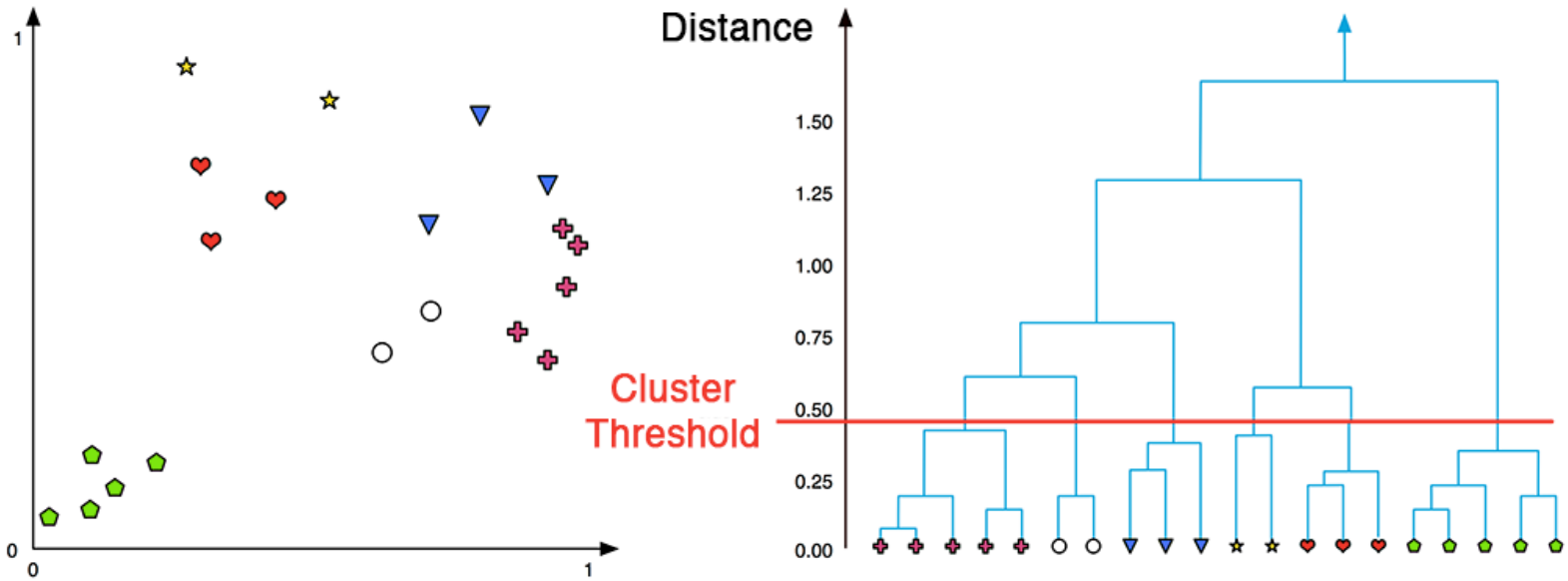
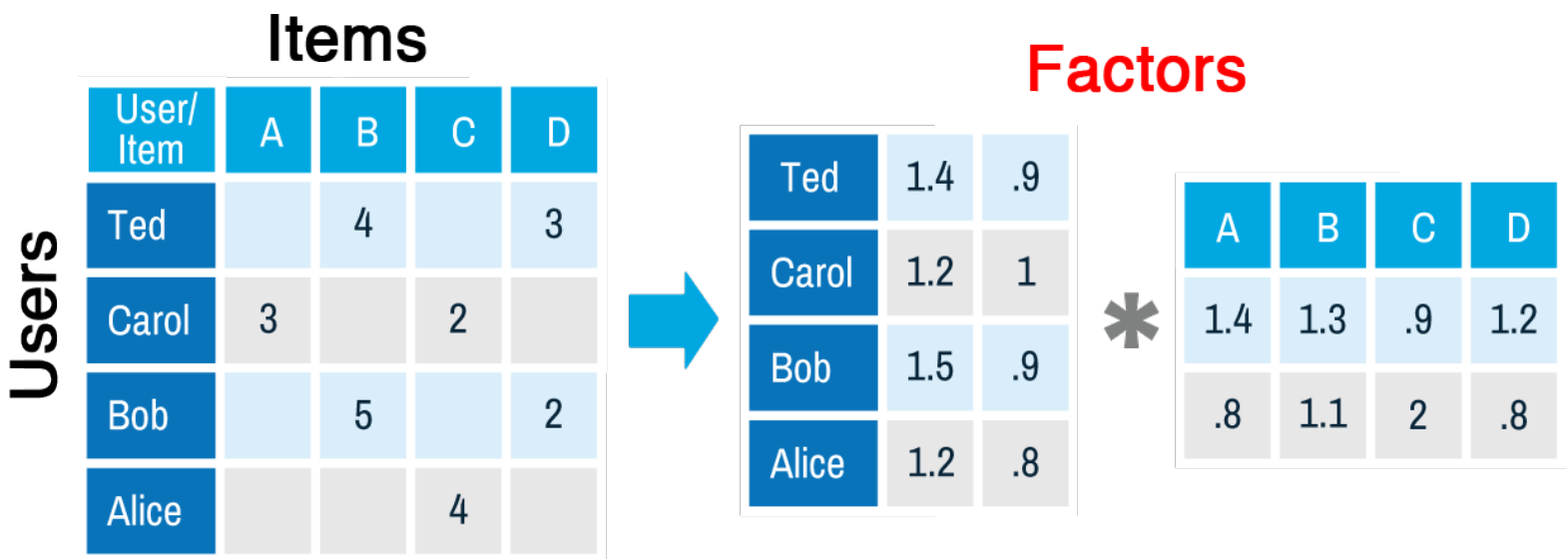


- Hierarchical clustering:



Factorization and Recommendation

- Goal: to uncover the ***factors*** behind data (rating matrix)



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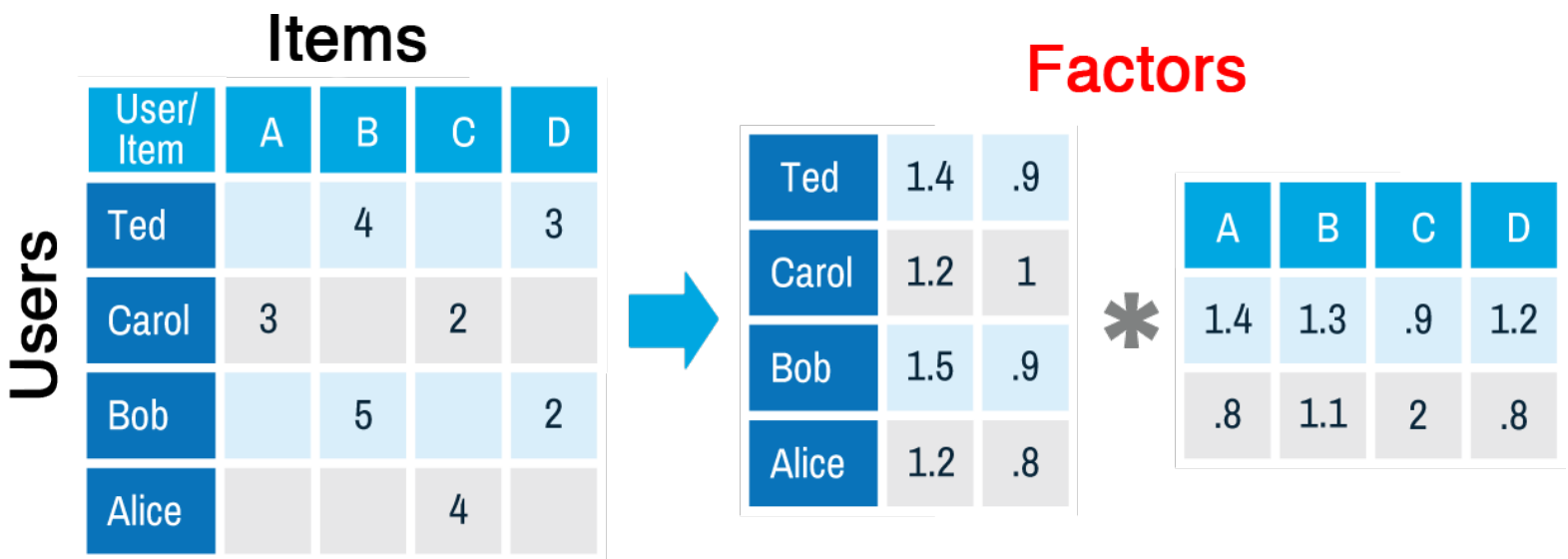

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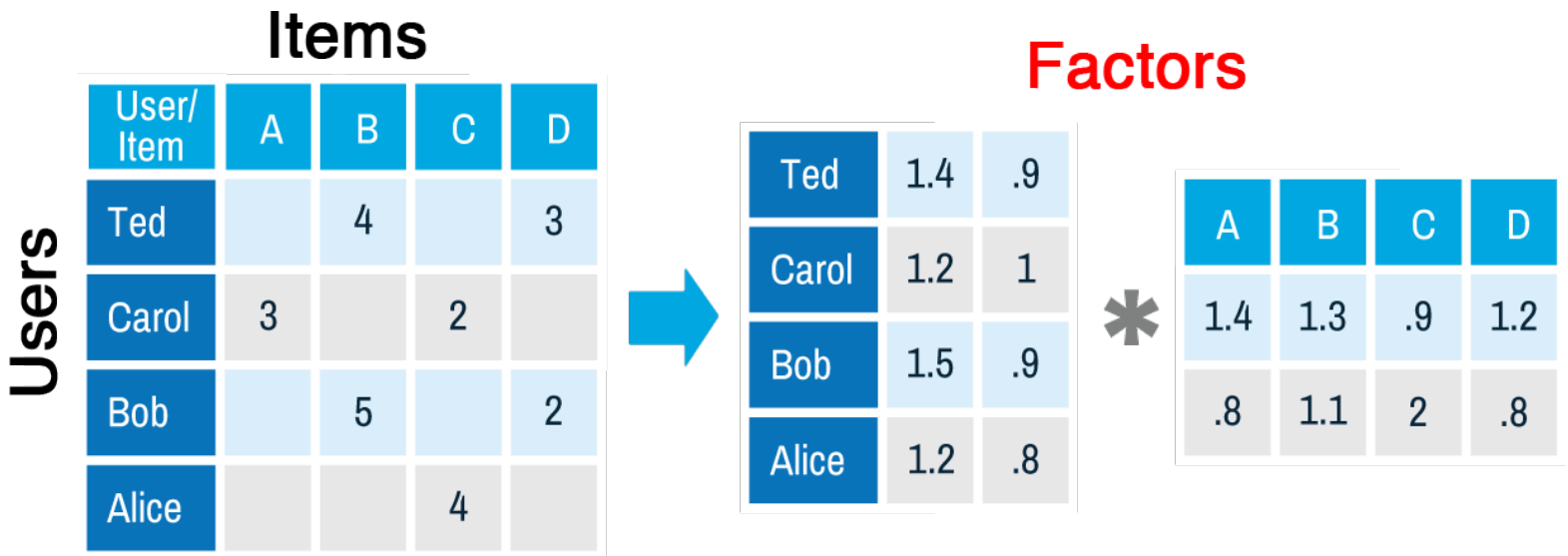

- Non-negative matrix factorization (NMF) [9, 10]

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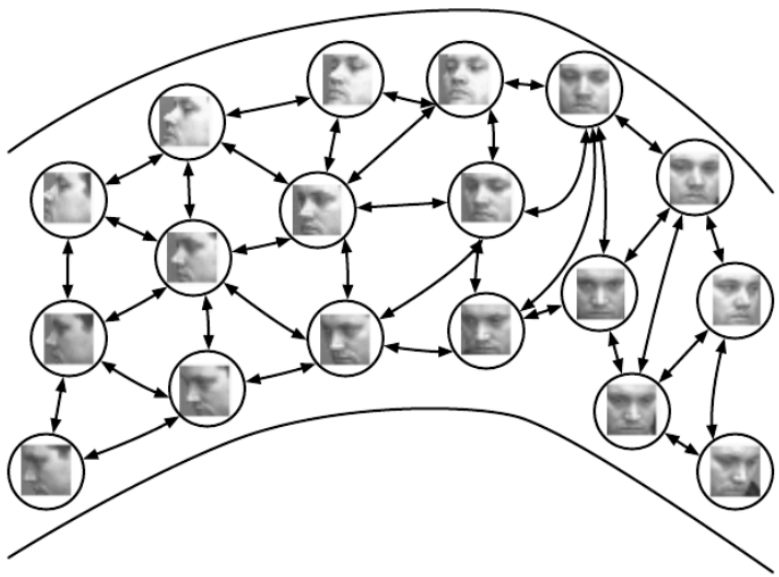
- ***Predictive learning***
  - Learn to "fill in the blanks"
- ***Manifold learning***
  - Learn tangent vectors of a given point



Data Generation I

- Goal: to generate new data points/samples

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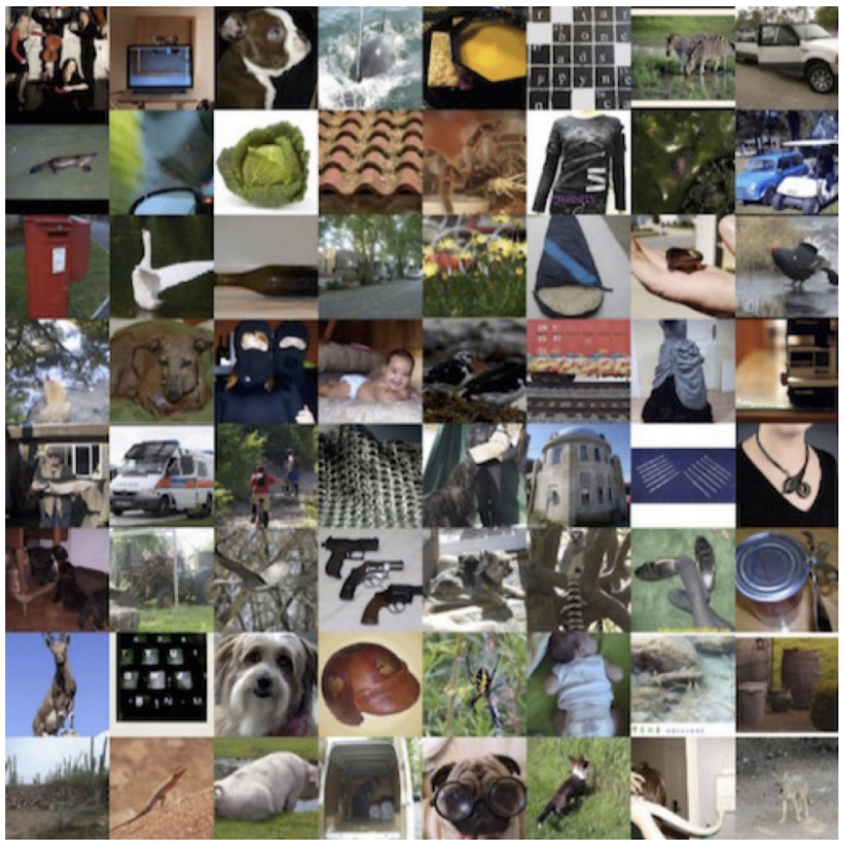
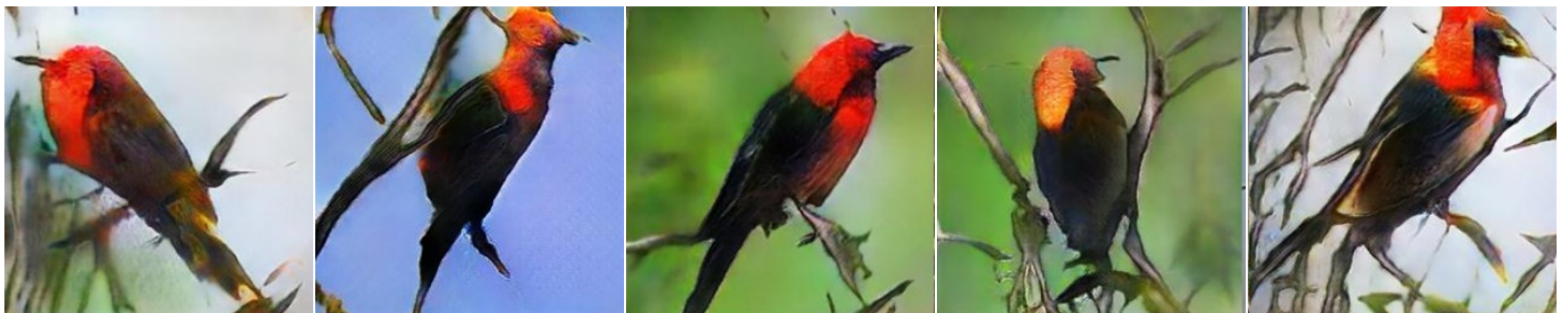
- *Generative adversarial networks* (GANs)



Data Generation II

- Text to image based on conditional GANs:

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



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Predictive Learning

- I.e., blank filling

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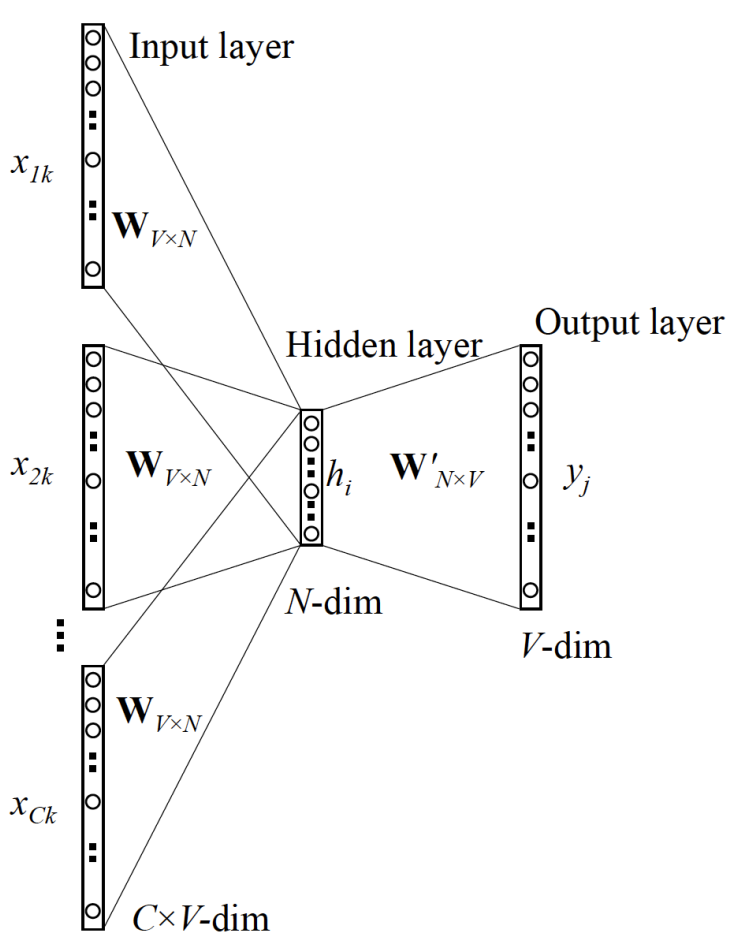
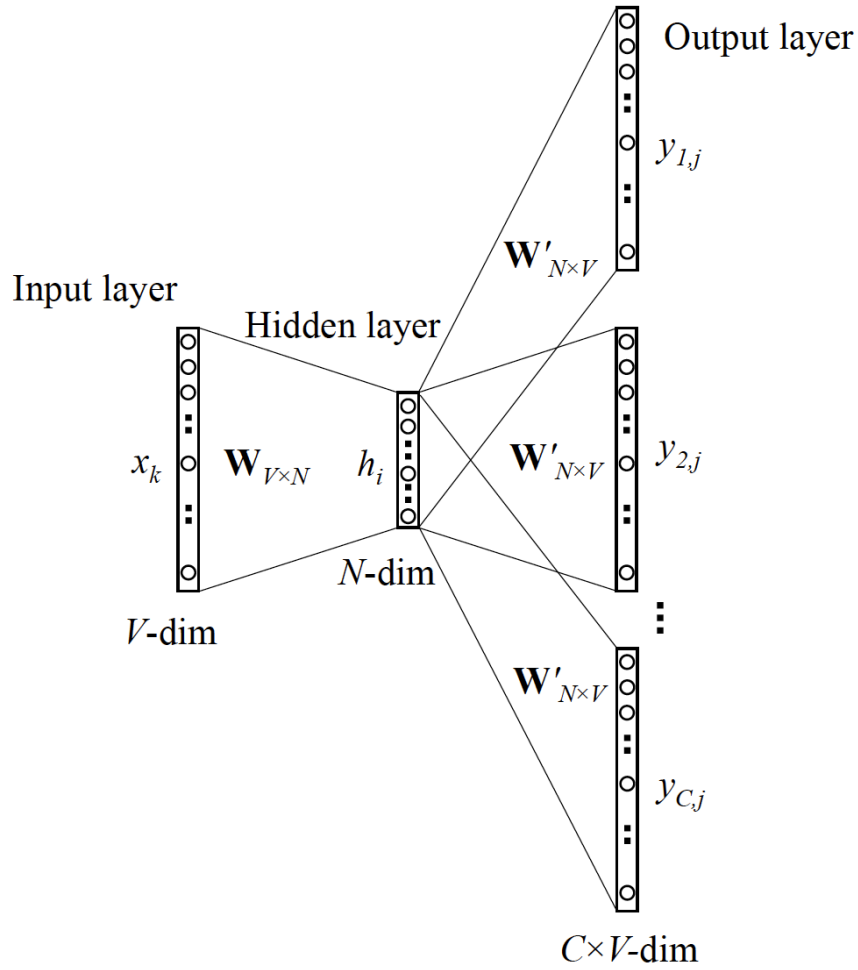
- E.g., word2vec [13, 12]: "*... the cat sat* ***on****...*"





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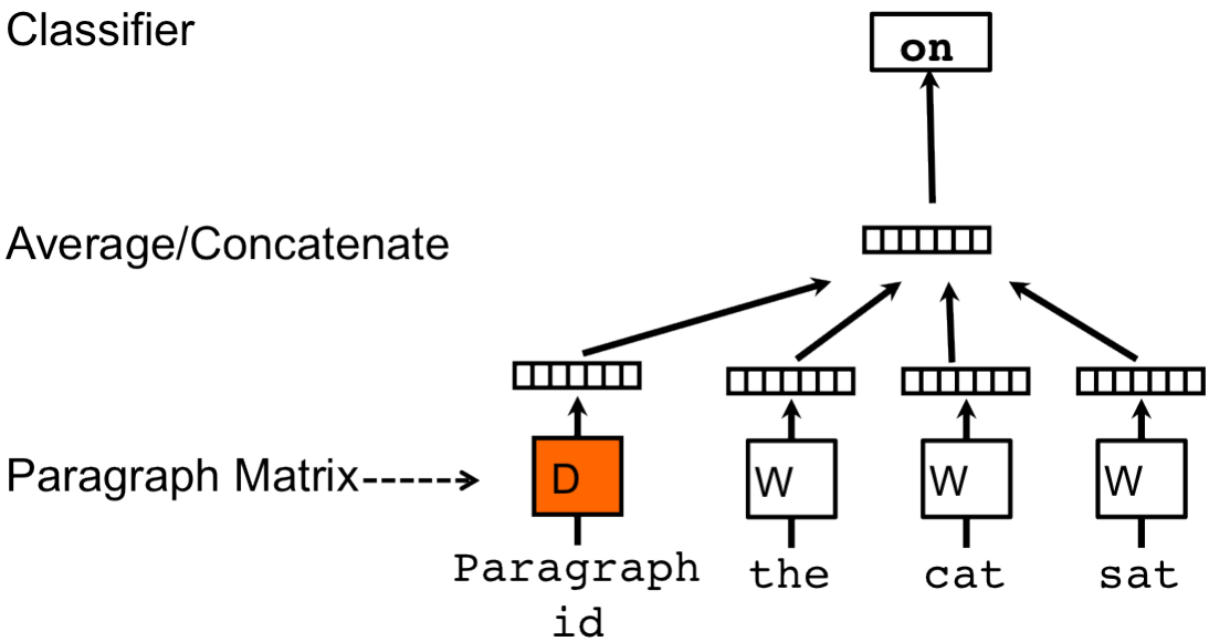
- Predictive learning for docs?
- Doc2vec [7]: to capture the ***context*** not explained by words



Filling Images

- How?

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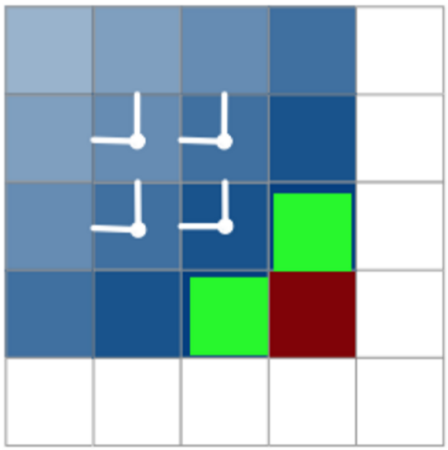
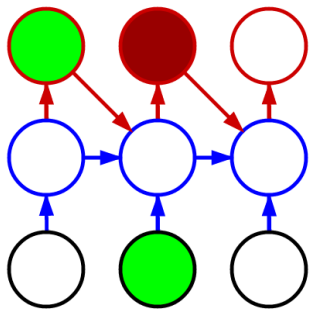
- PixelRNN [19]





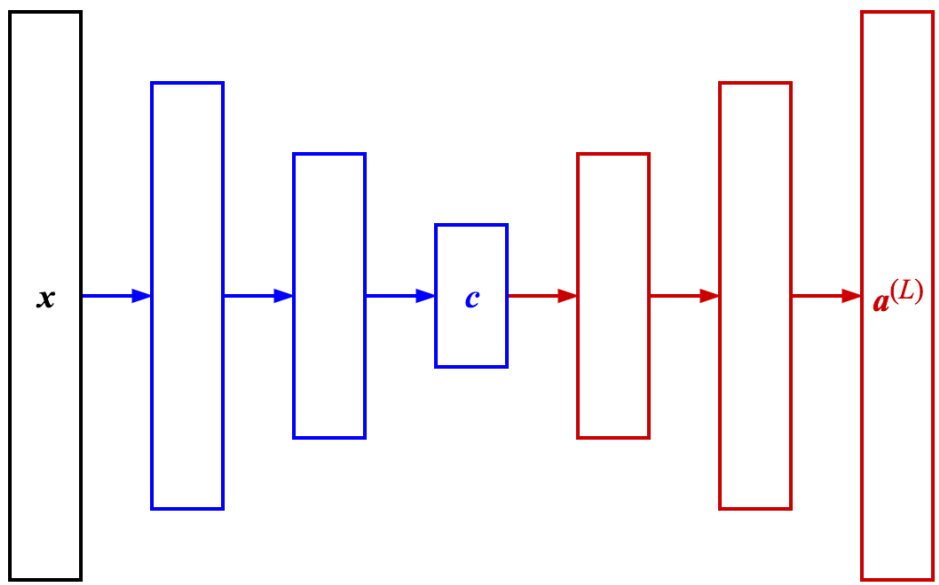
More

- Predicting the future by watching unlabeled videos [6, 21]:

Outline

Autoencoders I

- Encoder: to learn a low dimensional representation $\mathbf{c}$ (called ***code***) of input $\mathbf{x}$
- Decoder: to reconstruct $\mathbf{x}$ from $\mathbf{c}$



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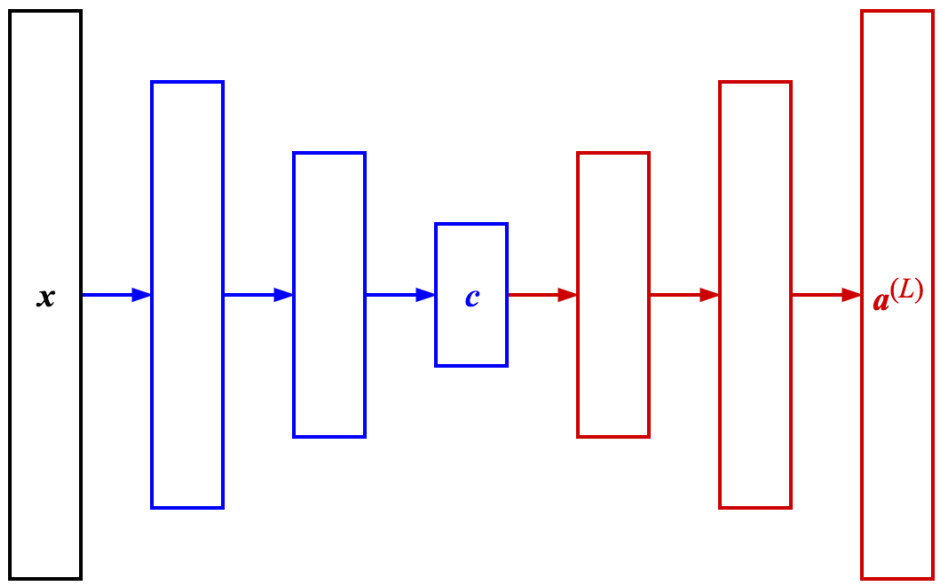

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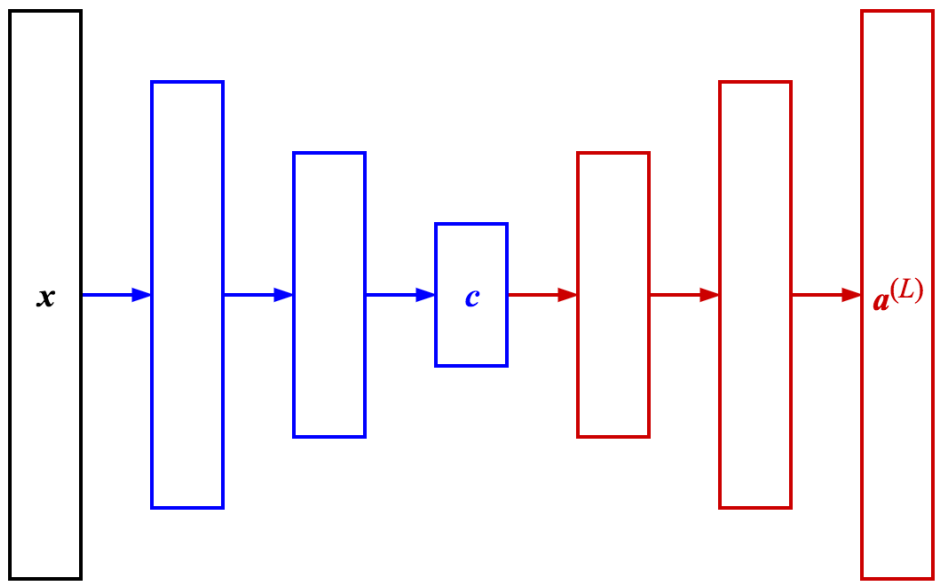
- Sigmoid output units $a_j^{(L)} = \hat{\rho}_j$ for $\mathrm{x}_j \sim \mathrm{Bernoulli}(\rho_j)$
  - $\mathrm{P}(x_j^{(n)} \mid \Theta) = (a_j^{(L)})^{x_j^{(n)}} (1 - a_j^{(L)})^{(1 - x_j^{(n)})}$



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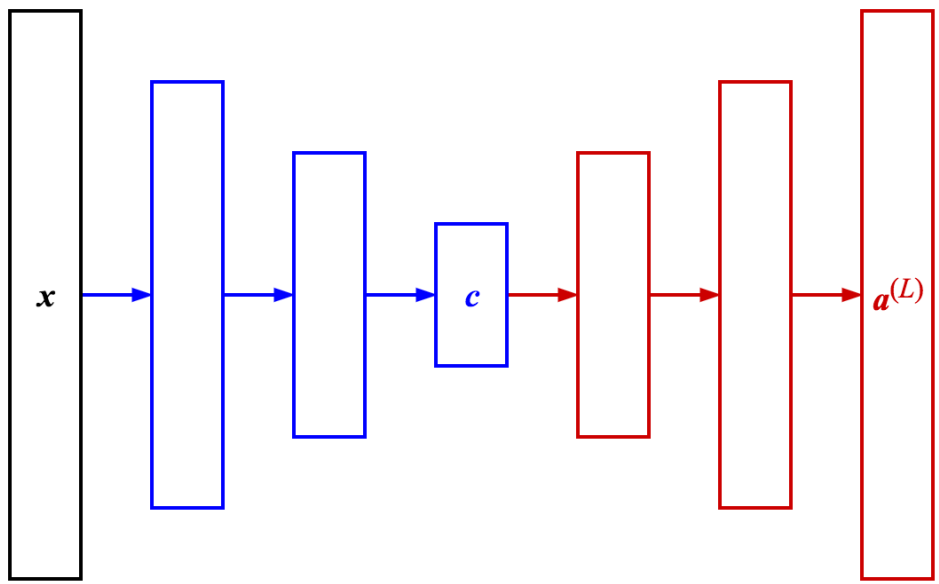
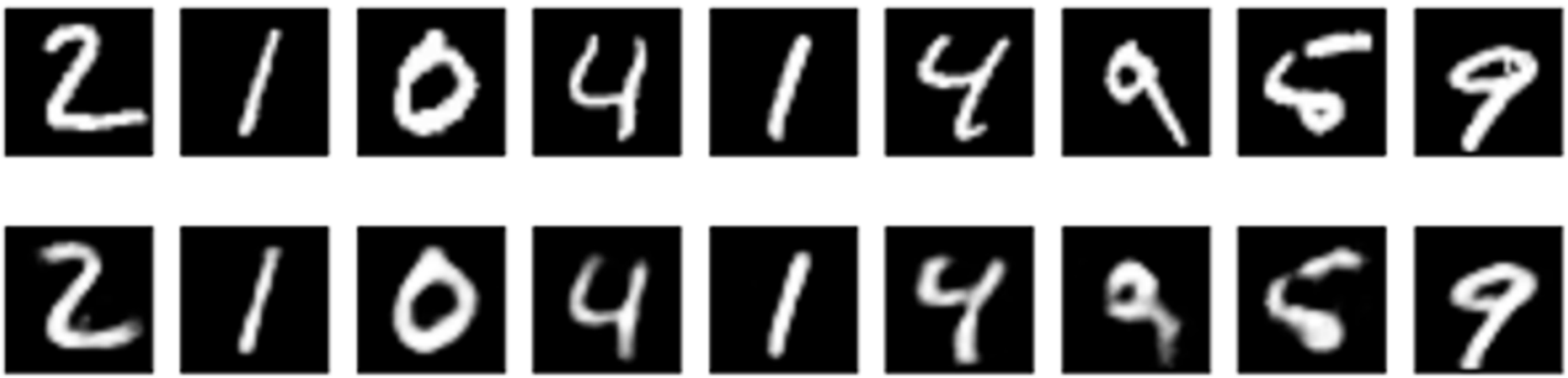
- Linear output units $\boldsymbol{a}^{(L)} = \boldsymbol{z}^{(L)} = \hat{\mu}$ for $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$
  - $-\log \mathrm{P}(\boldsymbol{x}^{(n)}\,|\,\Theta) = \|\boldsymbol{x}^{(n)} - \boldsymbol{z}^{(L)}\|^2$



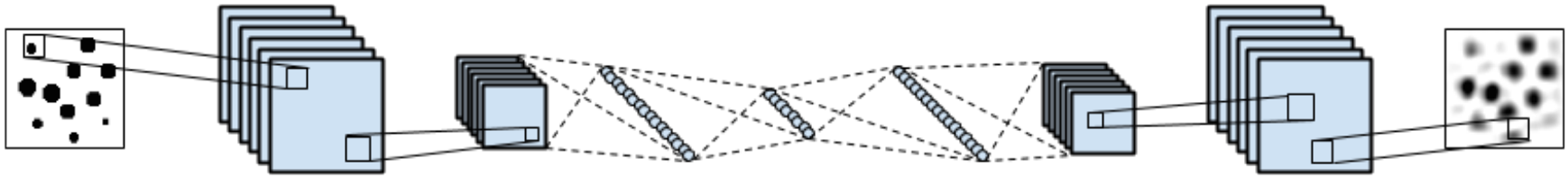
Autoencoders II

- A 32-bit code can roughly represents a 32×32 MNIST image



Convolutional Autoencoders

- Convolution + deconvolution:



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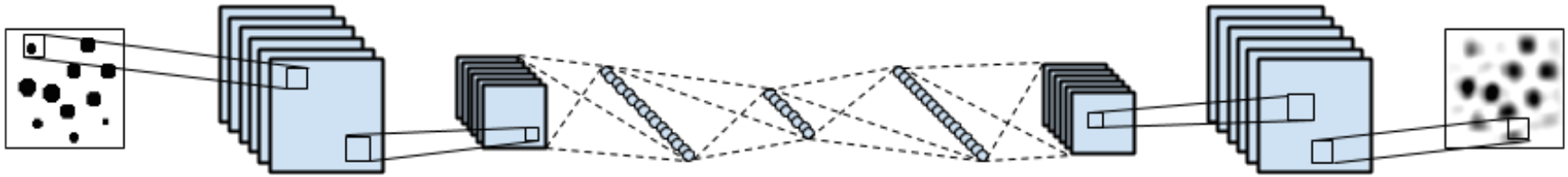

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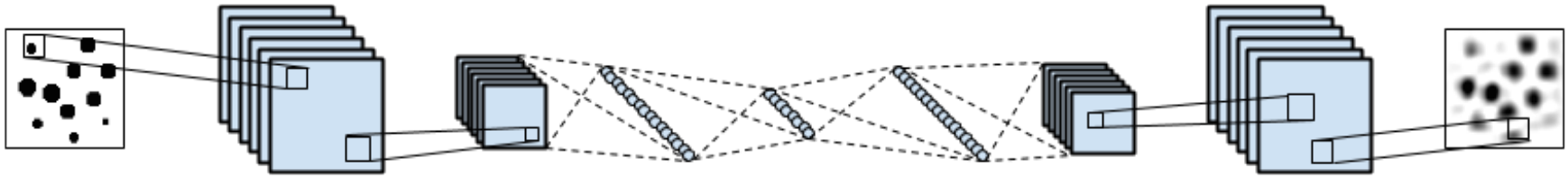
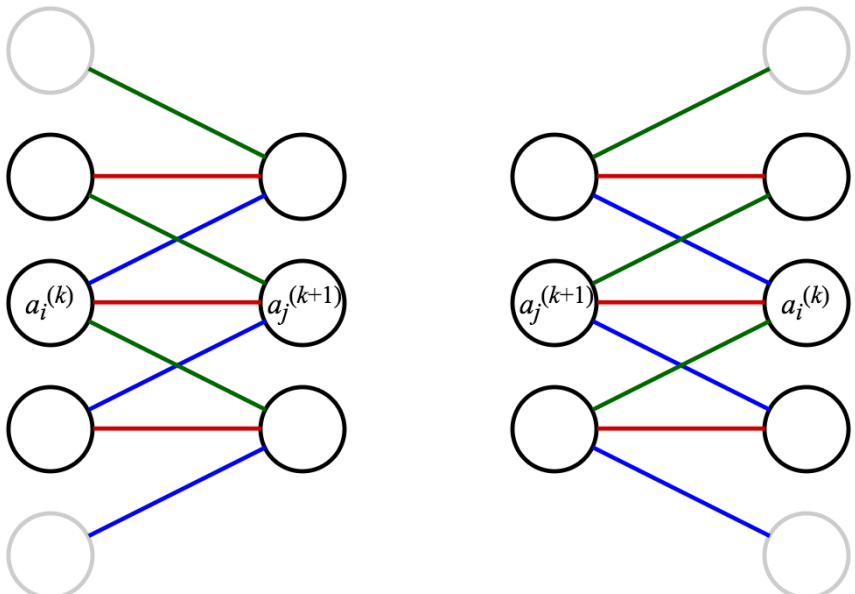


- How to train deconvolution layer? Treat it as convolution layer



Manifolds I

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

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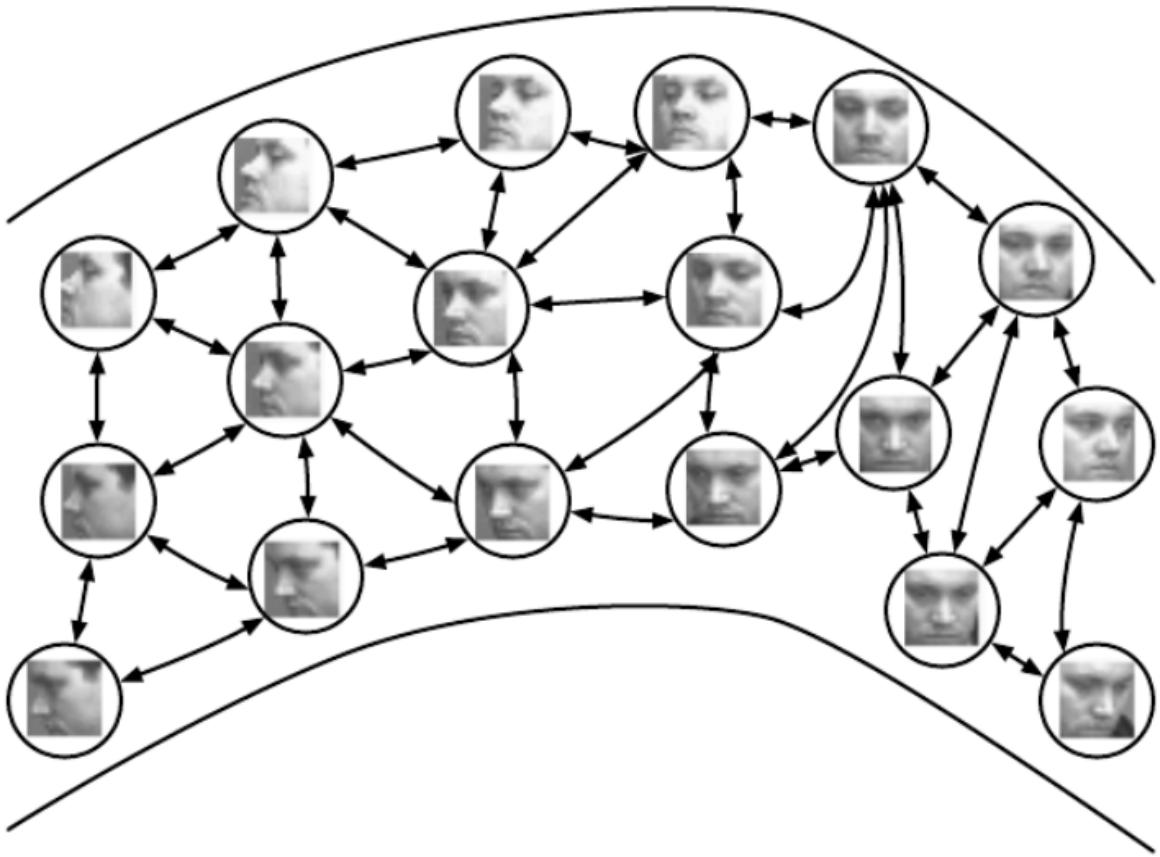
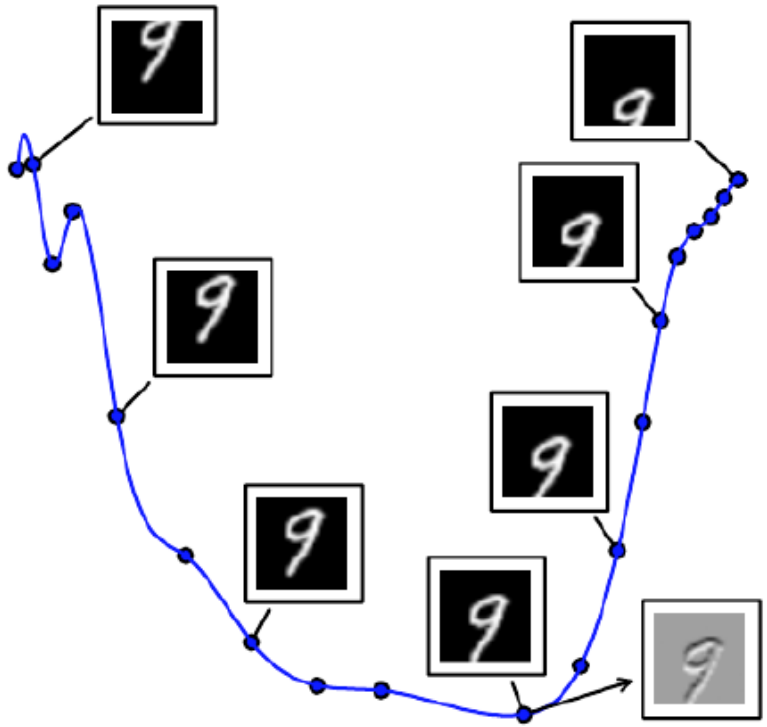
- A manifold is a topological space that are ***linear locally***



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 [16]: regularize the code $\mathbf{c}$ such that it is invariant to local changes of $\mathbf{x}$:

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

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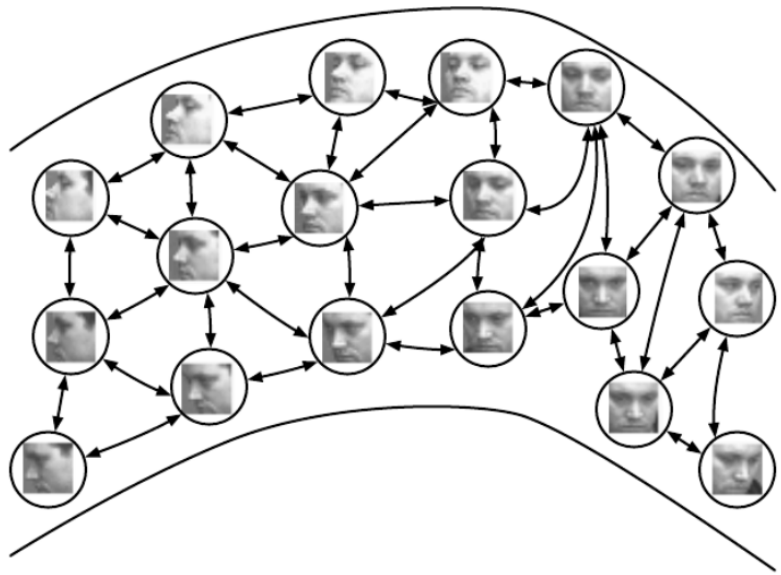
- Encoder preserves local structures in code space



Learning Manifolds II

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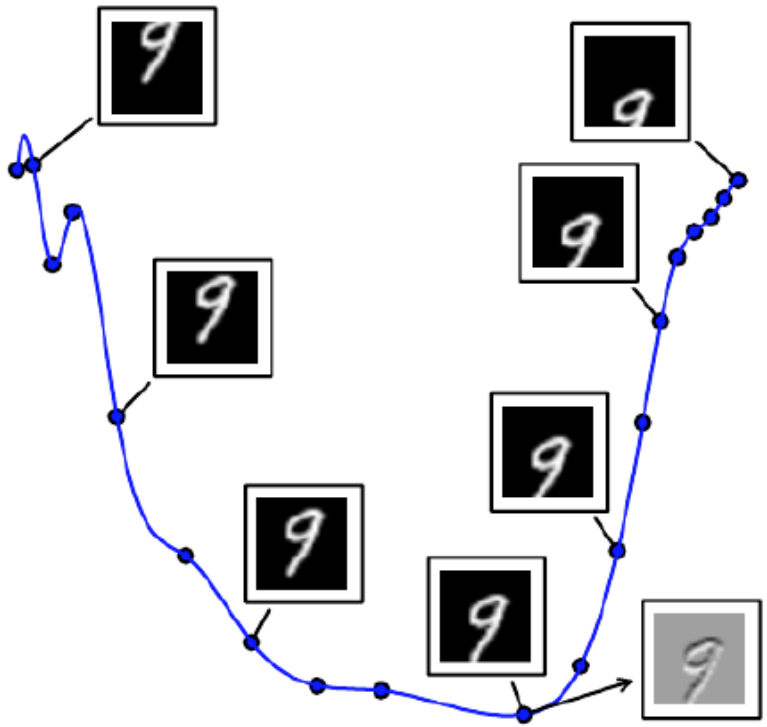
  - Encoder: to encode $\mathbf{x}$ ***with*** random noises
  - Decoder: to reconstruct $\mathbf{x}$ ***without*** noises

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 point?



Tangent Vectors II

- 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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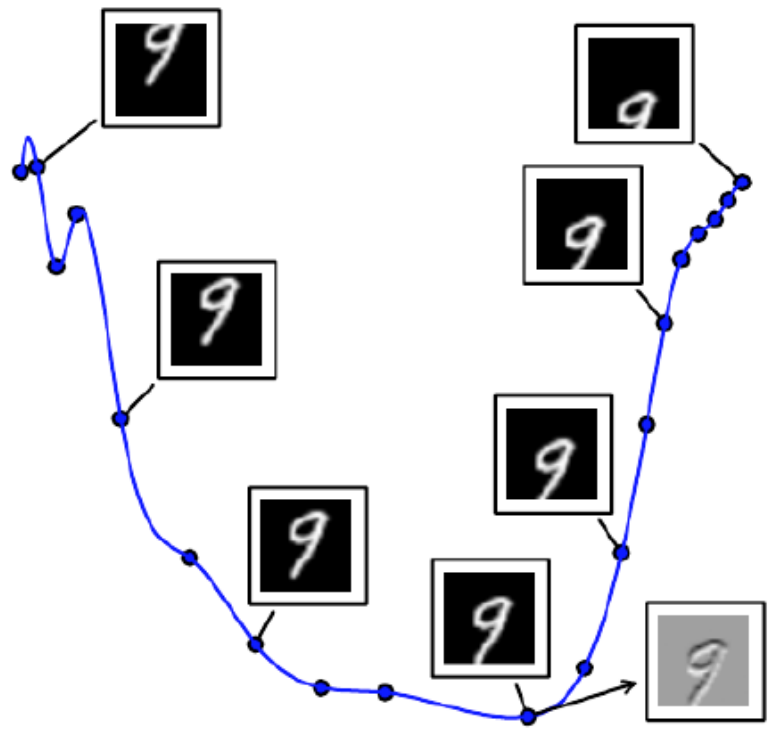
- Directions in the input space that ***changes $\boldsymbol{c}$ most*** should be tangent vectors



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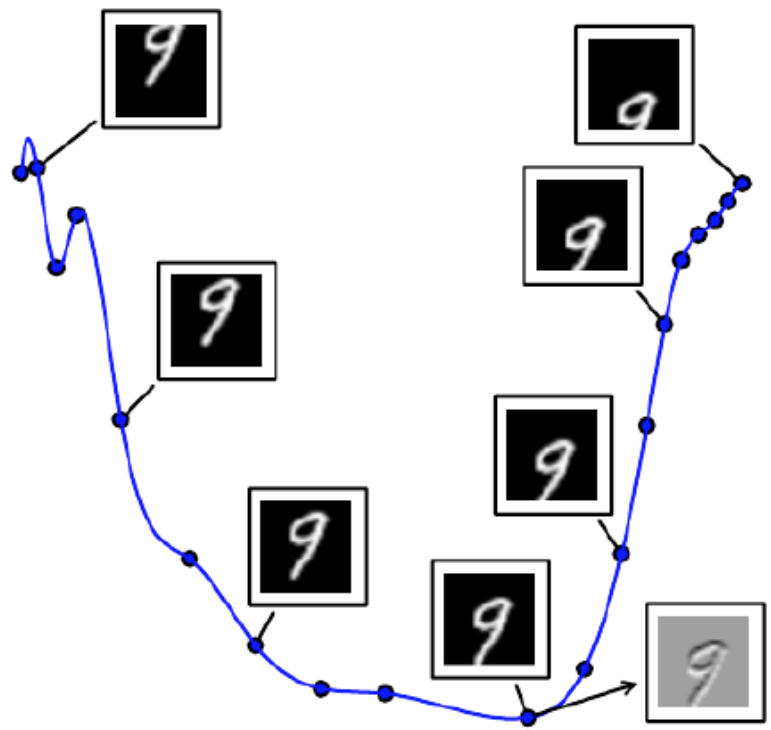
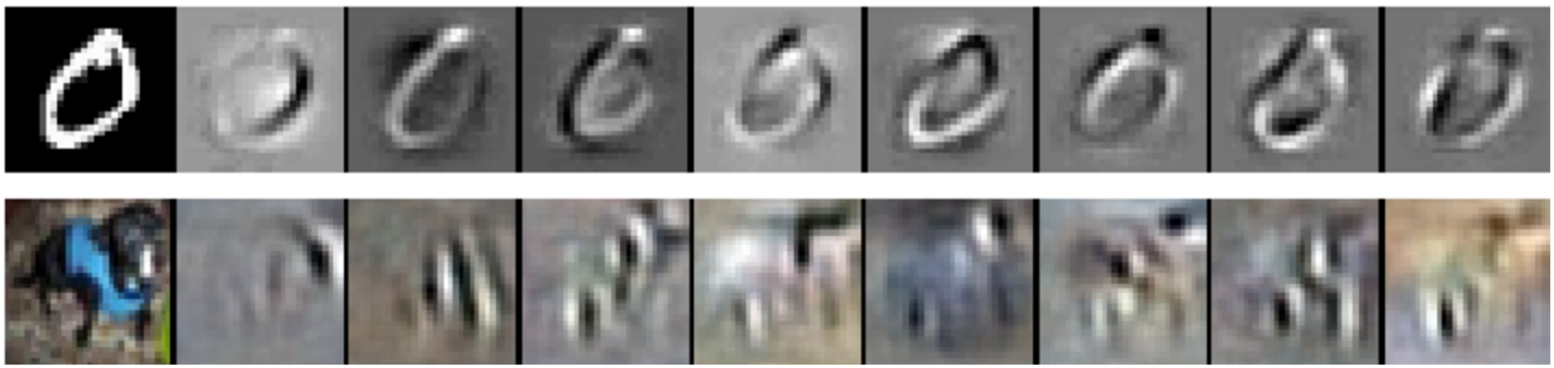
- Directions in the input space that ***changes $\boldsymbol{c}$ most*** should be tangent vectors

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 $\boldsymbol{D}$



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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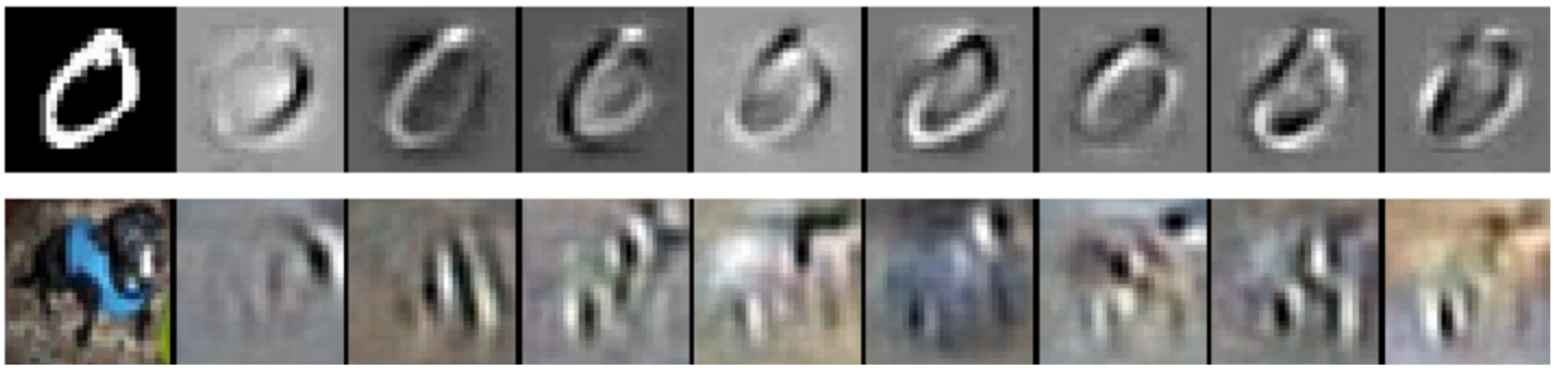
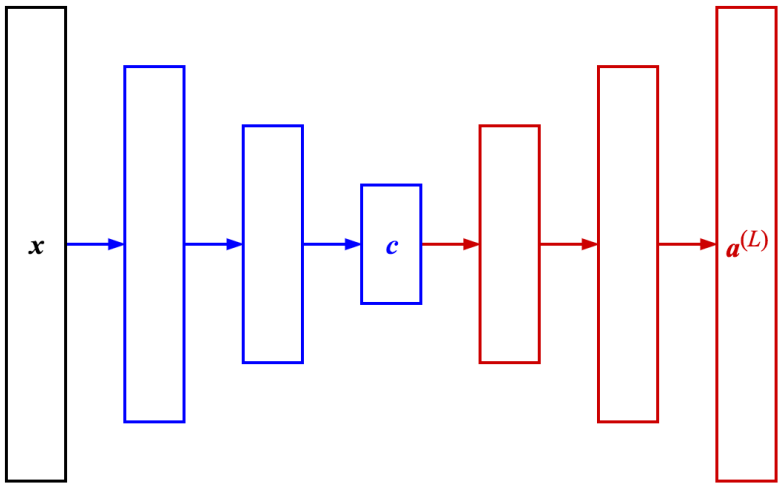


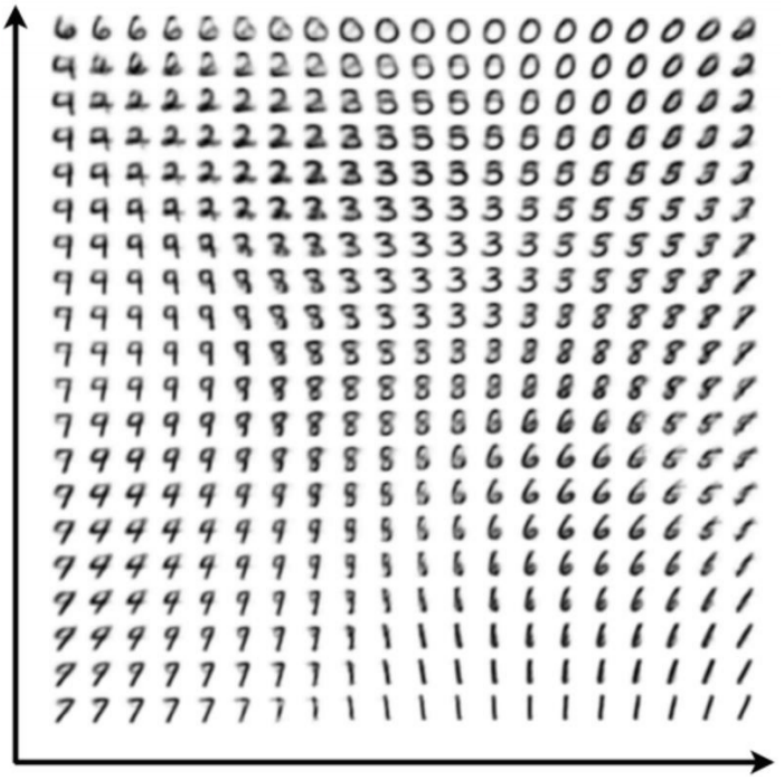
- Can be used by Tangent Prop [18]:
- Let $\{\boldsymbol{v}^{(i,j)}\}_j$ be tangent vectors of each example $\boldsymbol{x}^{(i)}$
- Trains an NN classifier f with cost penalty: $\Omega[f] = \sum_{i,j} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}^{(i)})^\top \boldsymbol{v}^{(i,j)}$
  - Points in the same manifold share the same label

Outline

Decoder as Data Generator

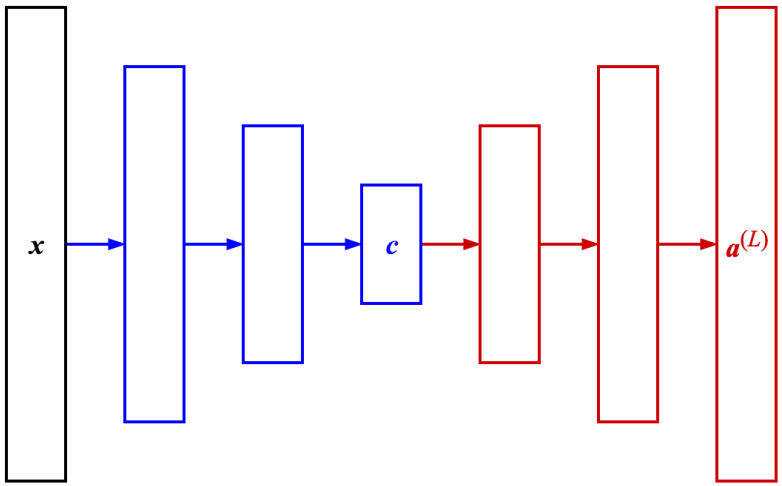
- Decoder can generate data points even with ***synthetic codes***

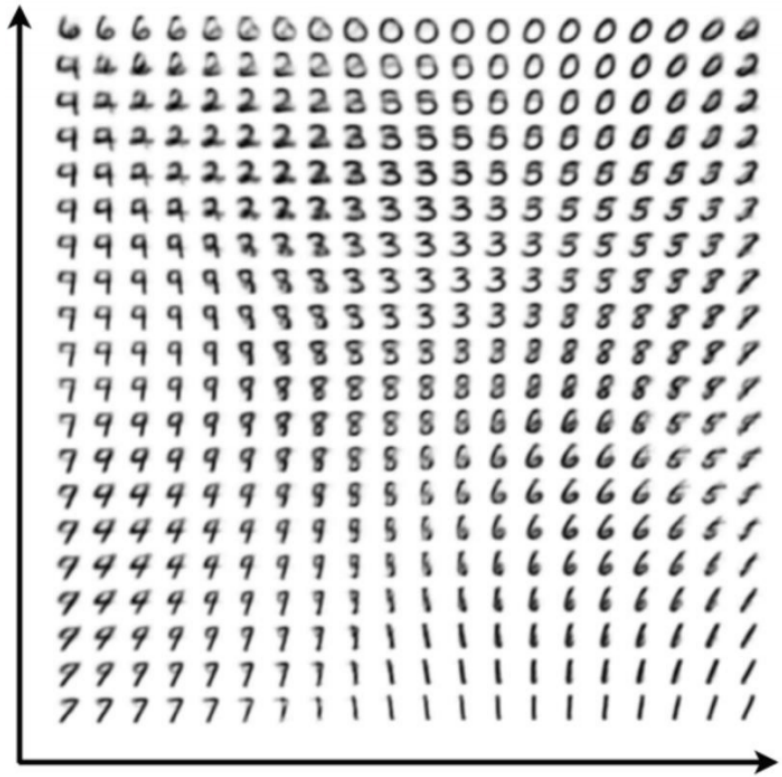




Decoder as Data Generator

- Decoder can generate data points even with ***synthetic codes***

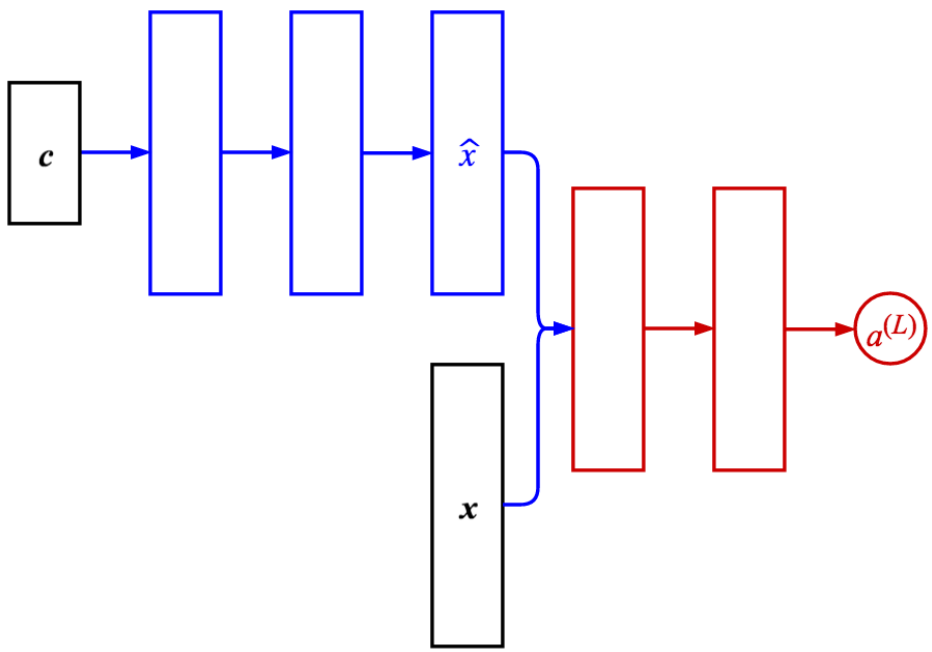




- However, decoder just "remembers" the samples it has seen
  - Generated data are just combinations of training examples

Generative Adversarial Networks (GANs)

- *Generative adversarial network* (*GAN*) [4]:
- Generator: to generate data points from random codes
- Discriminator: to separate generated points from true ones



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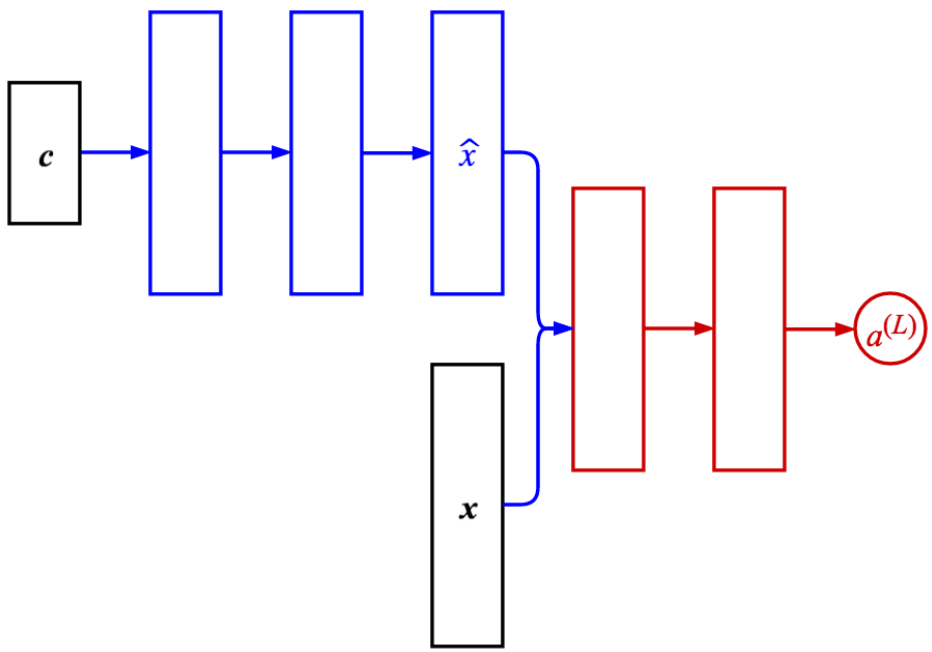

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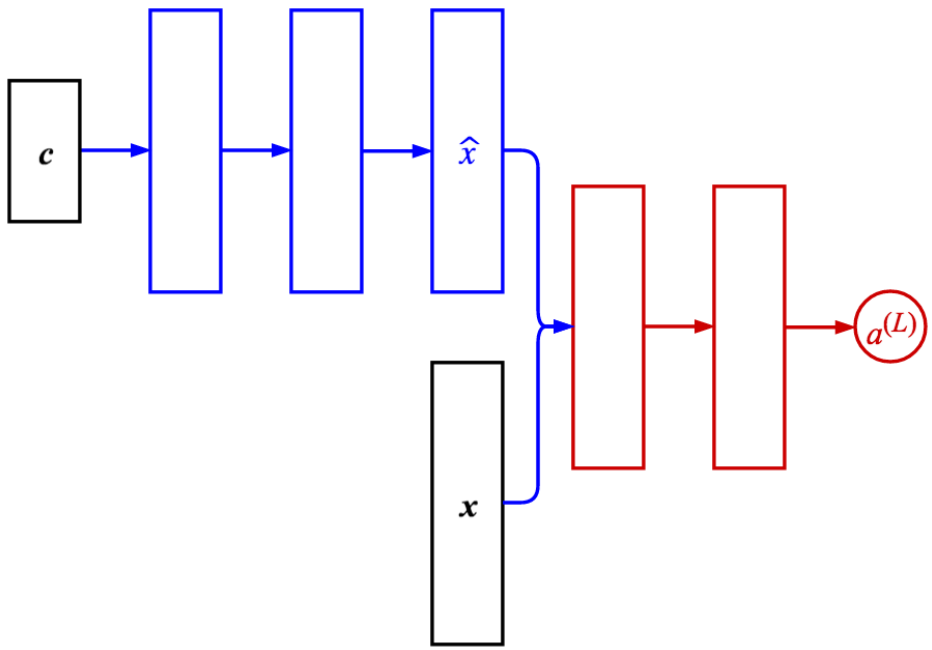
  - Weights for $\boldsymbol{x}$ and $\hat{\boldsymbol{x}}$ are tied

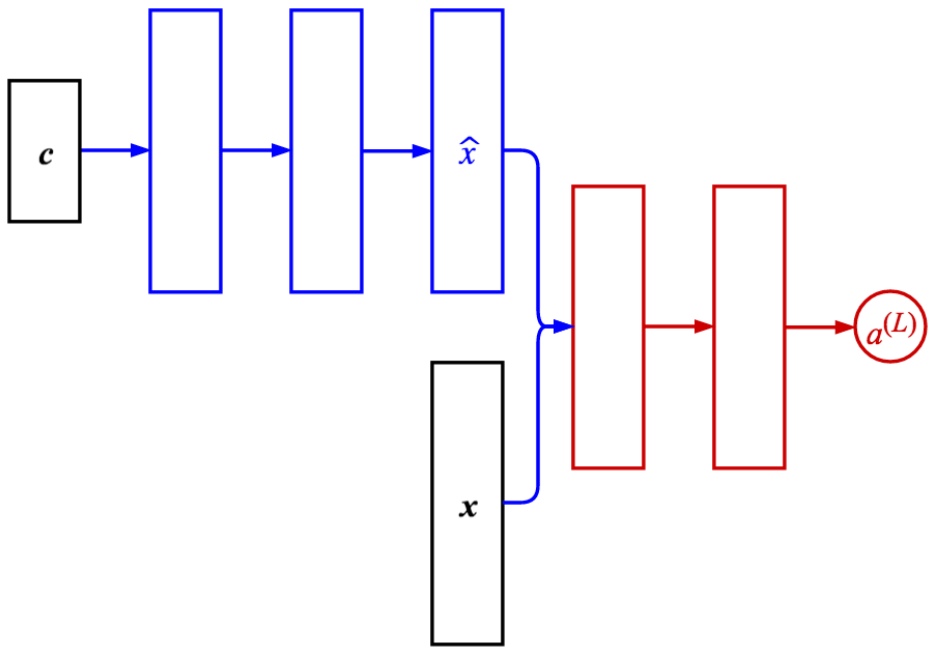


Cost Function

- In normal binary classification, we have the log likelihood
  $\log \mathrm{P}(\mathbb{X}|\Theta) = \sum_n \log \mathrm{P}(y^{(n)}|\boldsymbol{x}^{(n)}, \Theta) = \sum_n \log \left[(\hat{\rho}^{(n)})^{y^{(n)}} (1-\hat{\rho}^{(n)})^{(1-y^{(n)})} \right]$
- Cost function (N true points, M generated points):

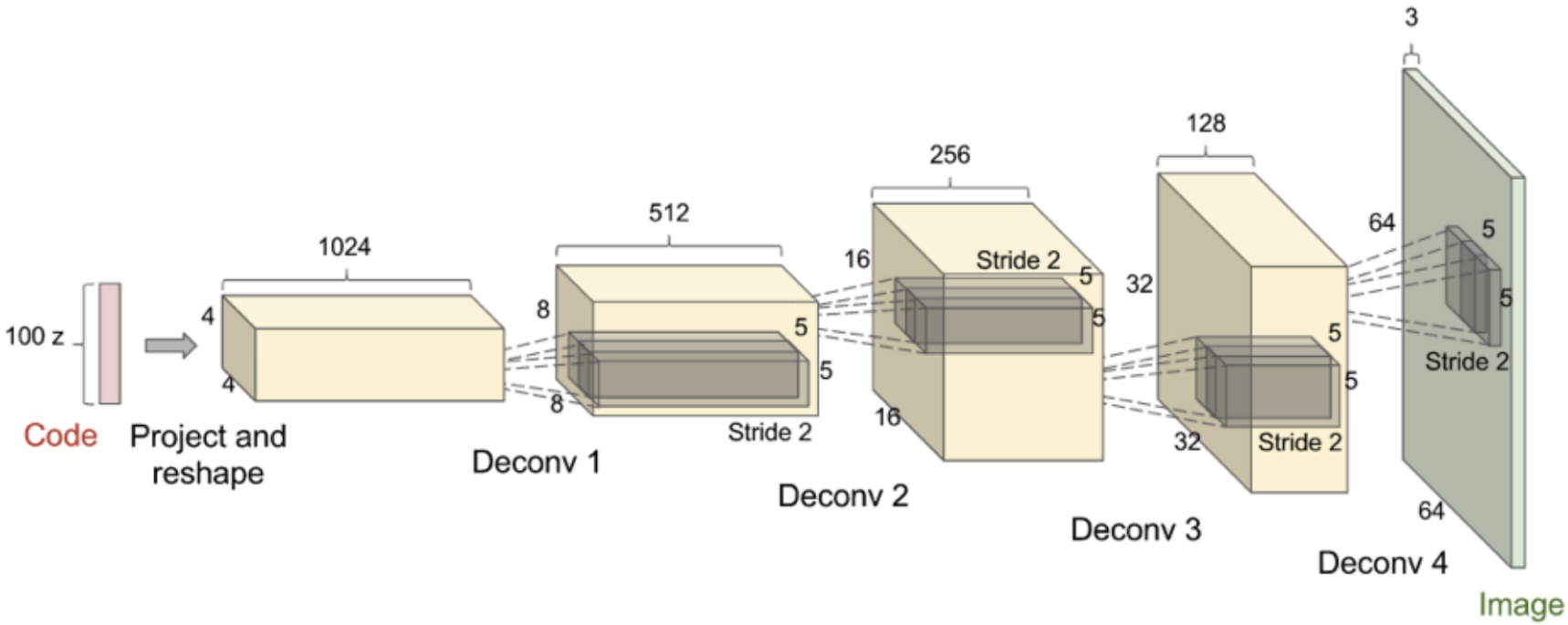
$$\arg \min_{\Theta_{\text{gen}}} \max_{\Theta_{\text{dis}}} \sum_n \log \hat{\rho}^{(n)} + \sum_m \log(1-\hat{\rho}^{(m)})$$

- $\hat{\rho}^{(n)}$ depends on Θ_{dis} only
- $\hat{\rho}^{(m)}$ depends on both Θ_{dis} and Θ_{gen}



Convolutional Generators

- DC-GAN [14] for generating images:



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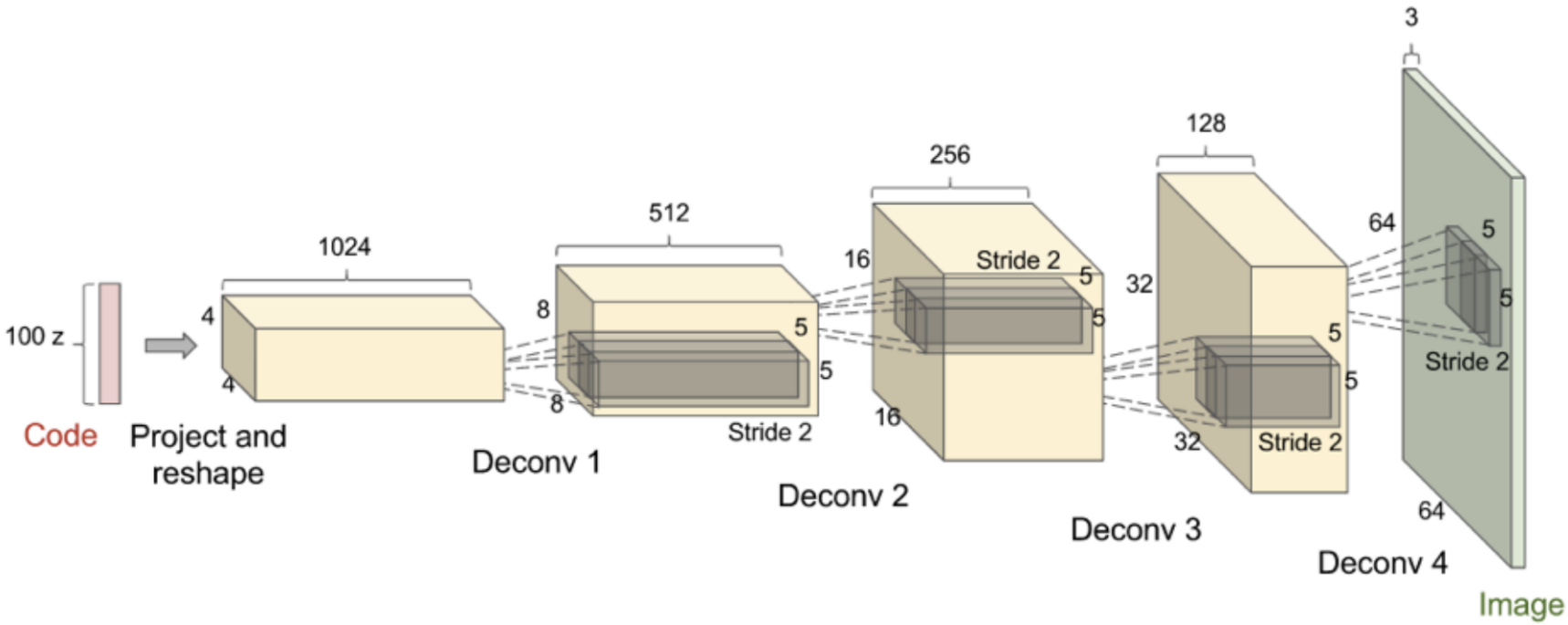

Training: Alternative SGD

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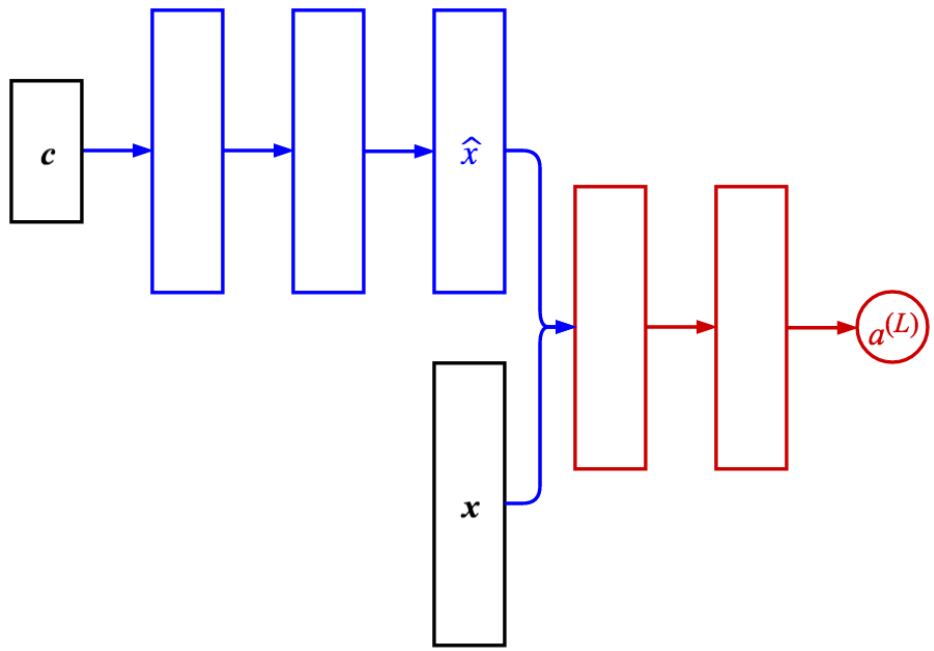

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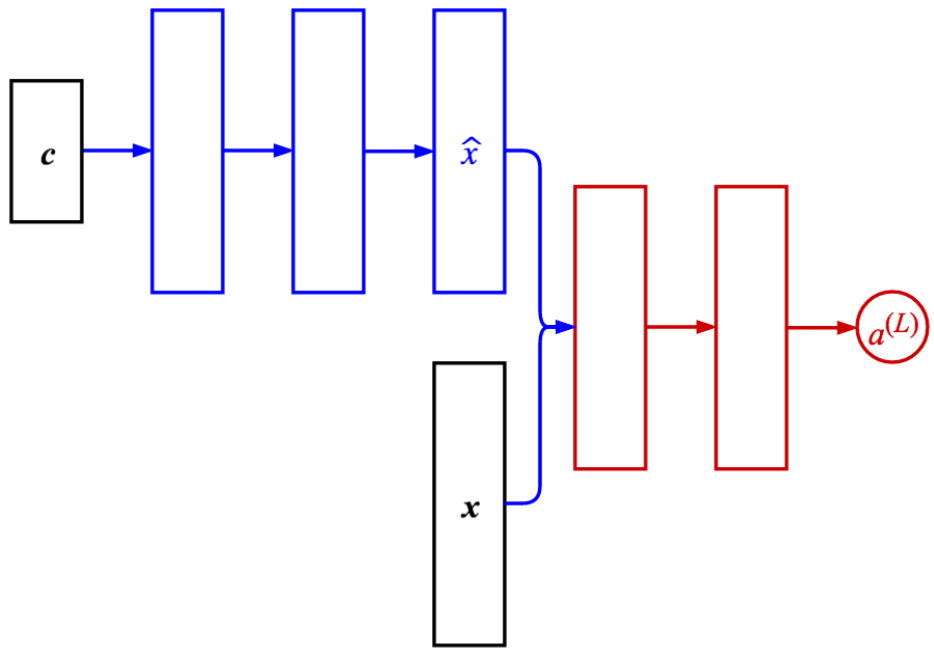

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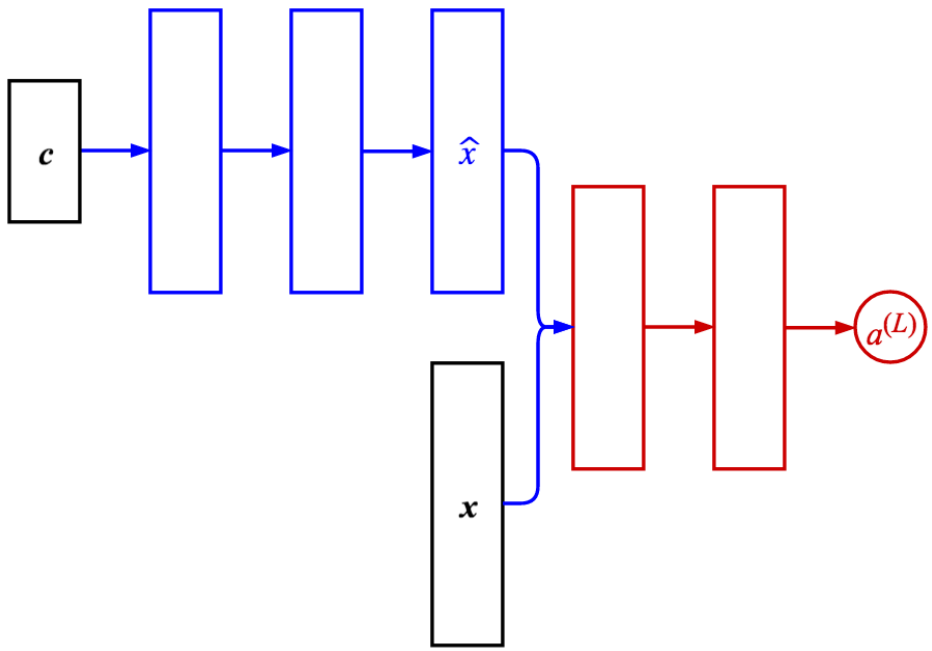

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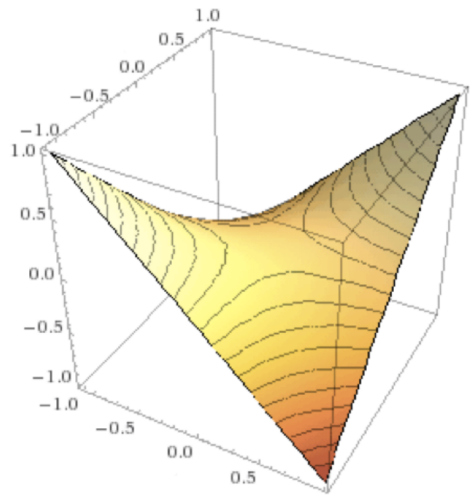
- The goal is to find a saddle point



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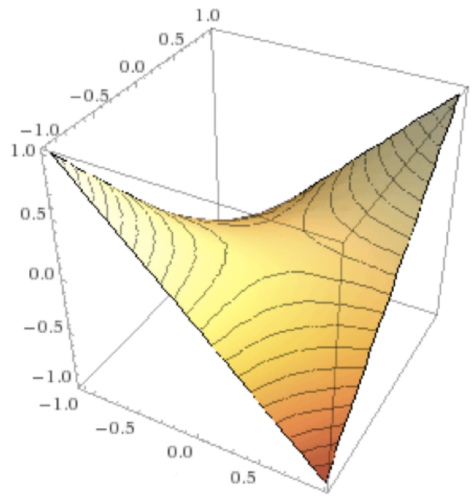

- However, most optimization algorithms are design to find minima
- Avoid momentum in training algorithm

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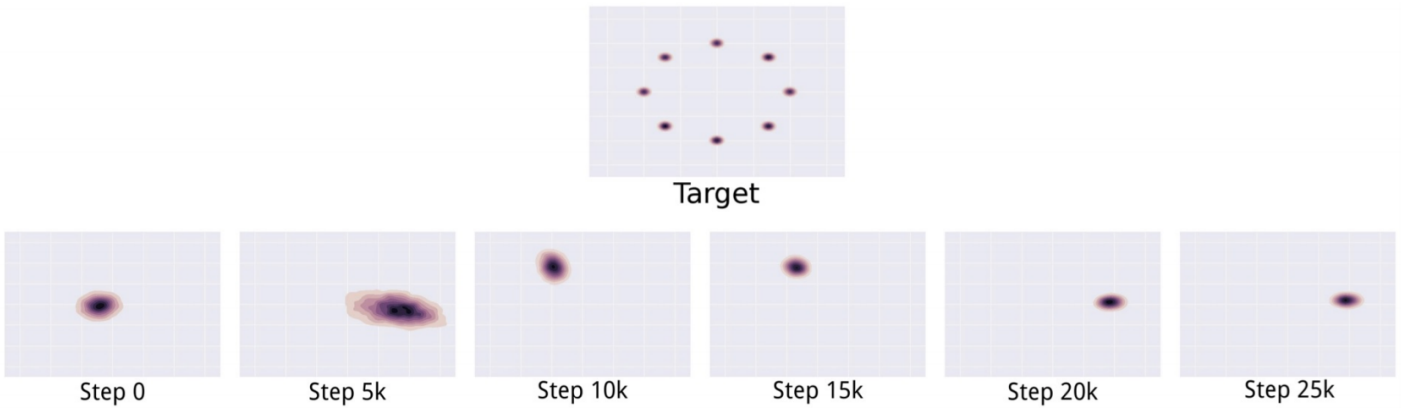
  - Then, discriminator can spot fake points by excluding the point
- Discriminator and generator cancel each other's progress during training steps



Unrolled GANs

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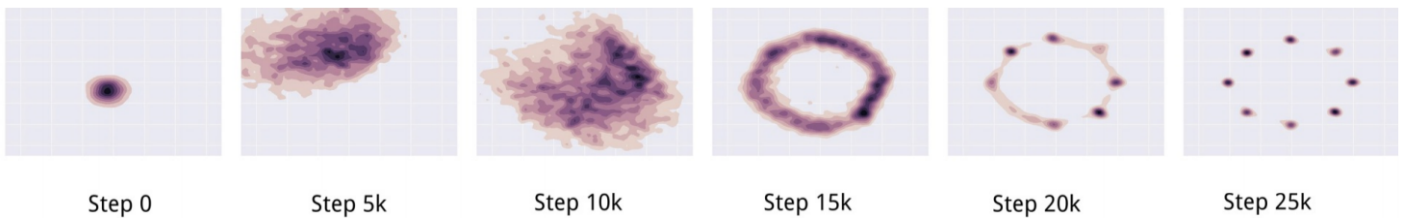
- Unrolled GANs [11]: to back-propagate through ***several*** max ***steps*** when computing $\nabla_{\Theta_{\text{gen}}} C$



Minibatch Discrimination

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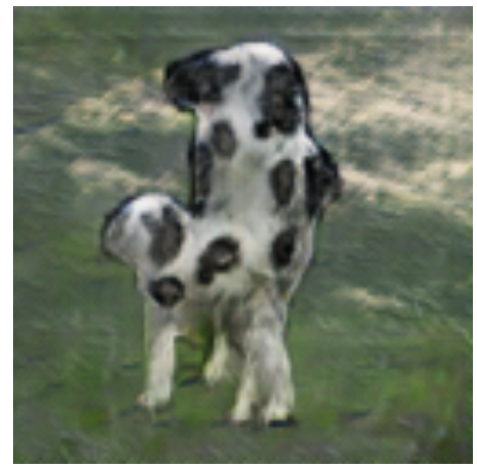
- Without vs. with minibatch discrimination:

Other Difficulties

Counting

Perspective

Global structure



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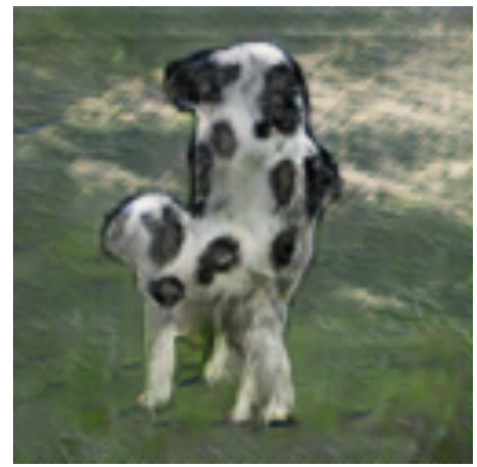
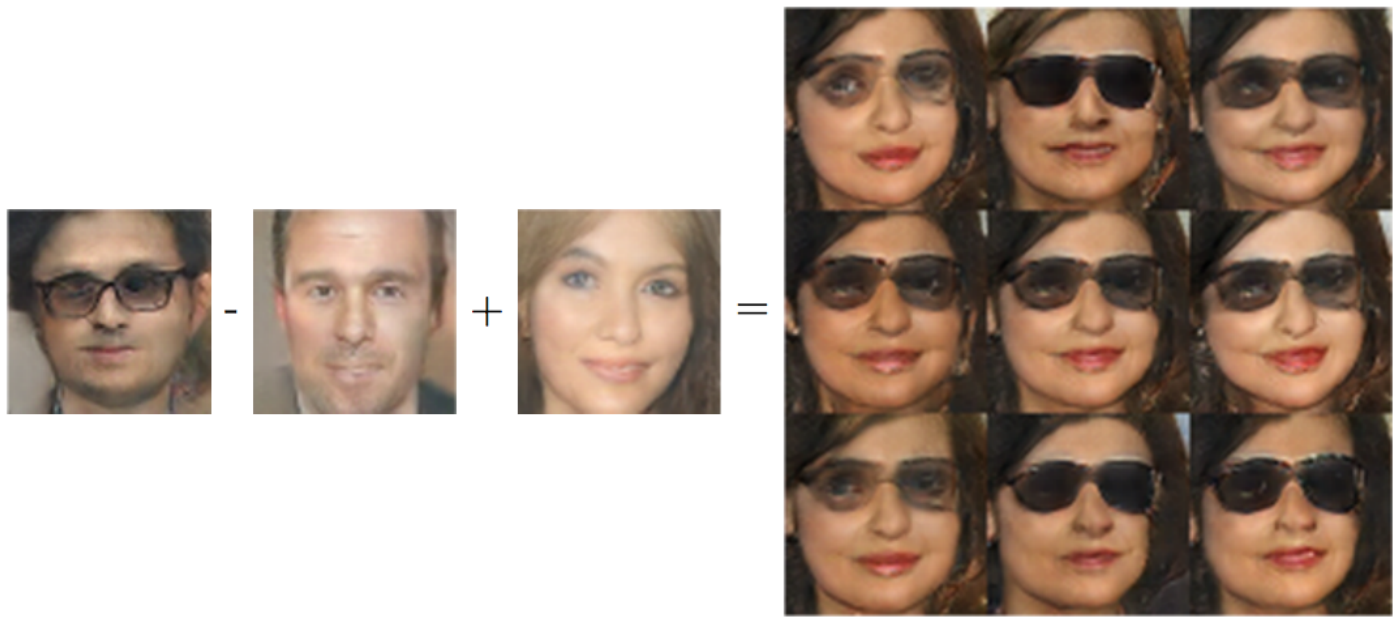


- Still are research problems

Code Space Arithmetics

- DC-GAN [14] can learn to use codes in meaningful ways:



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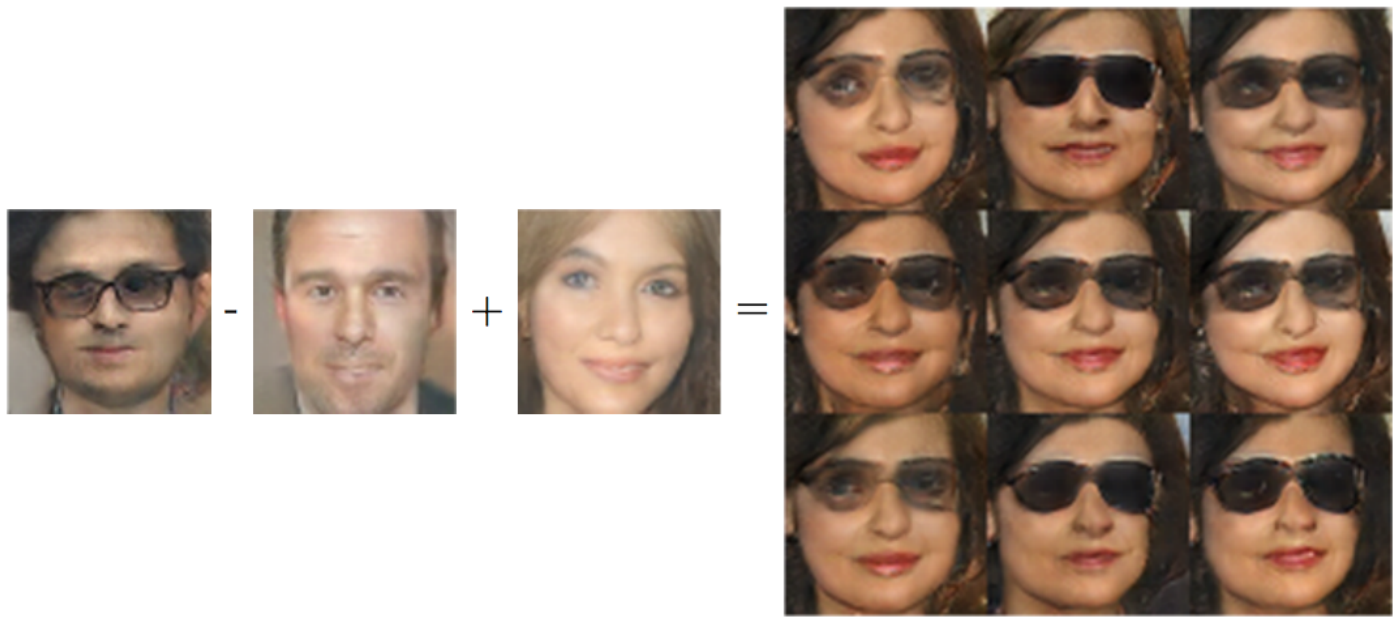
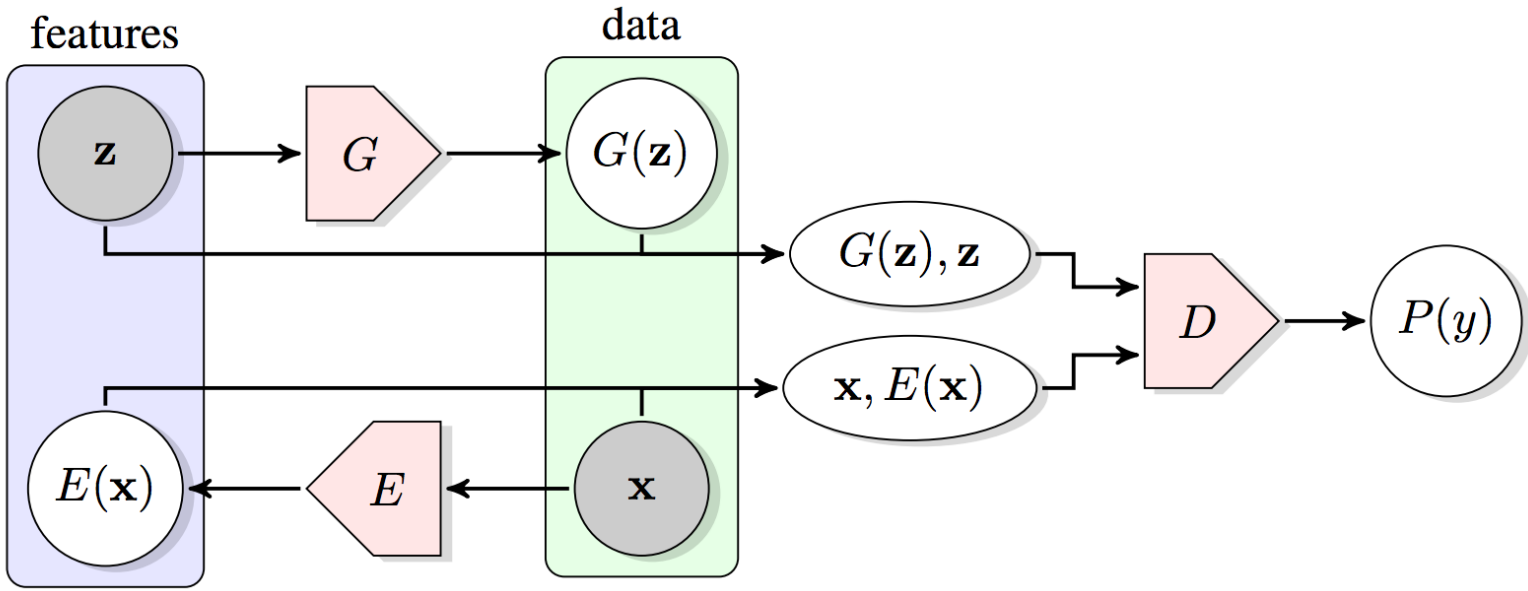


- Finding codes for images with constraints [22, 1] ▸ Demo 1 ▸ Demo 2

Learn to Encode in GANs

- Adversarial feature learning [2, 3]:



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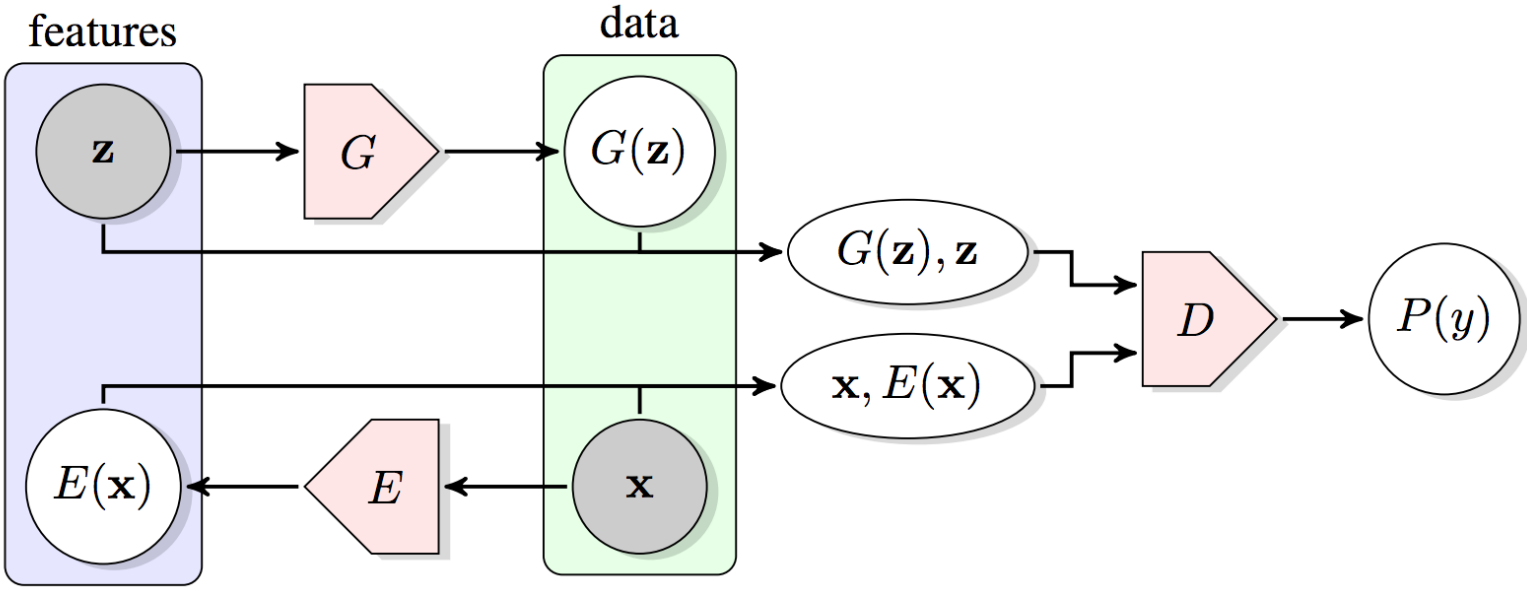
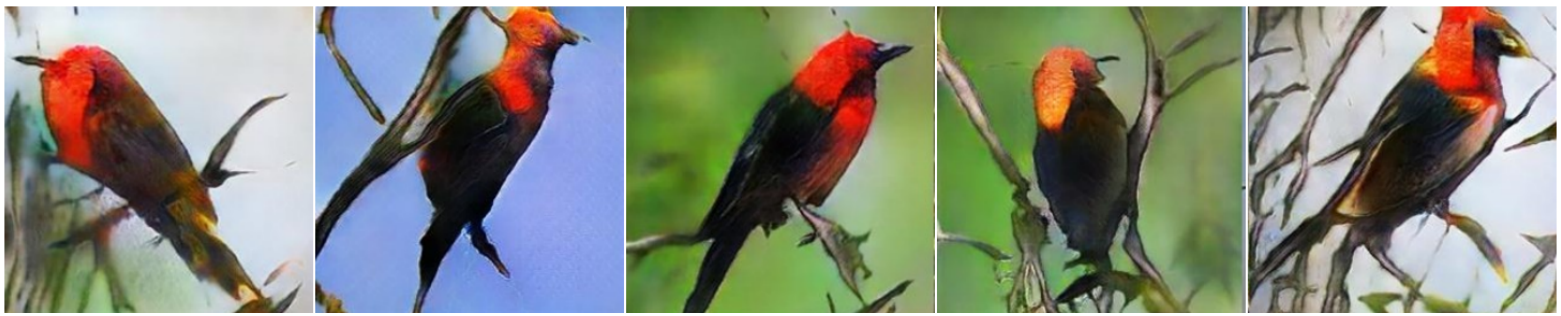


Conditional GAN I

- How?

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



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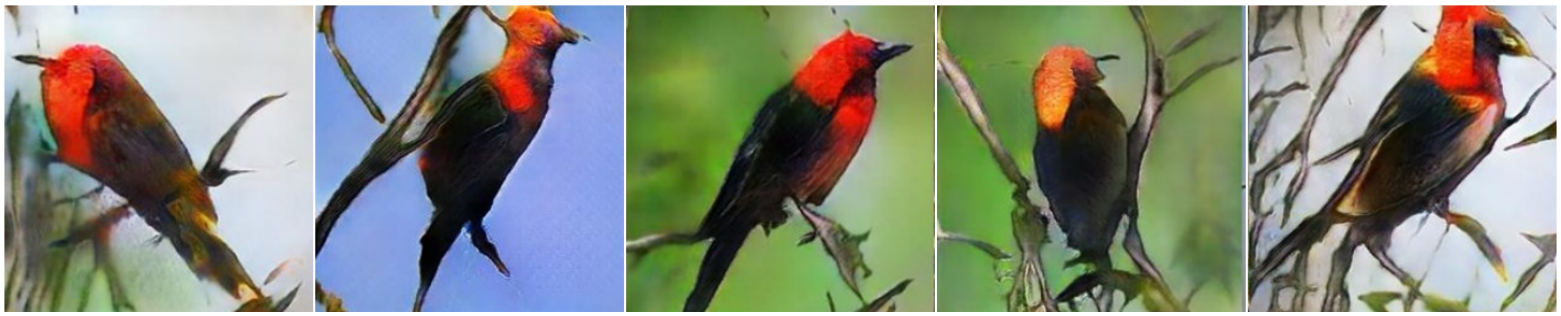
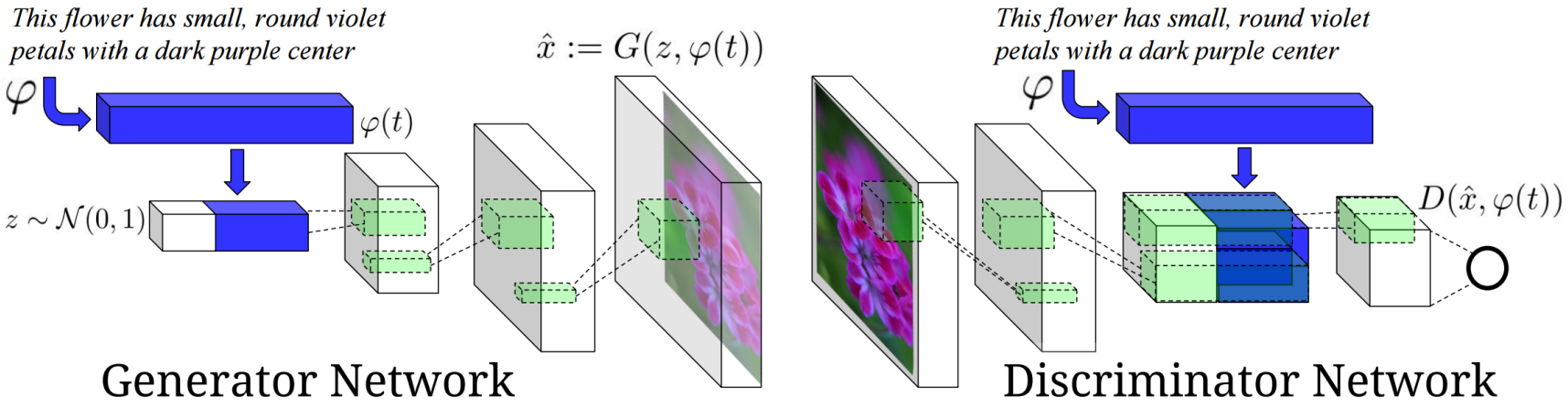
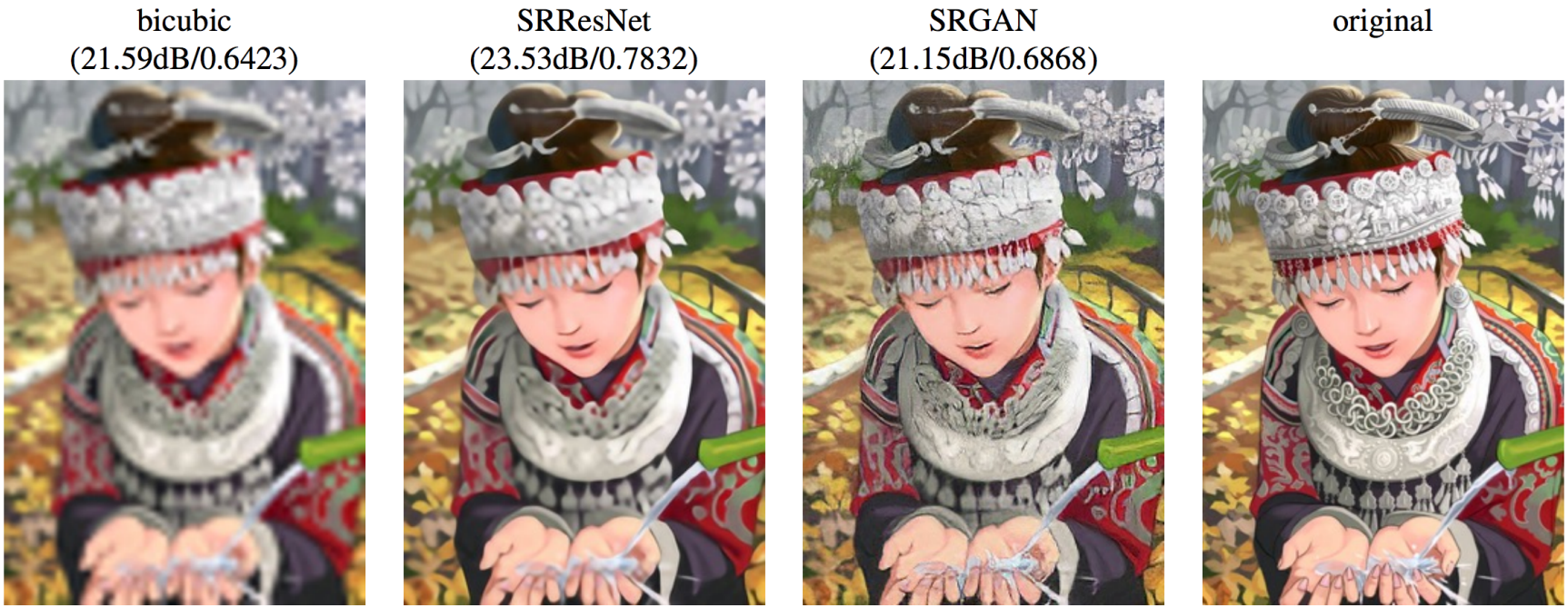


- Text to image [15]:



More GANs I

- Super resolution [8]:



More GANs II

- Image-to-image translation [5]:

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