Adversarially regularized GAE (ARGA) & Adversarially regularized VGAE (ARVGA)

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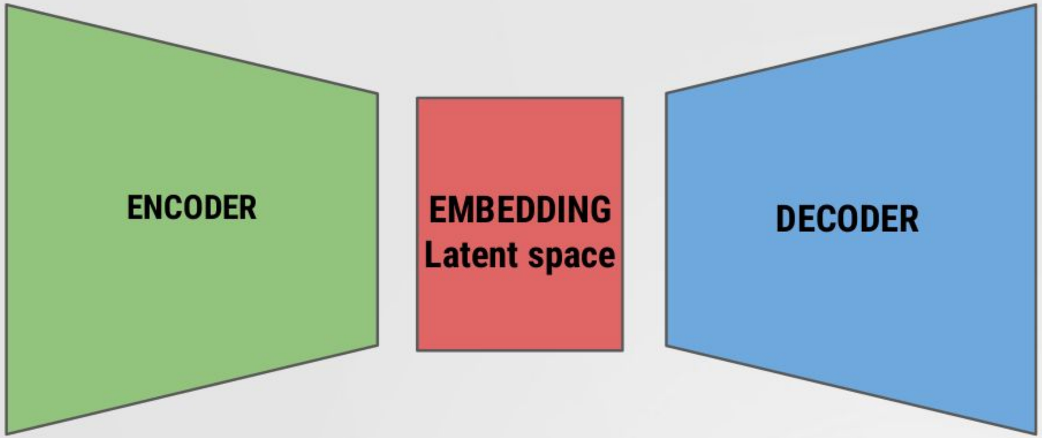
01 Recap



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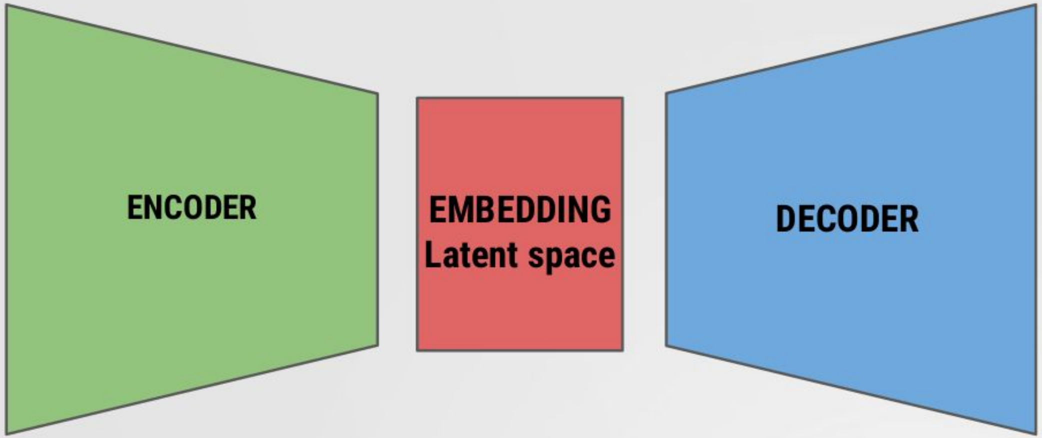

Input:
Graph with node features

- Adj. matrix A
- Data matrix X

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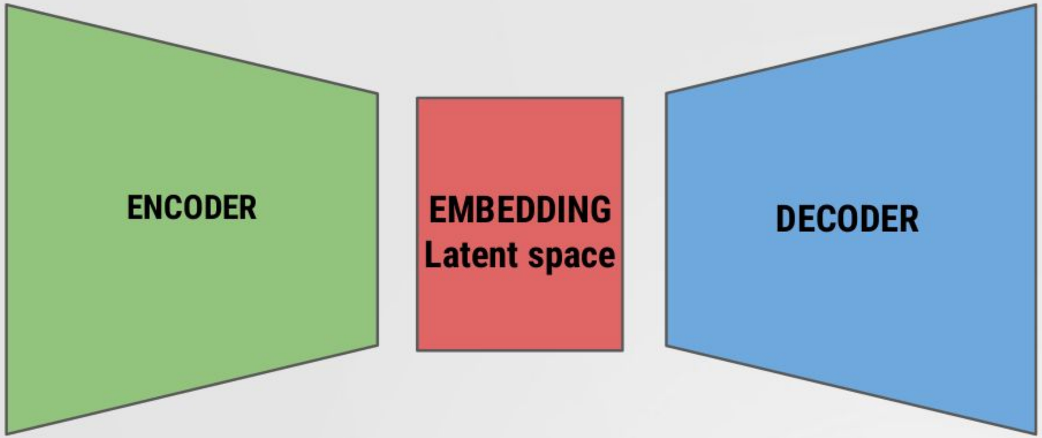

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Structural information

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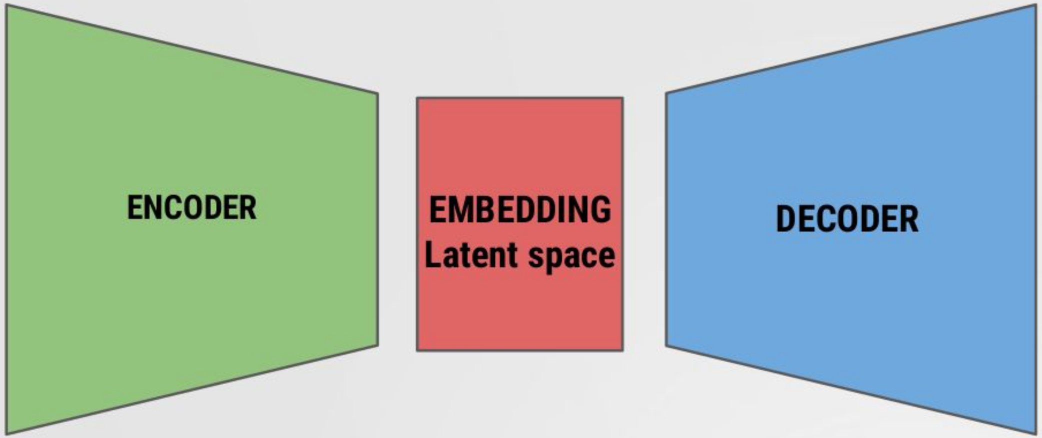

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Structural information

Feature information

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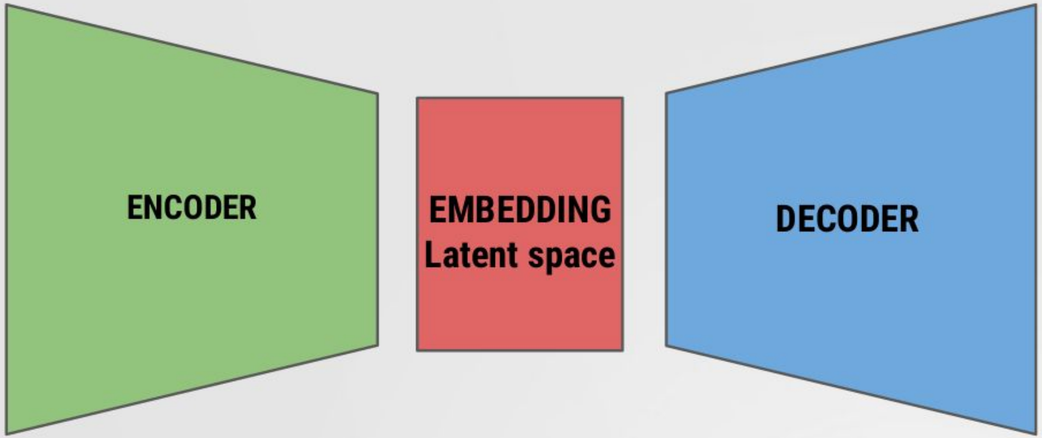

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Graph
- Approx. of A

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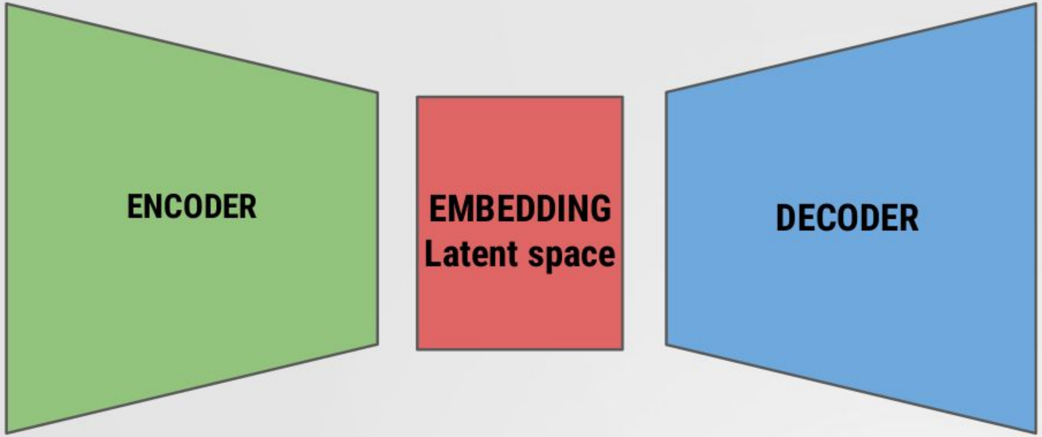

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Goal:

- Embedding
- Generation
- ...

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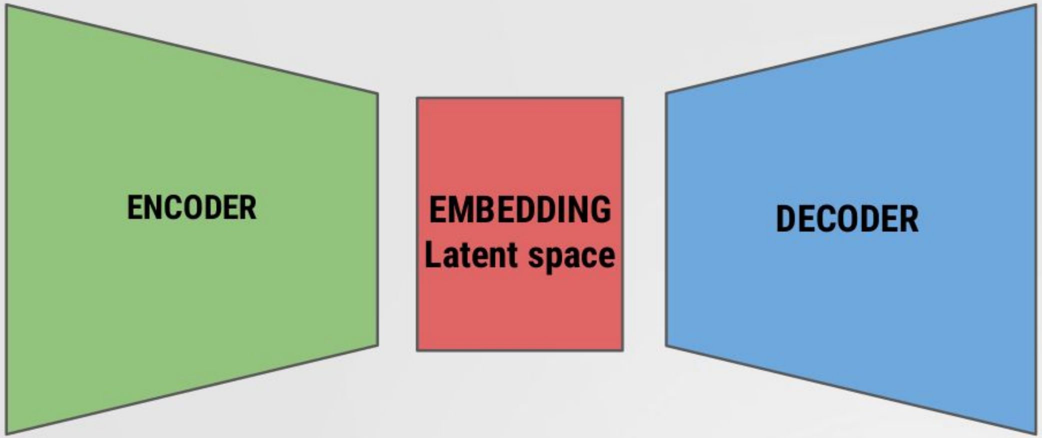

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Continuous feature space

01 Recap

GAE vs VGAE:

- Embedding on nodes
- Each nodes is mapped to its latent representation

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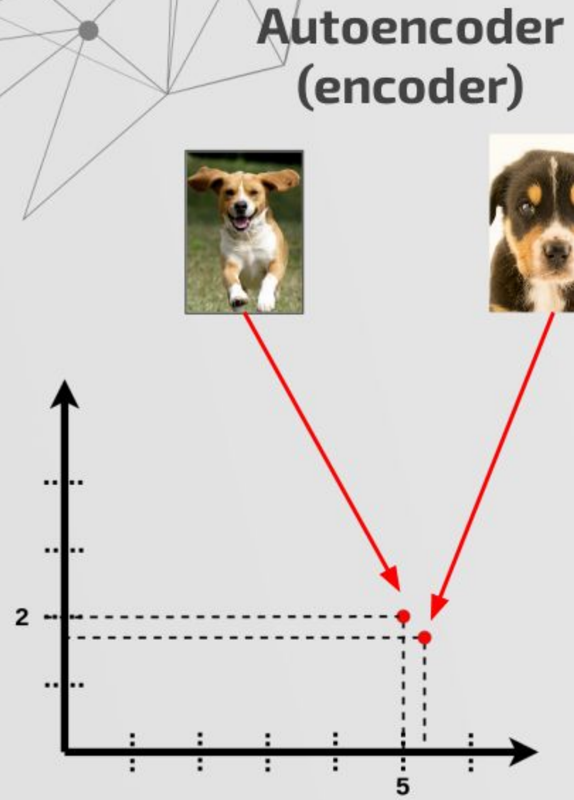

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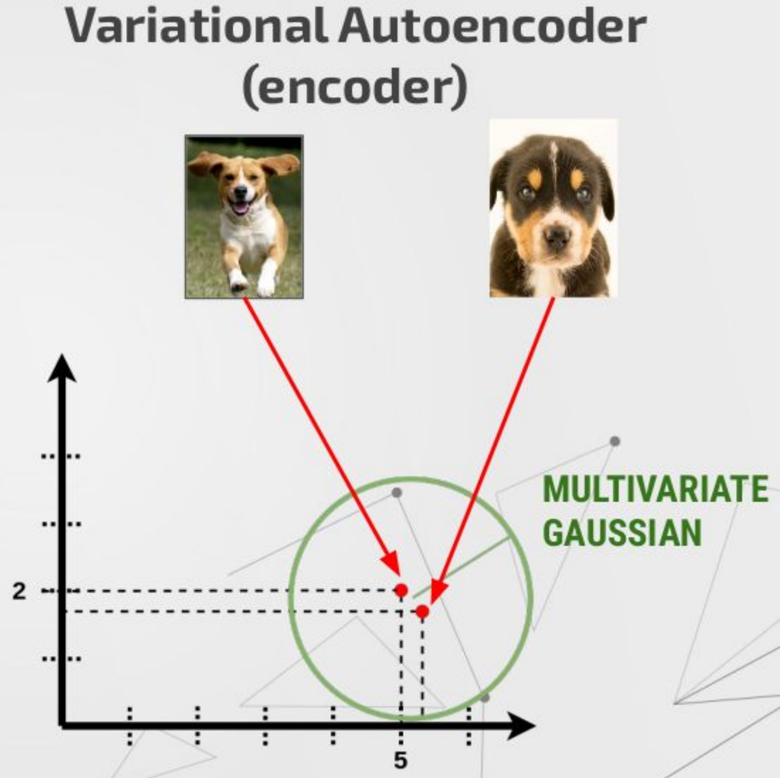

02 Motivation ARGA & ARVGA

Motivation:

The importance of the latent representation

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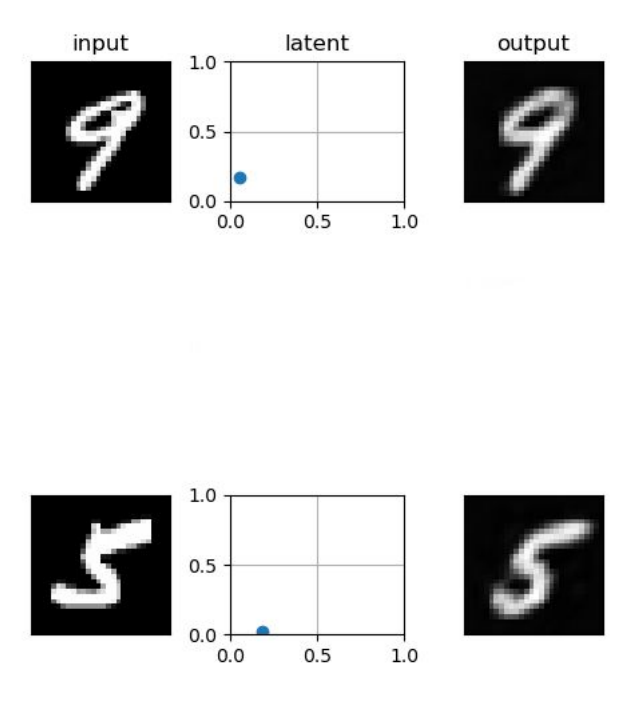

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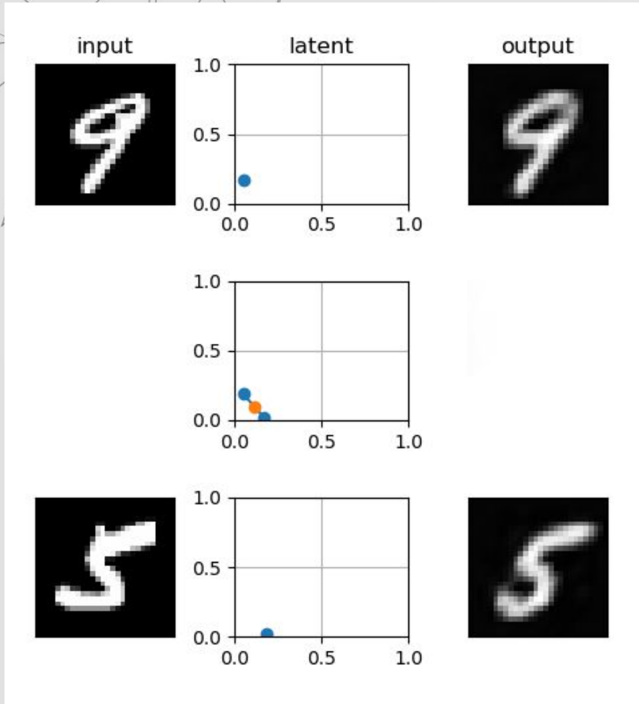

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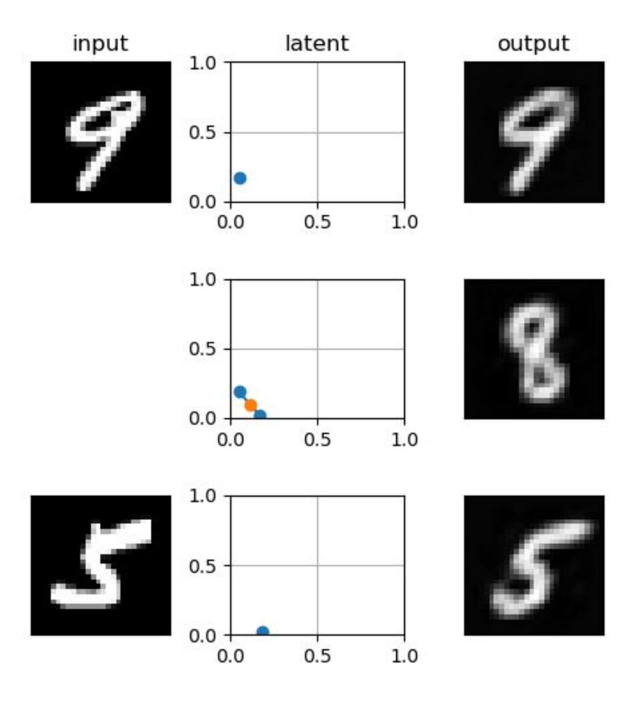

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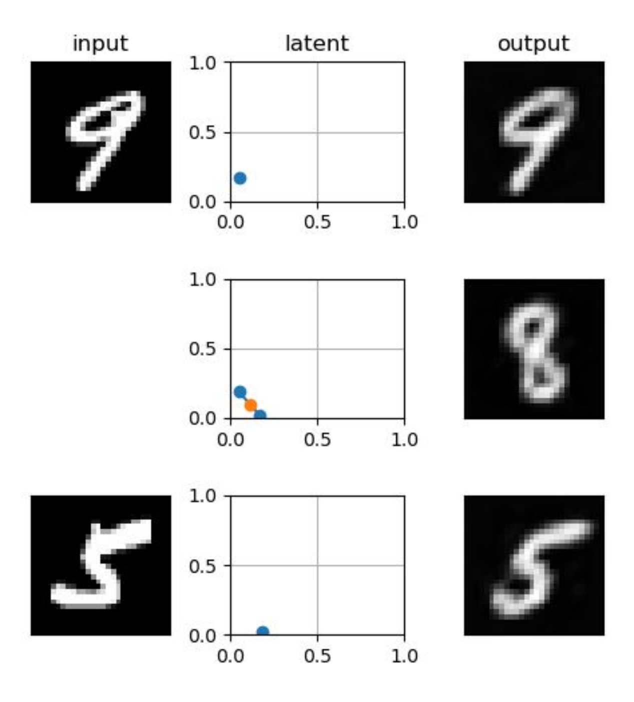

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The importance of the latent representation

AE and GAE: only reconstruction loss

VAE and VGAE: regularize to have continuous latent representation

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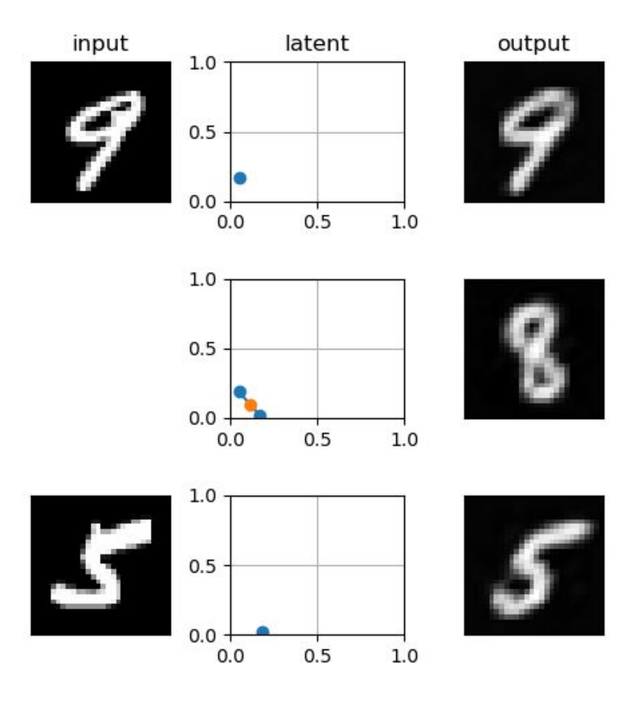

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AE and GAE: only reconstruction loss

VAE and VGAE: regularize to have continuous latent representation

ARGA & ARVGA improve it

02 Motivation ARGA & ARVGA

Motivation:
The importance of the latent representation

Adversarially regularized graph autoencoder (ARGA)
Adversarially regularized variational graph autoencoder (ARVGA)

S. Pan, R. Hu, G. Long, J. Jiang, L. Yao, and C. Zhang, *Adversarially regularized graph autoencoder for graph embedding*. in Proc. of IJCAI, 2018, pp. 2609–2615.

02 Motivation ARGA & ARVGA

Motivation:
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Adversarially regularized graph autoencoder (ARGA)
Adversarially regularized variational graph autoencoder (ARVGA)

We have a look at
adversarial training

S. Pan, R. Hu, G. Long, J. Jiang, L. Yao, and C. Zhang, *Adversarially regularized graph autoencoder for graph embedding*. in Proc. of IJCAI, 2018, pp. 2609–2615.

03 Ideas from adversarial models

Goal: generate fake objects (e.g. images) similar to real ones
Idea: play an adversarial game with two agents

I. Goodfellow et al., *Generative Adversarial Nets*. in Proc. of NIPS, 2014, pp. 2672--2680.

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Idea: play an adversarial game with two agents

↓

Generator: maps noise z to a fake object x
Discriminator: maps object x to probability of real/fake
Game: The generator tries to fool the discriminator
The discriminator tries to detect the fake objects

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$$\min_G \max_D \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

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The **Discriminator** wants to **max:**

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The **Discriminator** wants to **max:**

- Recall that D(x) is in [0, 1]
- **First term**:
  → large if D(x) is close to 1
  → assign high probability to real objects

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$$\min_G \max_D \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

The **Discriminator** wants to **max:**

- Recall that D(x) is in [0, 1]
- **First term**:
  ⟶ large if D(x) is close to 1
  ⟶ assign high probability to real objects
- **Second term**:
  ⟶ large if 1-D(G(z)) is close to 1
  ⟶ large if D(G(z)) is close to 0
  ⟶ assign low probability to fake objects

I. Goodfellow et al., *Generative Adversarial Nets*. in Proc. of NIPS, 2014, pp. 2672--2680.

03 Ideas from adversarial models

$$\min_G \max_D \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

The **Generator** wants to **min:**

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03 Ideas from adversarial models

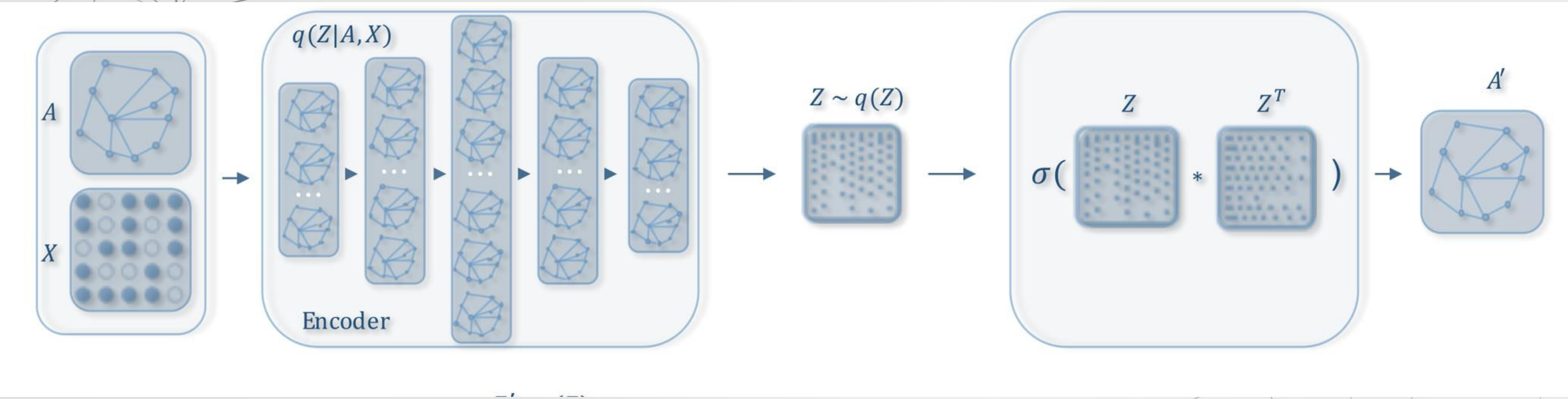
$$\min_G \max_D \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

The **Generator** wants to **min:**

- **Second term**:
  ⟶ small if 1-D(G(z) is close to 0
  ⟶ small if D(G(z) is close to 1
  ⟶ fool the discriminator into assigning high probability to fake objects

I. Goodfellow et al., *Generative Adversarial Nets*. in Proc. of NIPS, 2014, pp. 2672--2680.

04 ARGA & ARGVA



Picture from S. Pan et al.

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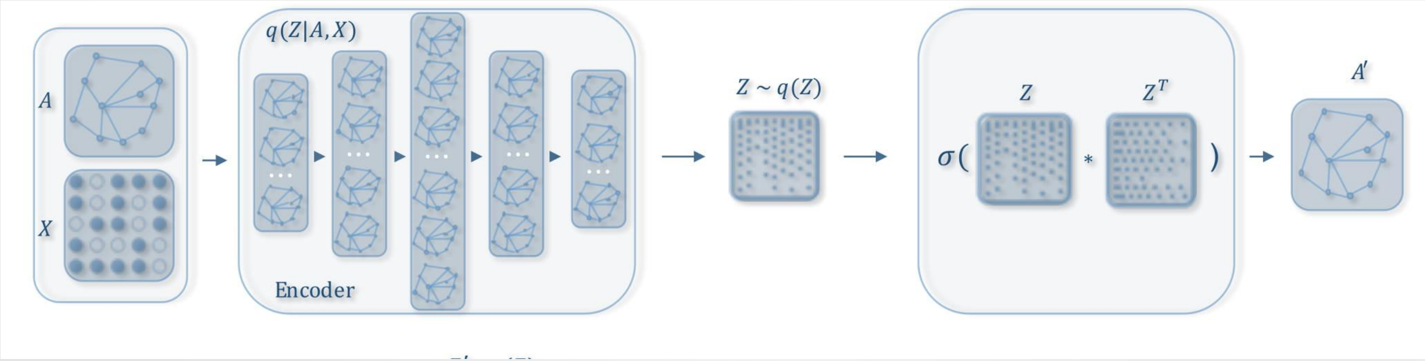


Architecture as in GAE/VGAE:

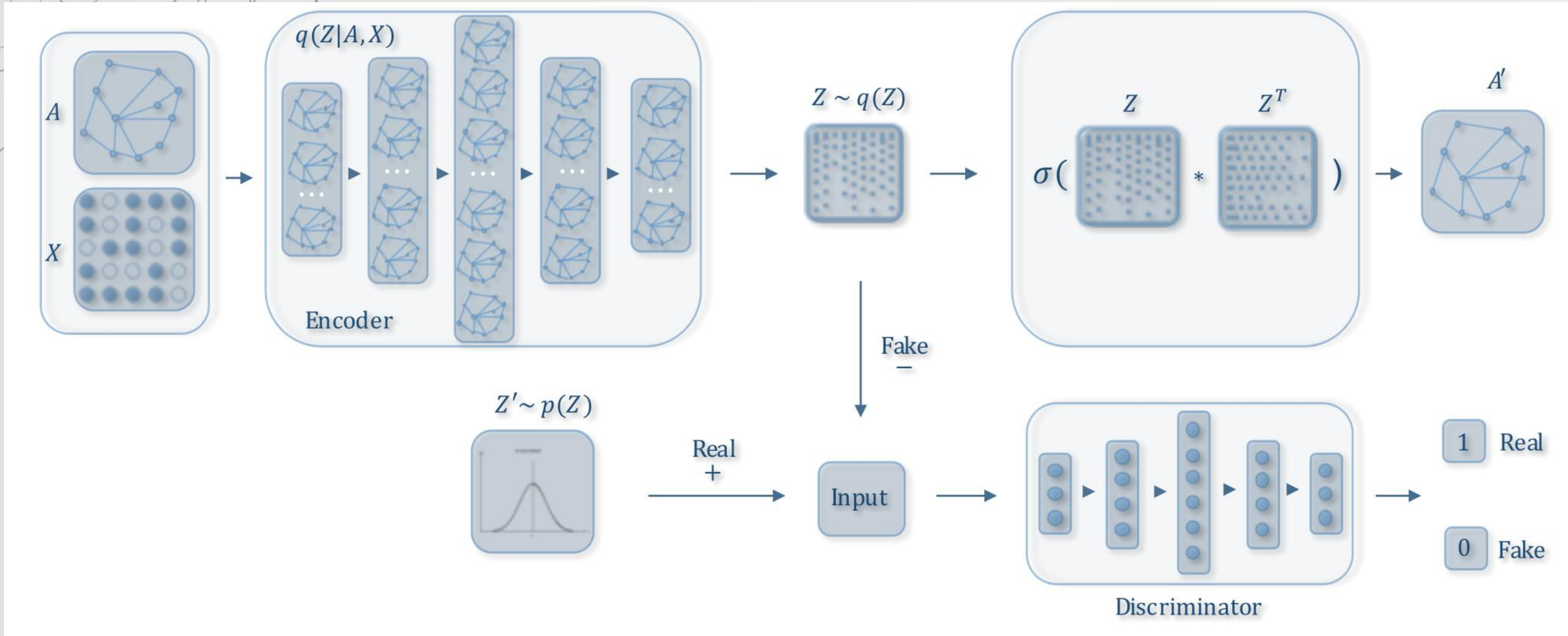
- **Encoder**: 2-layer GCN (with 2x for mean and logstd in VGAE)
- **Decoder**: inner product

→ Same **loss** as GAE/VGAE:

- **GAE**: reconstruction loss
- **VGAE**: rec. + KL regularization

Picture from S. Pan et al.

04 ARGA & ARGVA



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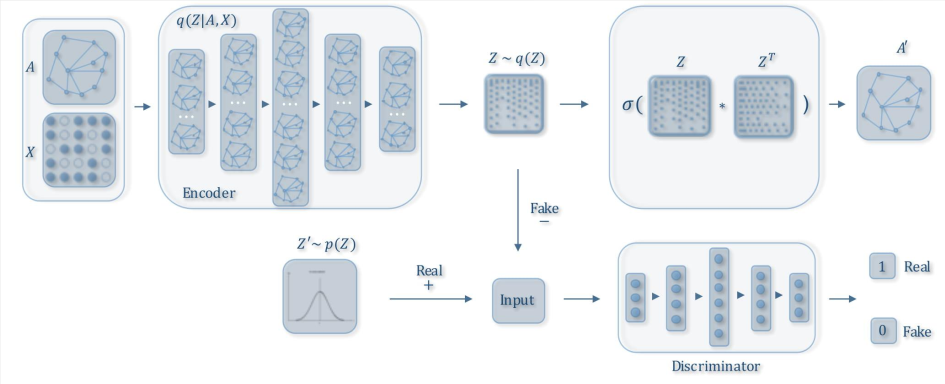

Architecture of the **discriminator:**

- Standard fully connected NN with 3 layers

Picture from S. Pan et al.

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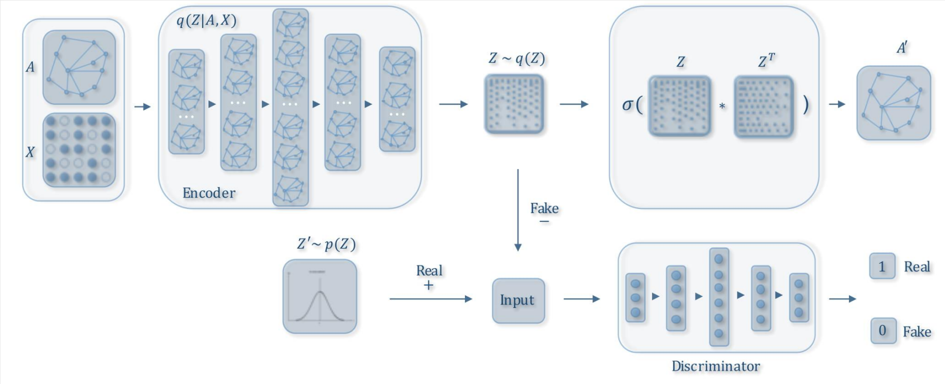

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Working on the latent space
→ continuous values!

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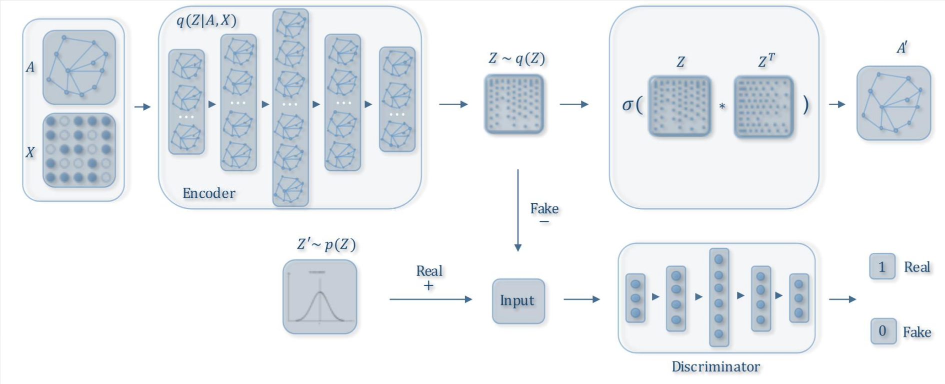

Architecture of the **discriminator:**

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Working on the latent space
→ continuous values!

→ Adversarial **loss**:
Real: samples from N(0, 1)
Fake: samples from the latent encoding

$$\min_{\mathcal{G}} \max_{\mathcal{D}} \mathbb{E}_{\mathbf{z}\sim p_z}[\log \mathcal{D}(\mathbf{Z})] + \mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}[\log(1-\mathcal{D}(\mathcal{G}(\mathbf{X},\mathbf{A})))]$$

Picture from S. Pan et al.

04 ARGA & ARGVA

Algorithm 1 Adversarially Regularized Graph Embedding

Require:
$\mathbf{G} = \{\mathbf{V}, \mathbf{E}, \mathbf{X}\}$: a Graph with links and features;
T: the number of iterations;
K: the number of steps for iterating discriminator;
d: the dimension of the latent variable
Ensure: $\mathbf{Z} \in \mathbb{R}^{n \times d}$

```
for iterator = 1,2,3, ······ , T do
    Generate latent variables matrix Z through Eq.(4);

    Update the graph autoencoder with its stochastic gradient by
    Eq. (10) for ARGA or Eq. (11) for ARVGA;
end for
return Z ∈ R^{n×d}
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This is: Z = E(X, A)

Picture from S. Pan et al.

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4:

5:

6:

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These are the usual GAE/VGAE losses

Picture from S. Pan et al.

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5: Sample m entities $\{\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(m)}\}$ from the prior distribution p_z
6: Update the discriminator with its stochastic gradient:

$$\bigtriangledown \frac{1}{m} \sum_{i=1}^{m} [\log \mathcal{D}(\mathbf{a}^{i}) + \log (1 - \mathcal{D}(\mathbf{z}^{(i)}))]$$

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K training loops of the discriminator

Picture from S. Pan et al.

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Sample fake gaussians

Picture from S. Pan et al.

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Sample true gaussians

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return Z ∈ R^{n×d}
```

Discriminator gradient (step 6):

$$\nabla \frac{1}{m} \sum_{i=1}^{m} [\log \mathcal{D}(\mathbf{a}^{i}) + \log (1 - \mathcal{D}(\mathbf{z}^{(i)}))]$$

K training loops of the discriminator

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Sample true gaussians

Update the discriminator

Picture from S. Pan et al.

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K training loops of the discriminator

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Sample true gaussians

Update the discriminator

Missing: update the encoder
(written in the text)

Picture from S. Pan et al.

05 ARGA & ARGVA

Jupyter Notebook