Graphite:
Iterative Generative Modeling of Graphs

GNN Study Group - Elian

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- Learning Deep Latent Variable Models

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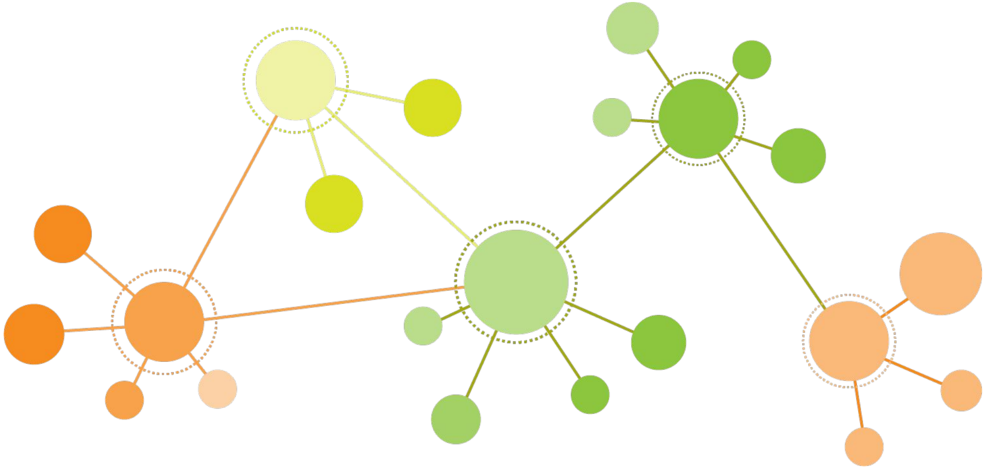
01

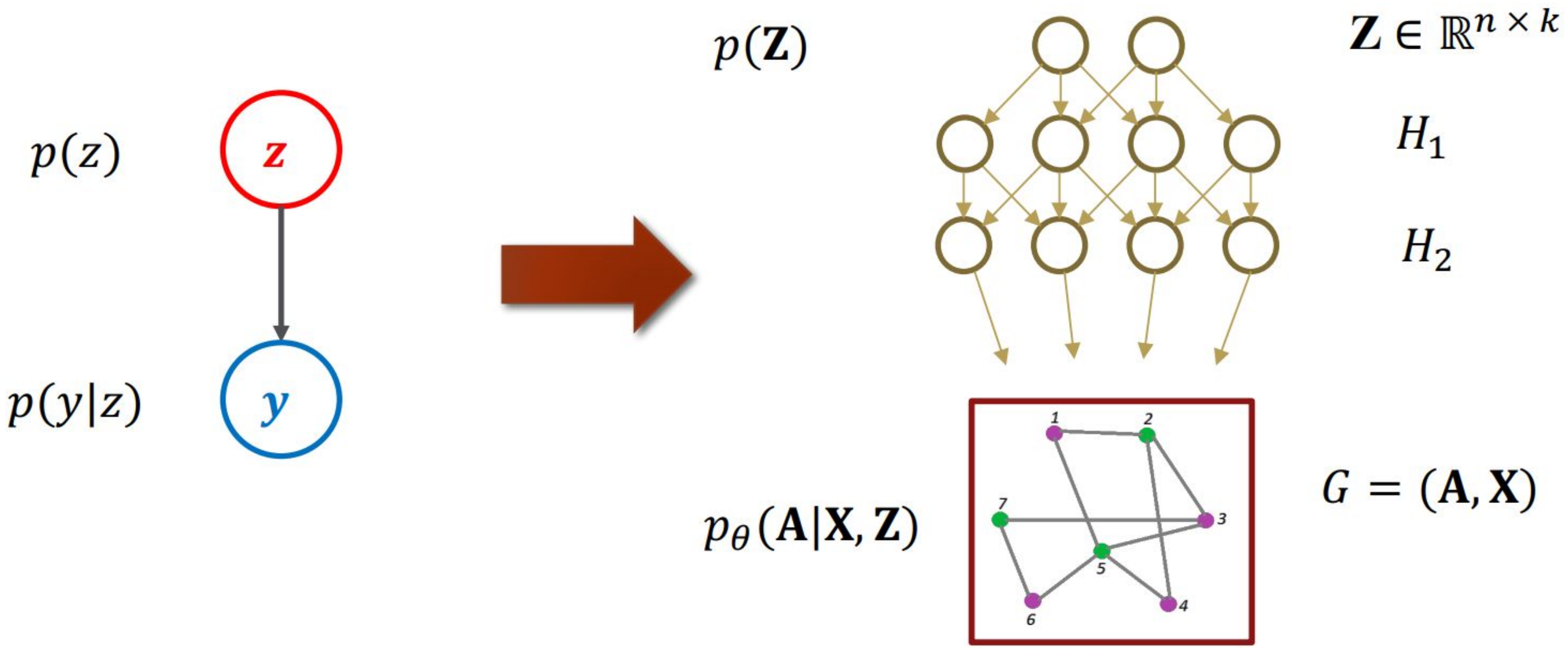
INTRODUCTION

Graph are Ubiquitous



- Ecology:
  - Food web networks
- Biology:
  - Brain networks
  - Protein-protein interaction networks
- Chemistry:
  - Molecules
  - Materials

Learning Deep Latent Variable Models of Graphs

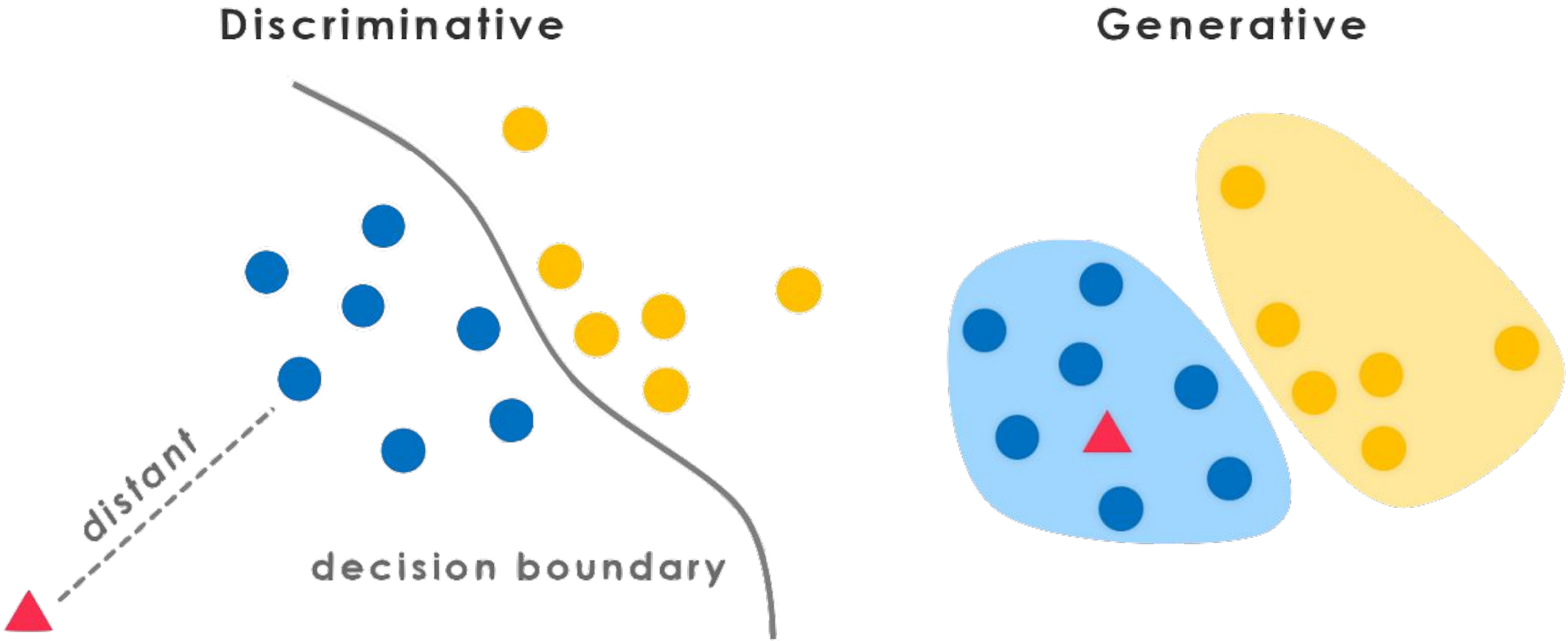


02

AUTOENCODER

What is the Modeling Means?

- Generative vs. Discriminative



What is the Modeling Means?

- Generative vs. Discriminative

What is the Modeling Means?

- Generative vs. Discriminative

Discriminative:

- Skin Color
- Hair Color
- Eye Color
- Facial Different
- Clothing Style
- etc...

Generative:

Asian:

- yellow skin
- small eyes
- black hair
- etc...

African:

- black skin
- black skin
- black skin
- etc...

How to Generate?

- Naive Bayes

Bayes' Theorem:

$$p(Y|\mathbf{X}) = \frac{p(\mathbf{X}, Y)}{p(\mathbf{X})} = \frac{p(Y)p(\mathbf{X}|Y)}{p(\mathbf{X})} \propto p(Y)p(\mathbf{X}|Y)$$

Naive Bayes Generator:

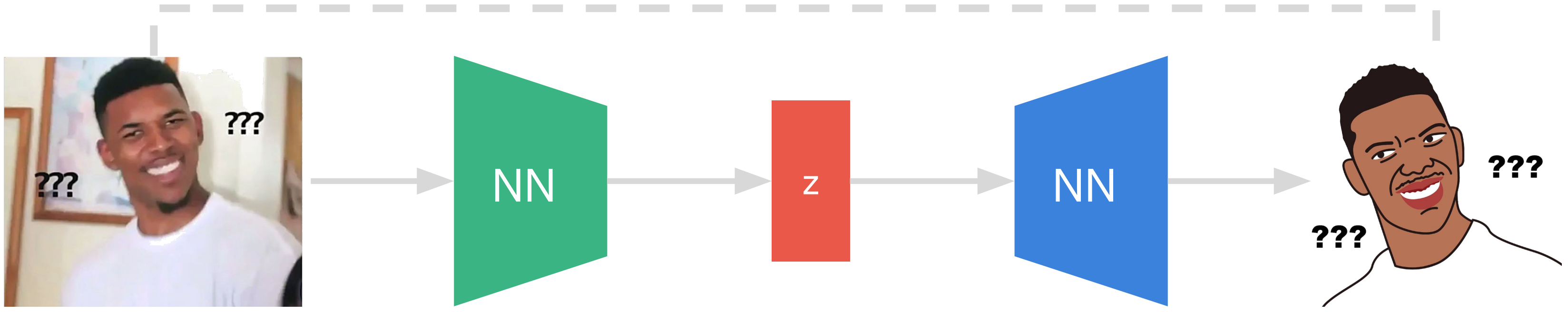
$$p(\mathbf{X}, Y) = p(Y) \times p(X_1, \cdots, X_d|Y) = p(Y) \times \prod_{i=1}^{d} p(X_i|Y)$$

How to Generate?

- AutoEncoder

$$loss = \frac{1}{n}\sum_{i}^{n}(x_i - G(x_i))^2$$

reconstruction loss

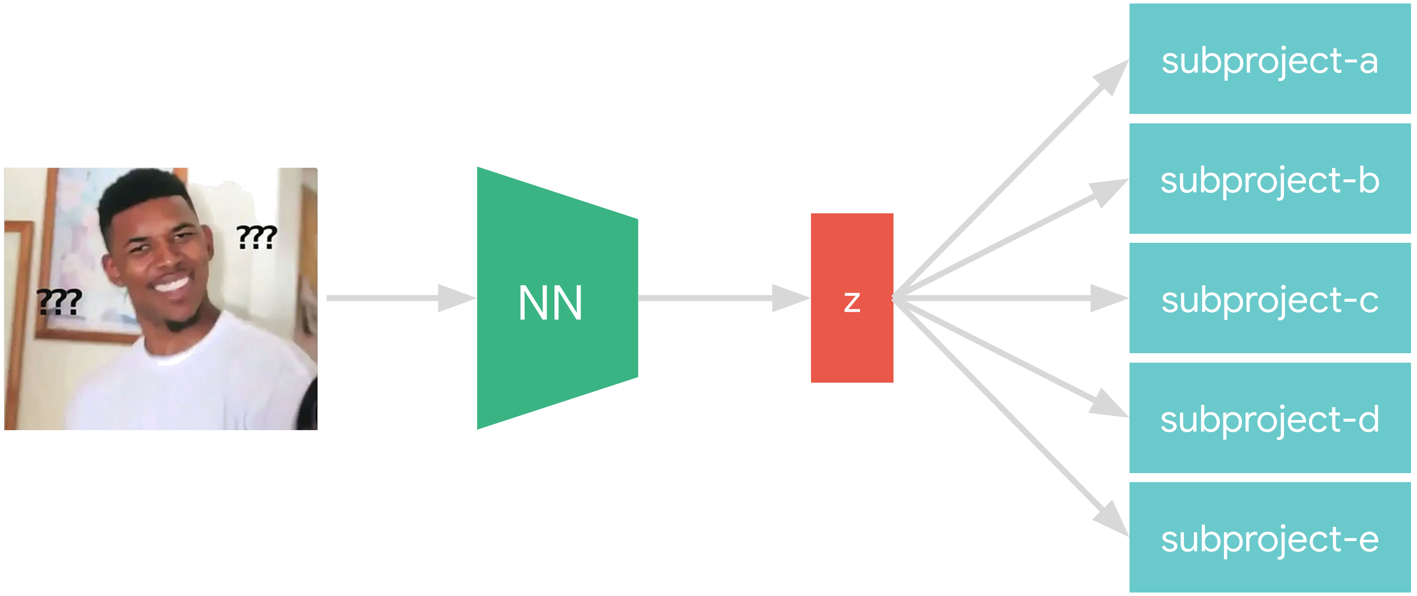


Encoder

Decoder

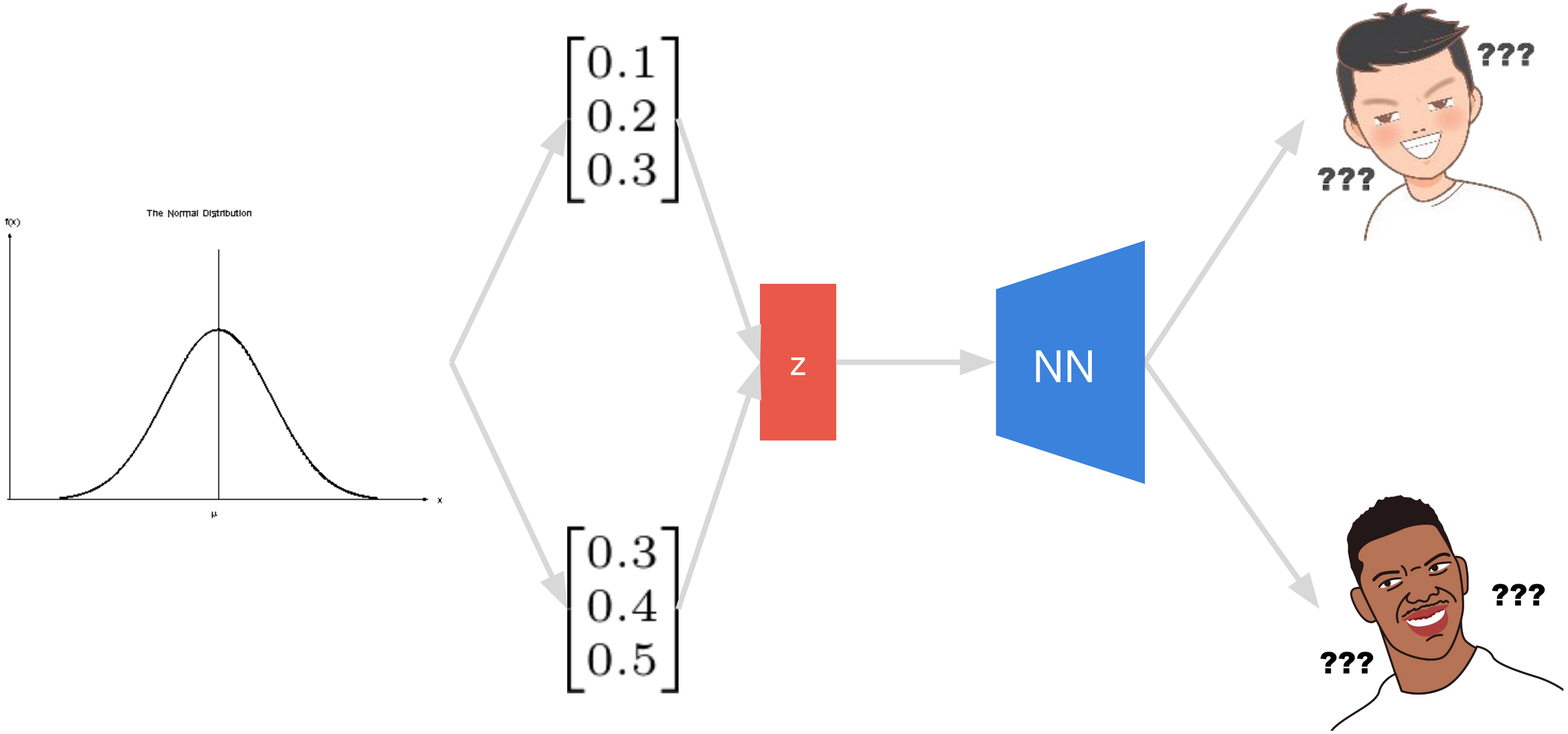
How to Generate?

- Image Compression

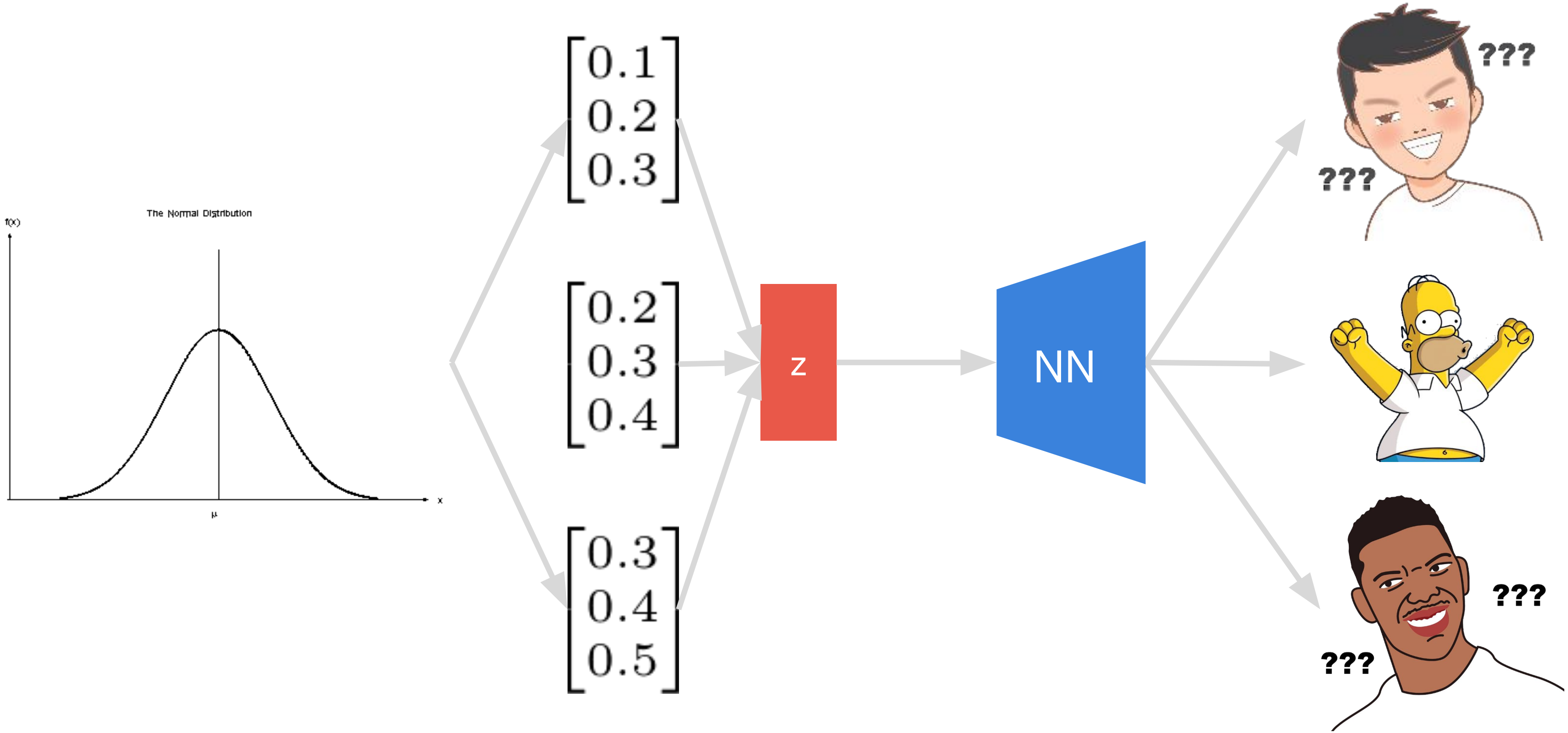


How to Generate?

- Image Generator



AutoEncoder Problem?

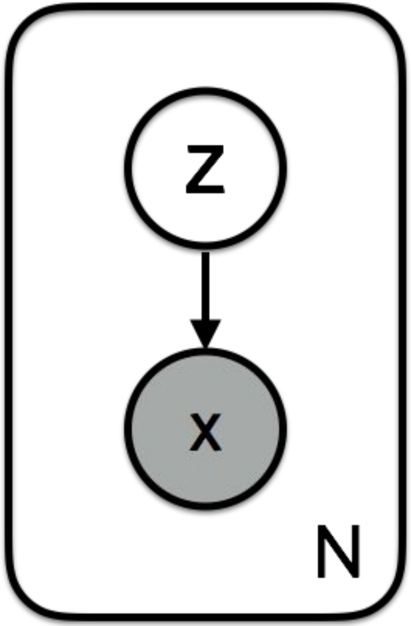


03

VARIANCE

Evidence Lower Bound (ELBO)

- Modeling



Latent Variables: $z_i \sim p(z)$

Data Points: $x_i \sim p_\theta(x \mid z)$

Joint Distribution: $p_\theta(x, z) = p_\theta(x \mid z)p(z)$

Model: $p_\theta(x) = \int p_\theta(x, z)dz$

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

$$p(z \mid \theta) \to p(z \mid x)$$

Evidence Lower Bound (ELBO)

- KL Divergence

KL Divergence: $\min_{\theta} D_{KL}\left[q(z \mid \theta) \parallel p(z \mid x)\right]$

$$
\begin{aligned}
D_{KL}\left[q(z \mid \theta) \parallel p(z \mid x)\right] &= \int q(z \mid \theta) \log \frac{q(z \mid \theta)}{p(z \mid x)} dz \\
&= \int q(z \mid \theta) \log \frac{q(z \mid \theta) p(x)}{p(x, z)} dz \\
&= \int q(z \mid \theta) \log \frac{q(z \mid \theta)}{p(x, z)} dz + \int q(z \mid \theta) \log \frac{p(x)}{p(x, z)} dz \\
&= \int q(z \mid \theta) \left(\log q(z \mid \theta) - \log p(z, x)\right) + \log p(x) \\
&= -\left(E_{q(z \mid \theta)}\left[\log \frac{p(x, z)}{q(z \mid \theta)}\right]\right) + \log p(x)
\end{aligned}
$$

Evidence Lower Bound (ELBO)

- KL Divergence

KL Divergence: $\min_{\theta} D_{KL}\left[q(z \mid \theta) \parallel p(z \mid x)\right]$

$$D_{KL}\left[q(z \mid \theta) \parallel \boxed{p(z \mid x)}\right] = -\boxed{\left(E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right]\right)} + \boxed{\log p(x)}$$

$$\log p(x) = E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right] + D_{KL}\left[q(z \mid \theta) \parallel p(z \mid x)\right]$$

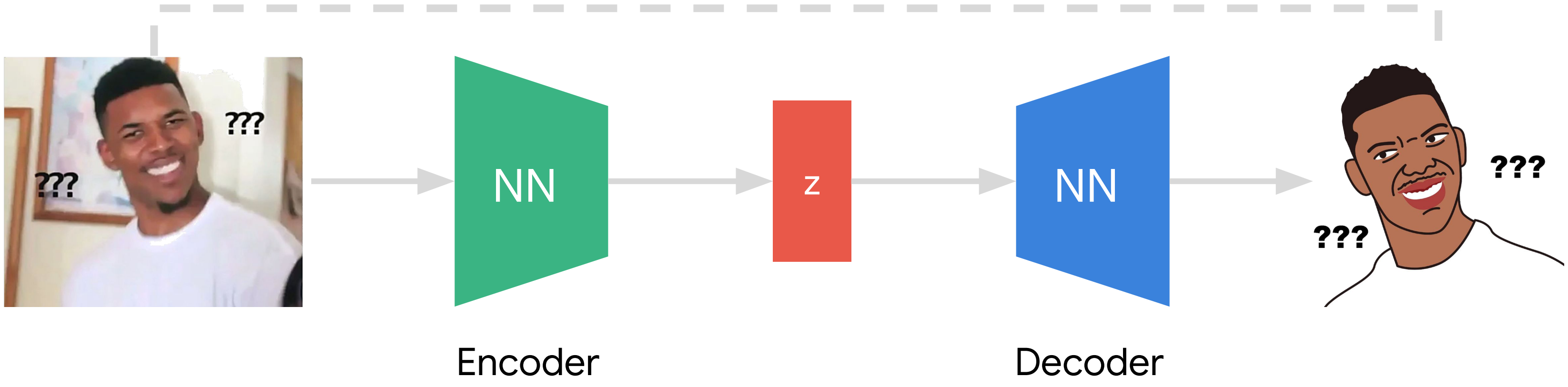
$$\log p(x) \geq E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right]$$

AutoEncoder Review

- AutoEncoder

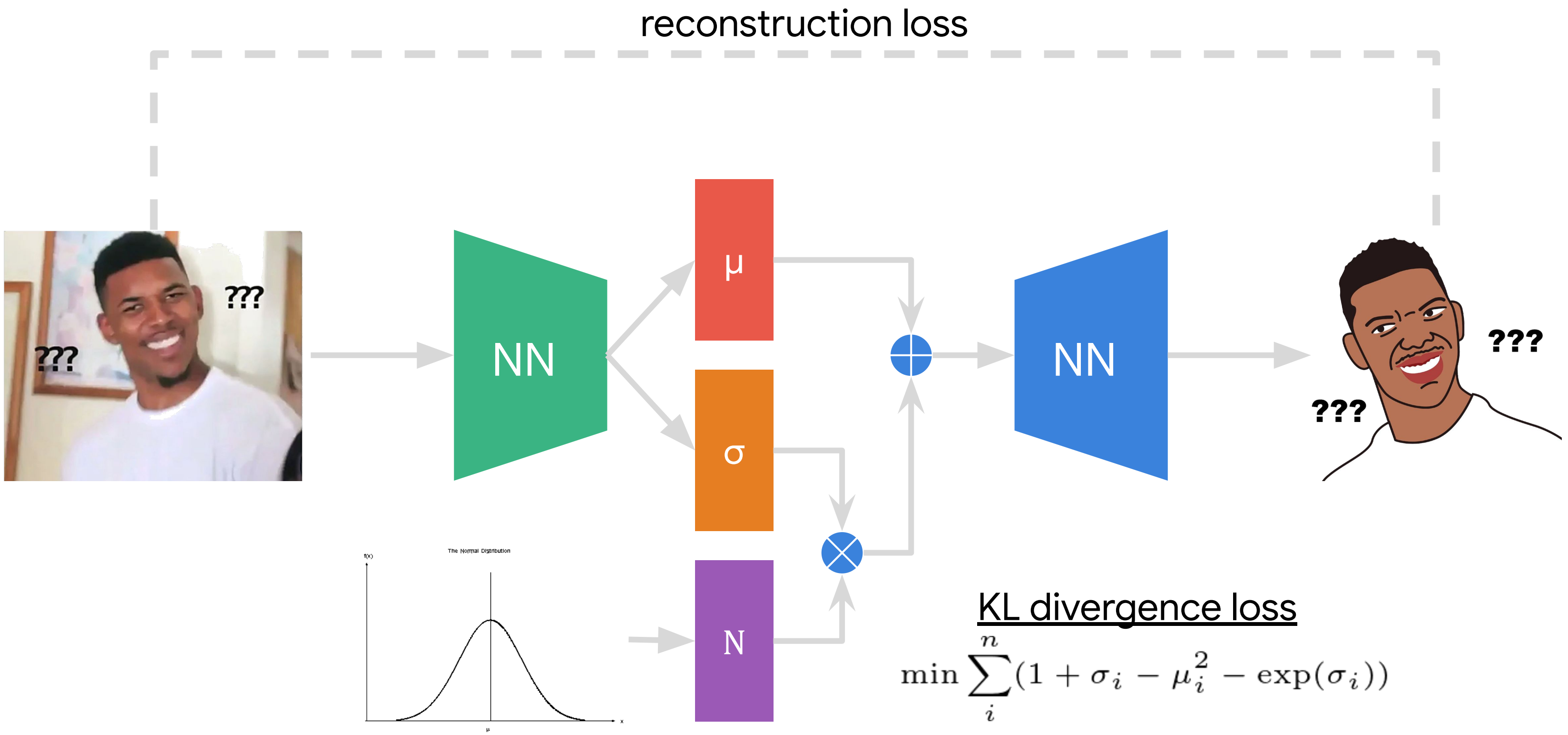
$$loss = \frac{1}{n}\sum_{i}^{n}(x_i - G(x_i))^2$$

reconstruction loss



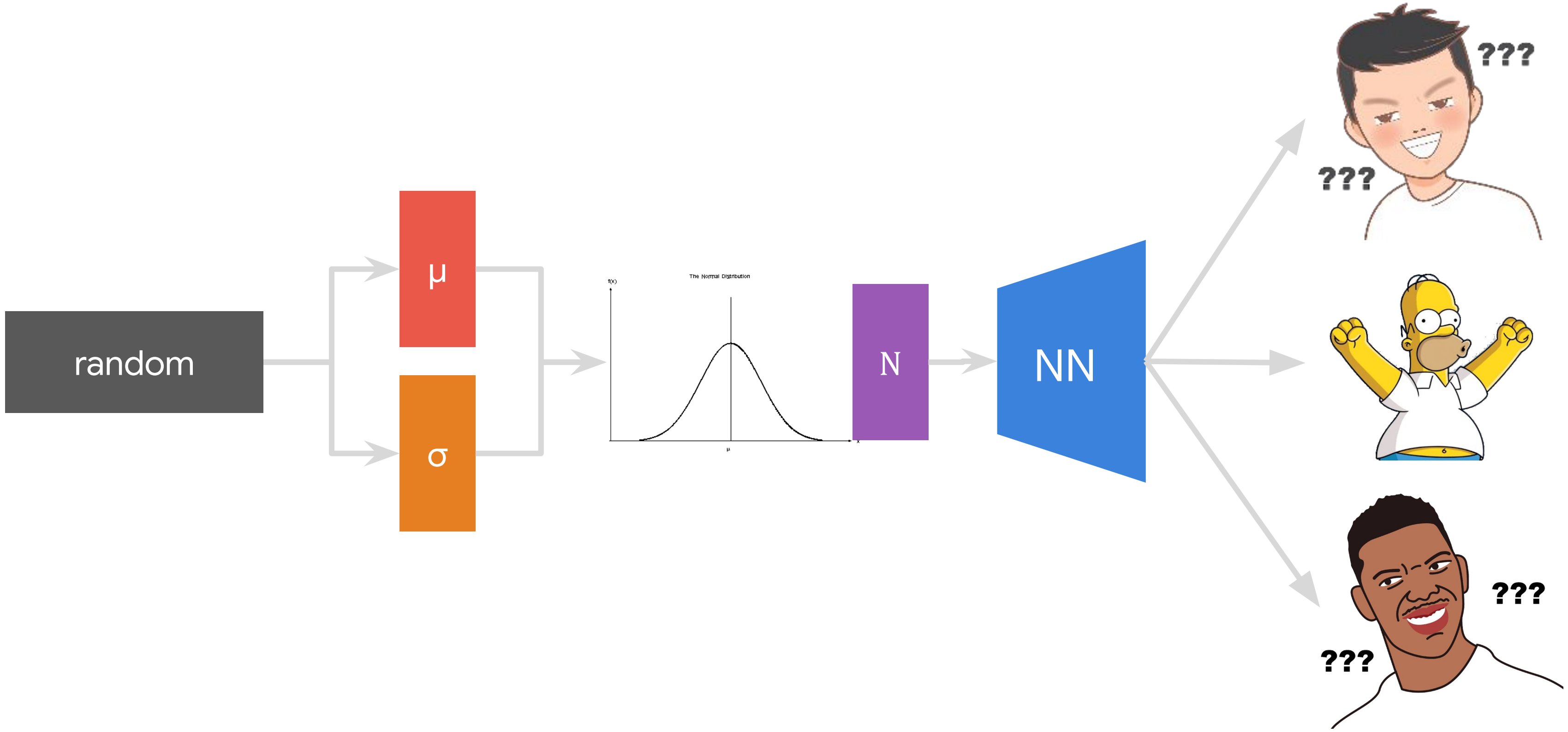
How to Generate?

- Variational AutoEncoder



How to Generate?

- Variational AutoEncoder

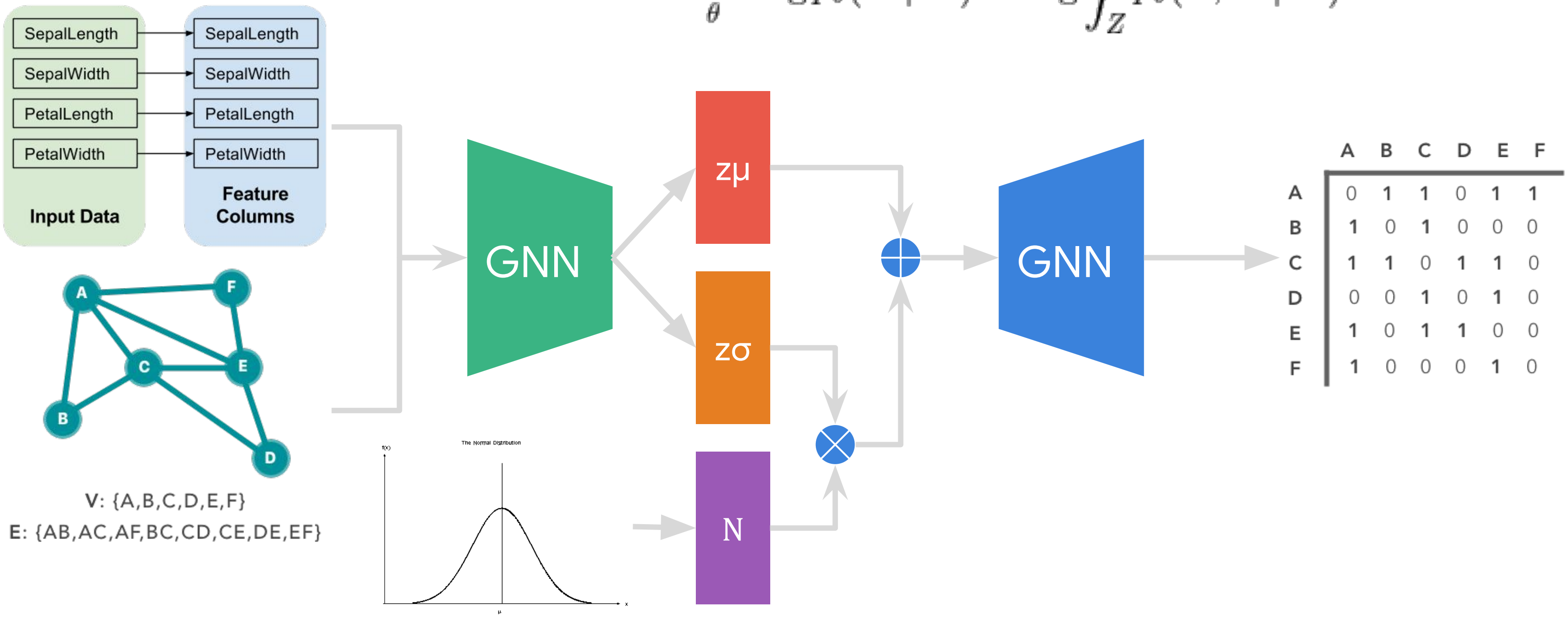


04

Graphite

Graphite Objective

$$\max_{\theta} \log p_{\theta}(A \mid X) = \log \int_{Z} p_{\theta}(A, Z \mid X) dz$$



Graphite Objective

KL Divergence $= E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right] + \log p(x)$

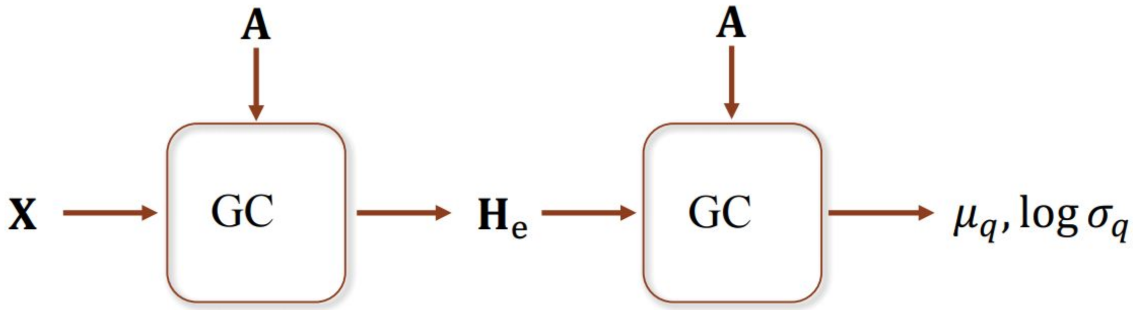
$$\log p(x) = E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right] + D_{KL}\left[q(z \mid \theta) \parallel p(z \mid x)\right]$$

$$\log p(x) \geq E_{q(z|\theta)}\left[\log \frac{p(x,z)}{q(z \mid \theta)}\right]$$

$$\log p(A \mid X) \geq E_{q_\phi}(Z \mid A, X)\left[\log \frac{p_\theta(A, Z \mid X)}{q_\phi(Z \mid A, X)}\right]$$

Graphite Encoder

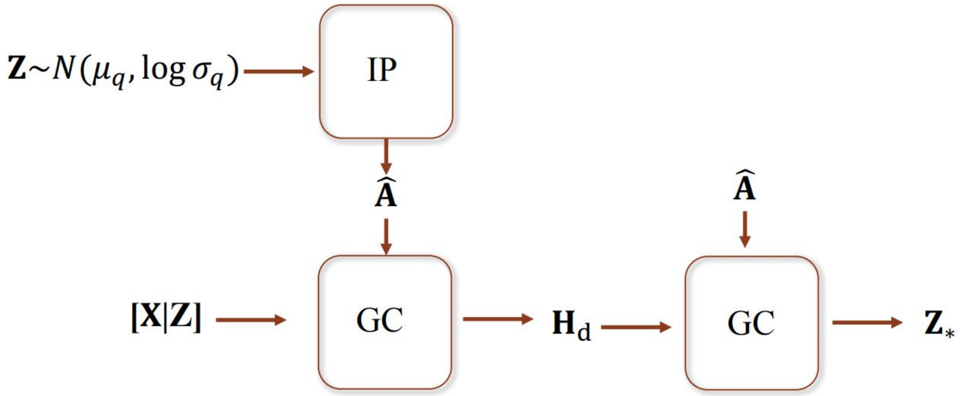
- Variational posterior $q_\theta(Z \mid A, X)$ is a multivariate Gaussian with diagonal covariance
- Encoder parameterized by a graph convolutional network



Forward pass of a two layer encoding GCN

Graphite Decoder

- Decoder is a hybrid that iterates between:
  - intermediate graph construction using an inner product decoder
  - message passing on the intermediate graph using graph convolutions



Graphite Decoder

- The final latent feature matrix is specified as a convex combination of the latent layers

$$Z' = \lambda Z + (1 - \lambda) Z_*$$

where λ ∈ [0,1] is a tunable hyperparameter.

- Observation model $p_\theta(A \mid X, Z)$ is a factorized multivariate Bernoulli

$$p_\theta(A \mid X, Z) = \prod_{i=1}^{n} \prod_{j=1}^{n} p_\theta(A_{ij} \mid X, Z)$$

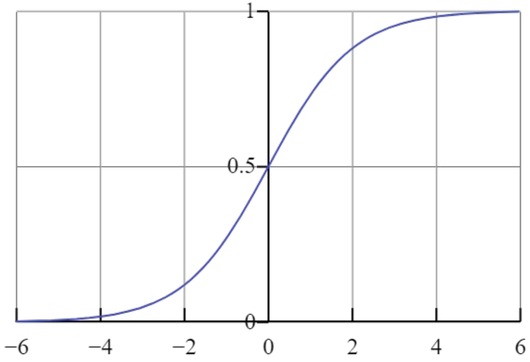
$$p_\theta(A_{ij} \mid X, Z) = \sigma(Z_i' Z_j')$$

05

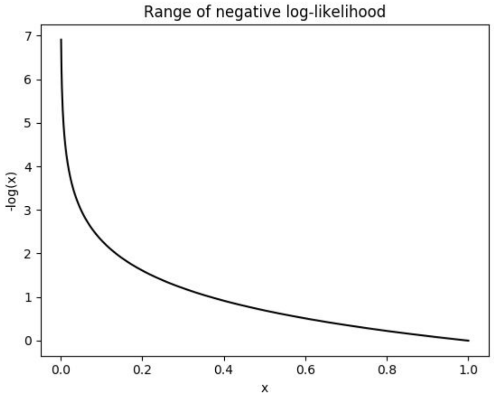
EXPERIMENTAL

Reconstruction Loss

- SCE and NLL




```
  z * -log(sigmoid(x)) + (1 - z) * -log(1 - sigmoid(x))
= z * -log(1 / (1 + exp(-x))) + (1 - z) * -log(exp(-x) / (1 + exp(-x)))
= z * log(1 + exp(-x)) + (1 - z) * (-log(exp(-x)) + log(1 + exp(-x)))
= z * log(1 + exp(-x)) + (1 - z) * (x + log(1 + exp(-x))
= (1 - z) * x + log(1 + exp(-x))
= x - x * z + log(1 + exp(-x))
```



$$
\begin{aligned}
L(b_0, b_1, s^2) &= \log \prod_{i=1}^{n} p(y_i | x_i; b_0, b_1, s^2) & (1)\\
&= \sum_{i=1}^{n} \log p(y_i | x_i; b_0, b_1, s^2) & (2)\\
&= -\frac{n}{2} \log 2\pi - n \log s - \frac{1}{2s^2} \sum_{i=1}^{n} (y_i - (b_0 + b_1 x_i))^2 & (3)
\end{aligned}
$$

Reconstruction Loss

- Sigmoid Cross Entropy

Table 1. Mean reconstruction errors and negative log-likelihood estimates (in nats) for autoencoders and variational autoencoders respectively on test instances from six different generative families. Lower is better.

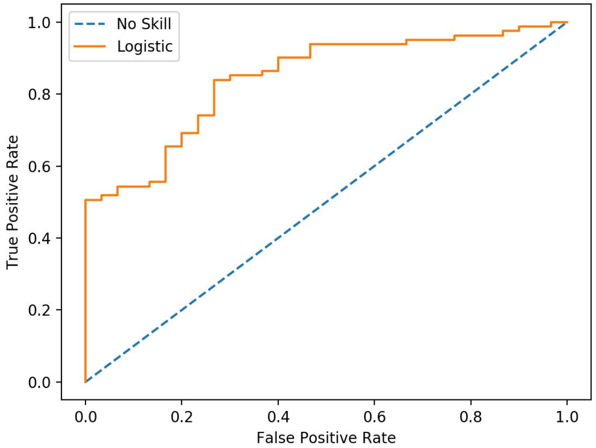
	Erdos-Renyi	Ego	Regular	Geometric	Power Law	Barabasi-Albert
GAE	221.79 ± 7.58	197.3 ± 1.99	198.5 ± 4.78	514.26 ± 41.58	519.44 ± 36.30	236.29 ± 15.13
Graphite-AE	$\mathbf{195.56} \pm 1.49$	$\mathbf{182.79} \pm 1.45$	$\mathbf{191.41} \pm 1.99$	$\mathbf{181.14} \pm 4.48$	$\mathbf{201.22} \pm 2.42$	$\mathbf{192.38} \pm 1.61$
VGAE	273.82 ± 0.07	273.76 ± 0.06	275.29 ± 0.08	274.09 ± 0.06	278.86 ± 0.12	274.4 ± 0.08
Graphite-VAE	$\mathbf{270.22} \pm 0.15$	$\mathbf{270.70} \pm 0.32$	$\mathbf{266.54} \pm 0.12$	$\mathbf{269.71} \pm 0.08$	$\mathbf{263.92} \pm 0.14$	$\mathbf{268.73} \pm 0.09$

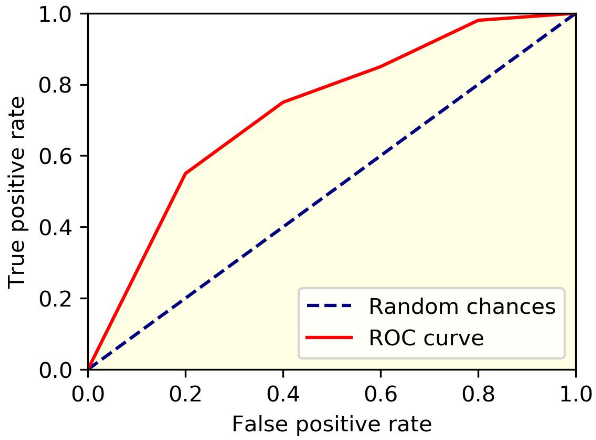
Link Prediction

- **Given two nodes in a graph, does an edge exist between the nodes?**
- **Baselines**:
  - Spectral Clustering (SC)
  - DeepWalk (DW): random walks and skip-gram objective
  - (Variational) Graph Autoencoder (VGAE, GAE):
    - GCN encoder but a single-step inner product decoder
- For Graphite, the task can be formulated as denoising.
- **Datasets**: Protein-protein Interaction, Cora, Citeseer, Pubmed
- **Evaluation metrics**:
  - Area Under the ROC Curve
  - Average Precision

Link Prediction

- AUC of ROC Curve





Link Prediction

- AUC of ROC curve

Table 3. Area Under the ROC Curve (AUC) for link prediction (* denotes dataset with features). Higher is better.

	Cora	Citeseer	Pubmed	Cora*	Citeseer*	Pubmed*
SC	89.9 ± 0.20	91.5 ± 0.17	$\mathbf{94.9} \pm 0.04$	-	-	-
DeepWalk	85.0 ± 0.17	88.6 ± 0.15	91.5 ± 0.04	-	-	-
node2vec	85.6 ± 0.15	89.4 ± 0.14	91.9 ± 0.04	-	-	-
GAE	90.2 ± 0.16	92.0 ± 0.14	92.5 ± 0.06	93.9 ± 0.11	94.9 ± 0.13	96.8 ± 0.04
VGAE	90.1 ± 0.15	92.0 ± 0.17	92.3 ± 0.06	94.1 ± 0.11	96.7 ± 0.08	95.5 ± 0.13
Graphite-AE	91.0 ± 0.15	92.6 ± 0.16	94.5 ± 0.05	94.2 ± 0.13	96.2 ± 0.10	$\mathbf{97.8} \pm 0.03$
Graphite-VAE	$\mathbf{91.5} \pm 0.15$	$\mathbf{93.5} \pm 0.13$	94.6 ± 0.04	$\mathbf{94.7} \pm 0.11$	$\mathbf{97.3} \pm 0.06$	97.4 ± 0.04

Link Prediction

- Average Precision

Table 4. Average Precision (AP) scores for link prediction (* denotes dataset with features). Higher is better.

	Cora	Citeseer	Pubmed	Cora*	Citeseer*	Pubmed*
SC	92.8 ± 0.12	94.4 ± 0.11	$\mathbf{96.0} \pm 0.03$	-	-	-
DeepWalk	86.6 ± 0.17	90.3 ± 0.12	91.9 ± 0.05	-	-	-
node2vec	87.5 ± 0.14	91.3 ± 0.13	92.3 ± 0.05	-	-	-
GAE	92.4 ± 0.12	94.0 ± 0.12	94.3 ± 0.5	94.3 ± 0.12	94.8 ± 0.15	96.8 ± 0.04
VGAE	92.3 ± 0.12	94.2 ± 0.12	94.2 ± 0.04	94.6 ± 0.11	97.0 ± 0.08	95.5 ± 0.12
Graphite-AE	92.8 ± 0.13	94.1 ± 0.14	95.7 ± 0.06	94.5 ± 0.14	96.1 ± 0.12	$\mathbf{97.7} \pm 0.03$
Graphite-VAE	$\mathbf{93.2} \pm 0.13$	$\mathbf{95.0} \pm 0.10$	$\mathbf{96.0} \pm 0.03$	$\mathbf{94.9} \pm 0.13$	$\mathbf{97.4} \pm 0.06$	97.4 ± 0.04

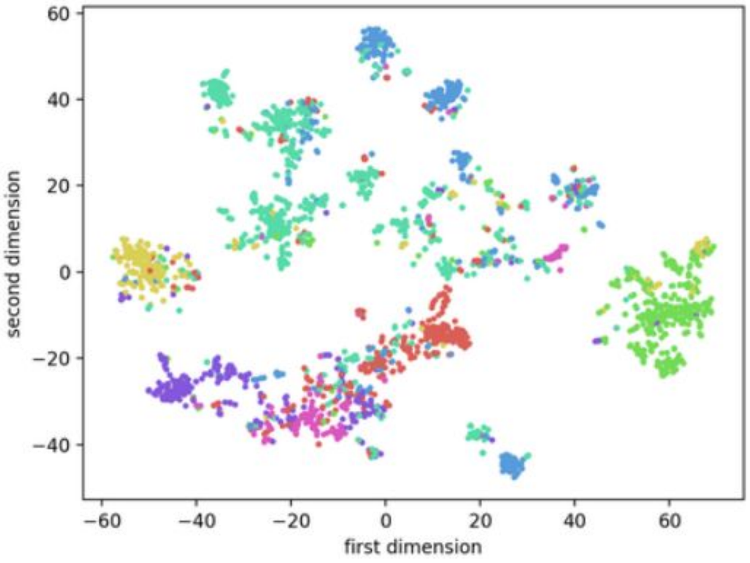
Node Classification

- Accuracy

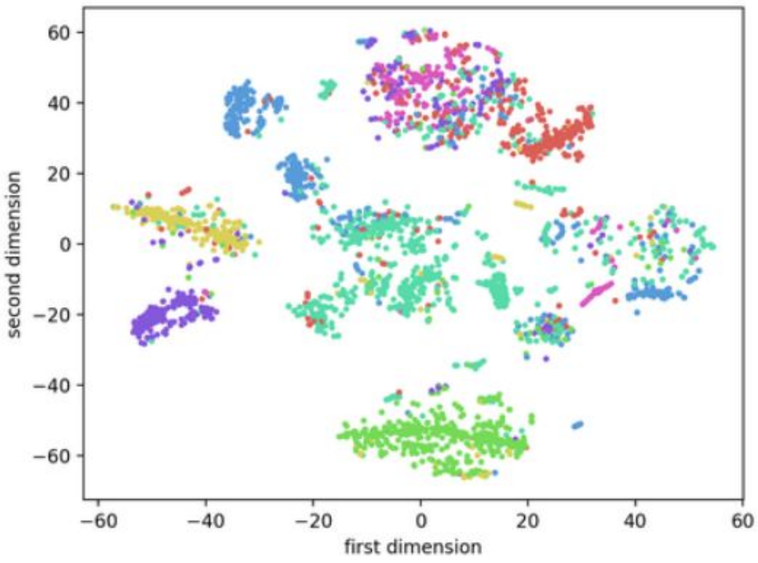
Table 5. Classification accuracies (* denotes dataset with features). Baseline numbers from Kipf & Welling (2017).

	Cora*	Citeseer*	Pubmed*
SemiEmb	59.0	59.6	71.1
DeepWalk	67.2	43.2	65.3
ICA	75.1	69.1	73.9
Planetoid	75.7	64.7	77.2
GCN	81.5	70.3	79.0
Graphite	**82.1** $\pm$ 0.06	**71.0** $\pm$ 0.07	**79.3** $\pm$ 0.03

Visualization of Latent Space



(a) Graphite-AE



(b) Graphite-VAE

DISCUSSION
CONCLUSION

Proposed Graphite, an algorithmic for generative modeling of graphs.

Future and ongoing work entail applications of Graphite to other inference tasks.

THANKS!

Do you have any questions?
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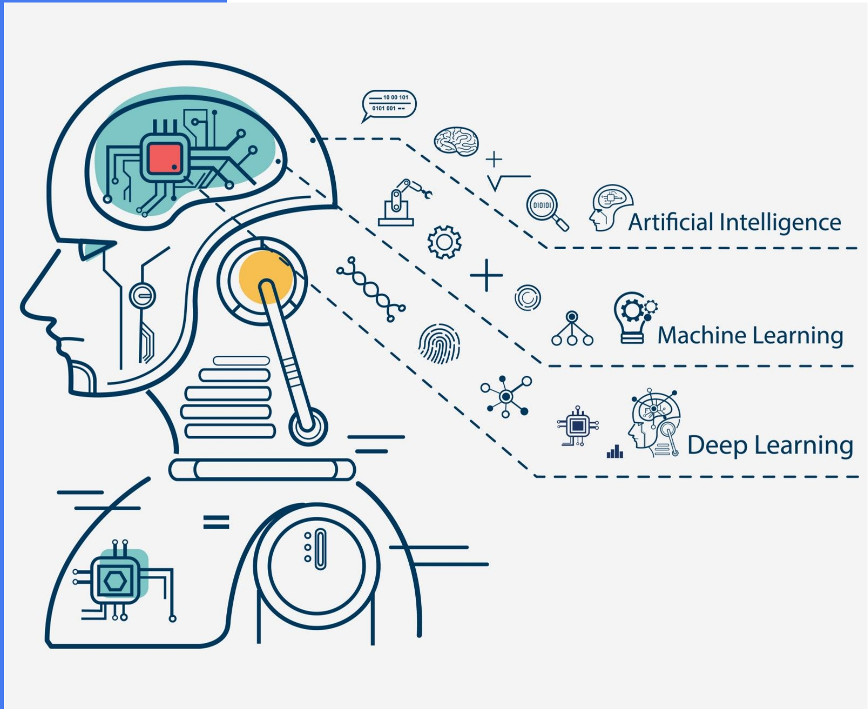

Elian Lu

Please feel free to contact me

ALTERNATIVE RESOURCES

- Study group GitHub link
- The paper link
- The code of this paper imple
- Variational graph auto-encoders(GAE)
- The code of GAE
- What is AutoEncoder?
- Variational AutoEncoder
- Variational Inference