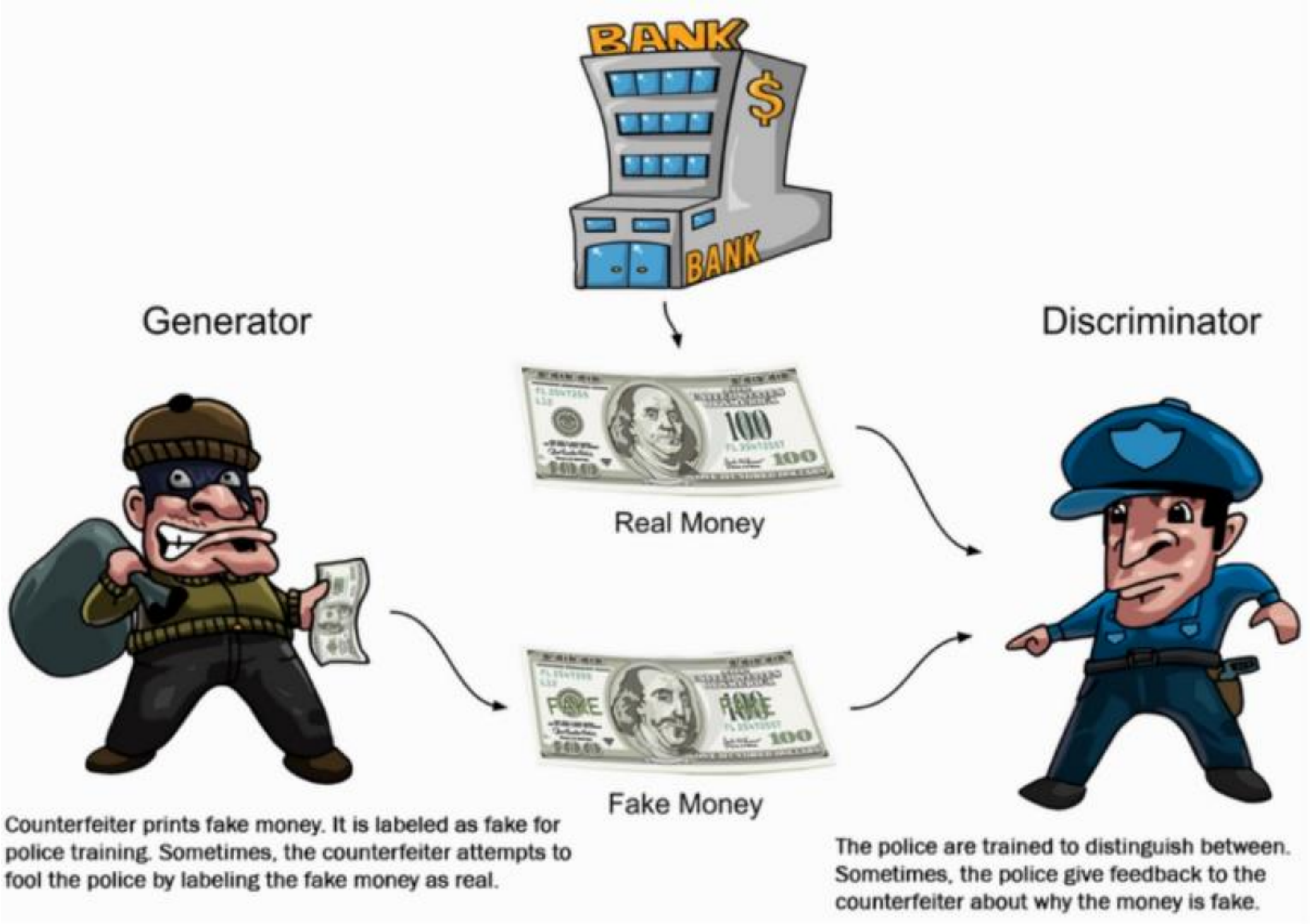
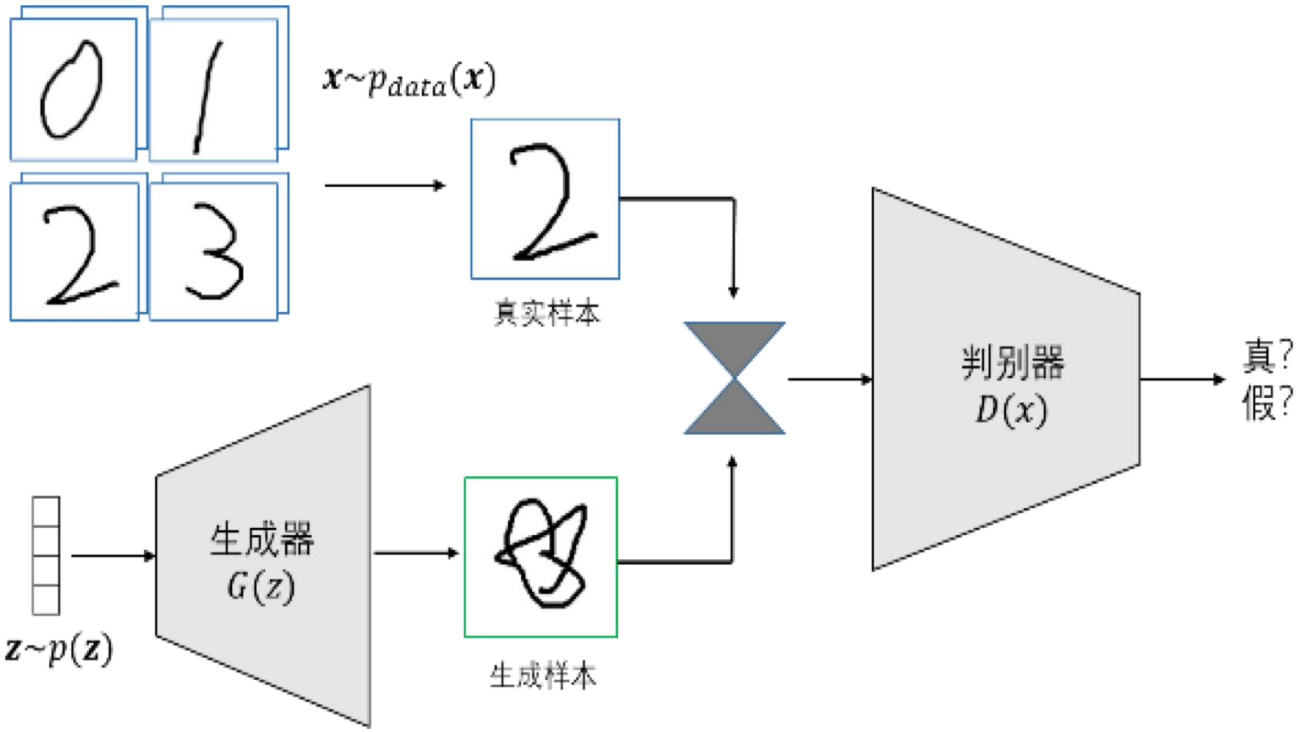
Generative Adversarial Networks

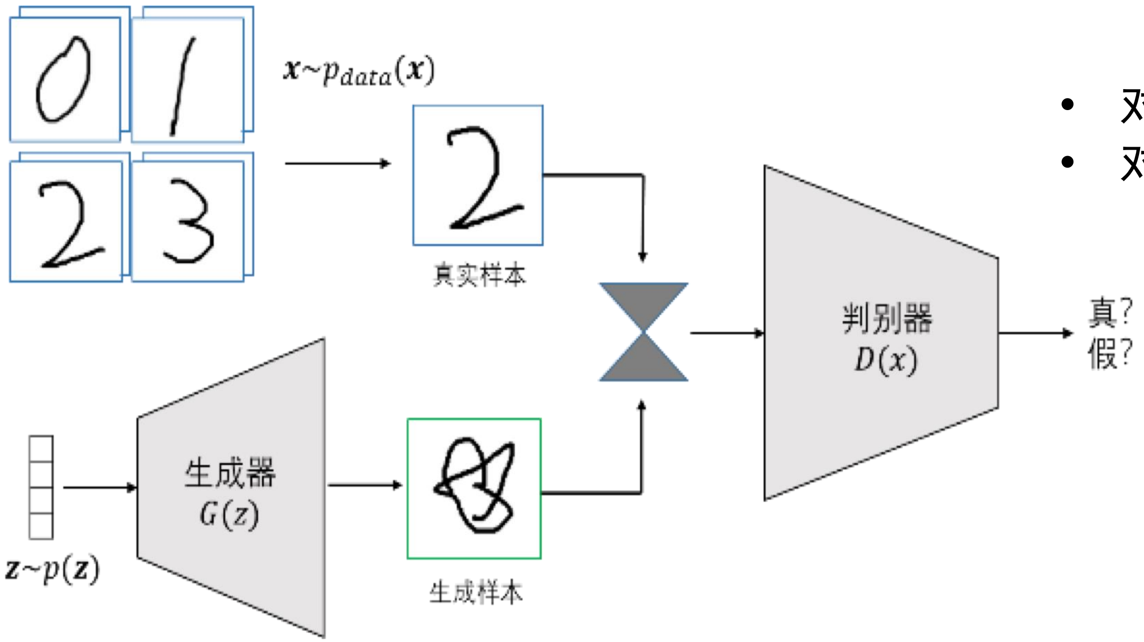


GAN



- 生成对抗网络包含两个神经网络，一个是生成器（generator），另一个是判别器（discriminator）
- 生成器的任务是在一定的隐变量控制下生成新样本，判别器的任务是对真实训练样本和生成器生成的“假样本”进行判别。
- “对抗”，就是指生成对抗网络在训练过程中，一方面训练判别器，使之尽可能准确地区分真样本和假样本；另一方面训练生成器，使之产生的假样本尽量不会被判别器识别出来。

GAN



- 对真样本x，希望D(x)判别为1
- 对假样本G(z)，希望D(G(z))判别为0

$$\min_G \max_D V(D,G) = E_{\boldsymbol{x} \sim p_{data}(\boldsymbol{x})}[log D(\boldsymbol{x})] + E_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[log\left(1 - D(G(\boldsymbol{z}))\right)]$$

- maxD 使得分类器尽量准确的区分真实样本和生成样本， 即最大化log(D(x))和log(1-D(G(z))
- minG 使得生成器尽量骗过分类器，即log(1-D(G(z))最小

GAN

对固定的生成器：z->x的映射关系固定

$$V(D,G) = \int_x p_{data}(x)log\big(D(x)\big)dx + \int_z p_z(z)log\Big(1 - D\big(G(z)\big)\Big)dz$$

$$= \int_x p_{data}(x)log\big(D(x)\big)\,dx + \int_x p_g(x)log\big(1 - D(x)\big)\,dx$$

$$= \int_x \Big(p_{data}(x)log\big(D(x)\big) + p_g(x)log\big(1 - D(x)\big)\Big)\,dx$$

对判别器求V(D,G)最大，最优解需满足

$$\frac{\partial}{\partial D(x)}\Big(p_{data}(x)log\big(D(x)\big) + p_g(x)log\big(1 - D(x)\big)\Big) = 0$$

可得最优判别器D*(x) 为

$$D^*(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

GAN

对于固定的判别器，需要对生成器求V(D,G)最小

将 $D^*(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$ 代入

$$V(D^*, G) = E_{x\sim p_{data}}\left[log\frac{p_{data}(x)}{p_{data}(x) + p_g(x)}\right] + E_{x\sim p_g}\left[log\frac{p_g(x)}{p_{data}(x) + p_g(x)}\right]$$

$$V(D^*, G) = -log(4) + KL\left(p_{data}||\frac{p_{data} + p_g}{2}\right) + KL\left(p_g||\frac{p_{data} + p_g}{2}\right)$$

$$V(D^*, G) = -log(4) + 2JSD(p_{data}||p_g)$$

$JSD(p_{data}||p_g)$是$p_{data}(x)$和$p_g(x)$的J-S散度（Jensen-Shannon divergence）

对生成器最小化V(D*,G)就是最小化$p_{data}(x)$和$p_g(x)$的差异，最优解是$p_{data}(x) = p_g(x)$，
即生成样本与真实样本相同

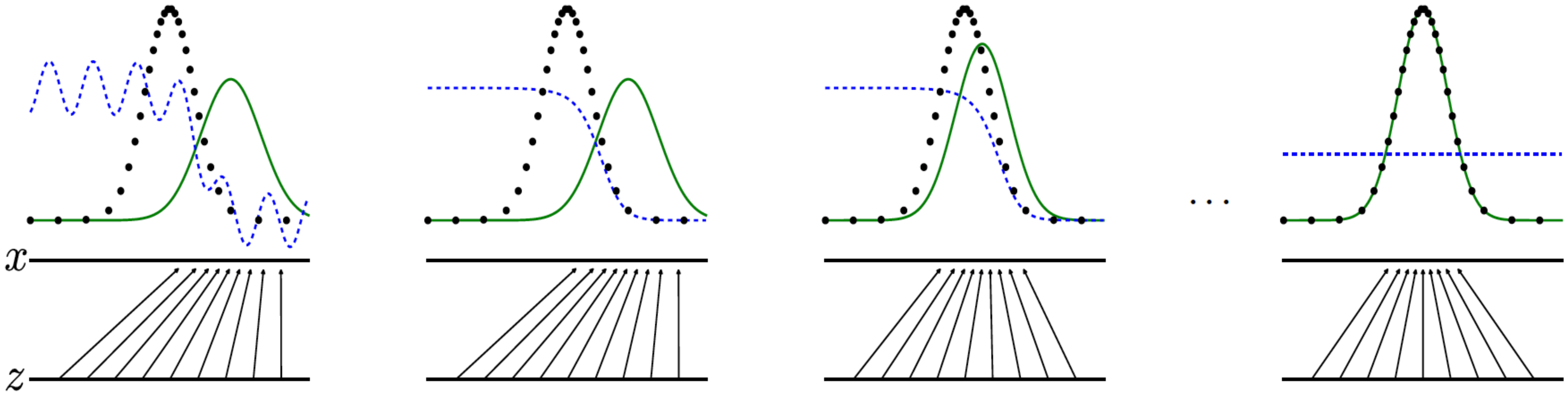
GAN

初始化的D和G

$$D^*(\boldsymbol{x}) = \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_g(\boldsymbol{x})}$$

$$p_g = p_{\text{data}}$$

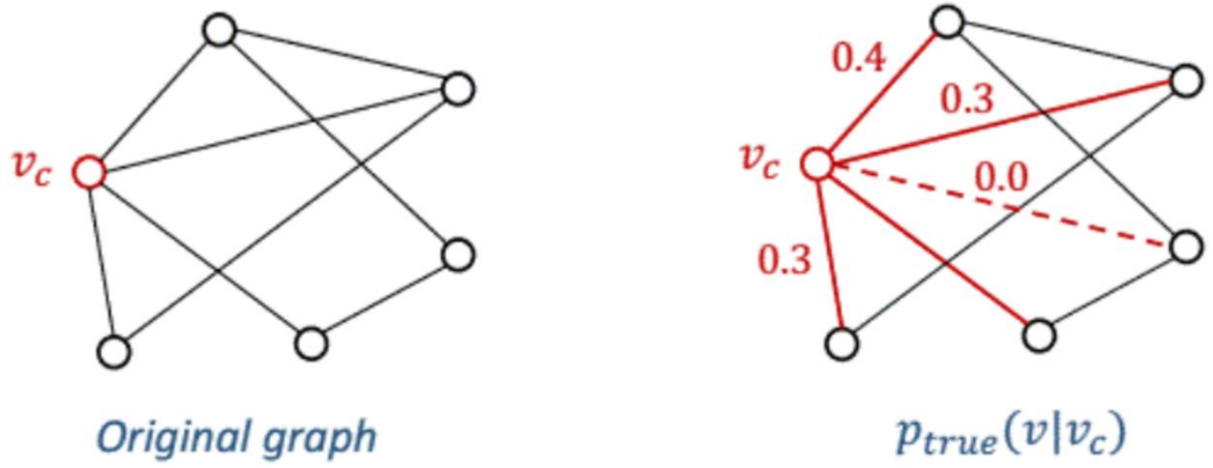
$$D(\boldsymbol{x}) = \frac{1}{2}$$



(a) (b) (c) (d)

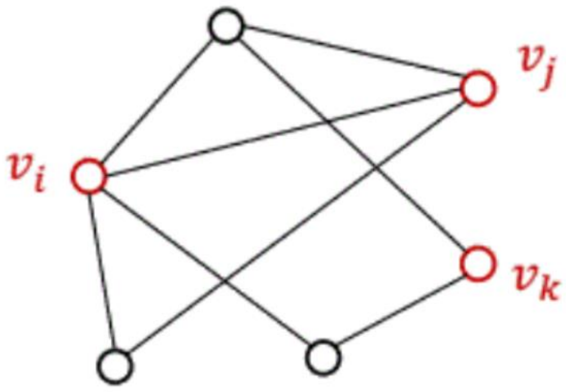
graphGAN

- Generative graph representation learning model assumes an **underlying true connectivity distribution** $p_{true}(v|v_c)$ for each vertex v_c
  - The edges can be viewed as observed samples generated by $p_{true}(v|v_c)$
  - Vertex embeddings are learned by maximizing the likelihood of edges
  - E.g., DeepWalk (KDD 2014) and node2vec (KDD 2016)



graphGAN

- Discriminative graph representation learning model aim to learn a **classifier** for predicting the existence of edges directly
  - Consider two vertices v_i and v_j jointly as features
  - Predict the probability of an edge existing between them, i.e., $p(edge|v_i, v_j)$
  - E.g., SDNE (KDD 2016) and PPNE (DASFAA, 2017)



$p(edge|v_i, v_j) = 0.8$

$p(edge|v_i, v_k) = 0.3$

……

Key point: positive and negative sample imbalance

graphGAN

- $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, $\mathcal{V} = \{v_1, \ldots, v_V\}$, $\mathcal{E} = \{e_{ij}\}_{i,j=1}^{V}$
- $\mathcal{N}(v_c)$: set of neighbors of v_c
- $p_{true}(v_c)$: underlying true connectivity distribution for v_c

- The objective of GraphGAN is to learn the following two models:
  - $G(v|v_c; \theta_G)$ which tries to approximate $p_{true}(v_c)$
  - $D(v, v_c; \theta_D)$ which aims to discriminate the connectivity for the vertex pair (v, v_c)
- The two-player minimax game:

$$\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^{V} \Big(\mathbb{E}_{v \sim p_{\mathrm{true}}(\cdot|v_c)} \big[\log D(v, v_c; \theta_D) \big] + \mathbb{E}_{v \sim G(\cdot|v_c; \theta_G)} \big[\log \big(1 - D(v, v_c; \theta_D)\big) \big] \Big)$$

Optimization of D

$$\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^{V} \Big(\mathbb{E}_{v \sim p_{\text{true}}(\cdot|v_c)} \big[\log D(v, v_c; \theta_D) \big] + \mathbb{E}_{v \sim G(\cdot|v_c;\theta_G)} \big[\log \big(1 - D(v, v_c; \theta_D)\big) \big] \Big) \tag{1}$$

- Implementation of D:

$$D(v, v_c; \theta_D) = \sigma(\mathbf{d}_v^\top \mathbf{d}_{v_c}) = \frac{1}{1 + \exp(-\mathbf{d}_v^\top \mathbf{d}_{v_c})}, \tag{2}$$

where $\mathbf{d}_v, \mathbf{d}_{v_c} \in \mathbb{R}^k$ are the k-dimensional vectors of v and v_c for D

- Gradient of $V(G, D)$ w.r.t θ_D:

$$\nabla_{\theta_D} V(G, D) = \begin{cases} \nabla_{\mathbf{d}_v, \mathbf{d}_{v_c}} \log D(v, v_c; \theta_D), & if\ v \sim p_{\text{true}}; \\ \nabla_{\mathbf{d}_v, \mathbf{d}_{v_c}} (1 - \log D(v, v_c; \theta_D)), & if\ v \sim G. \end{cases} \tag{3}$$

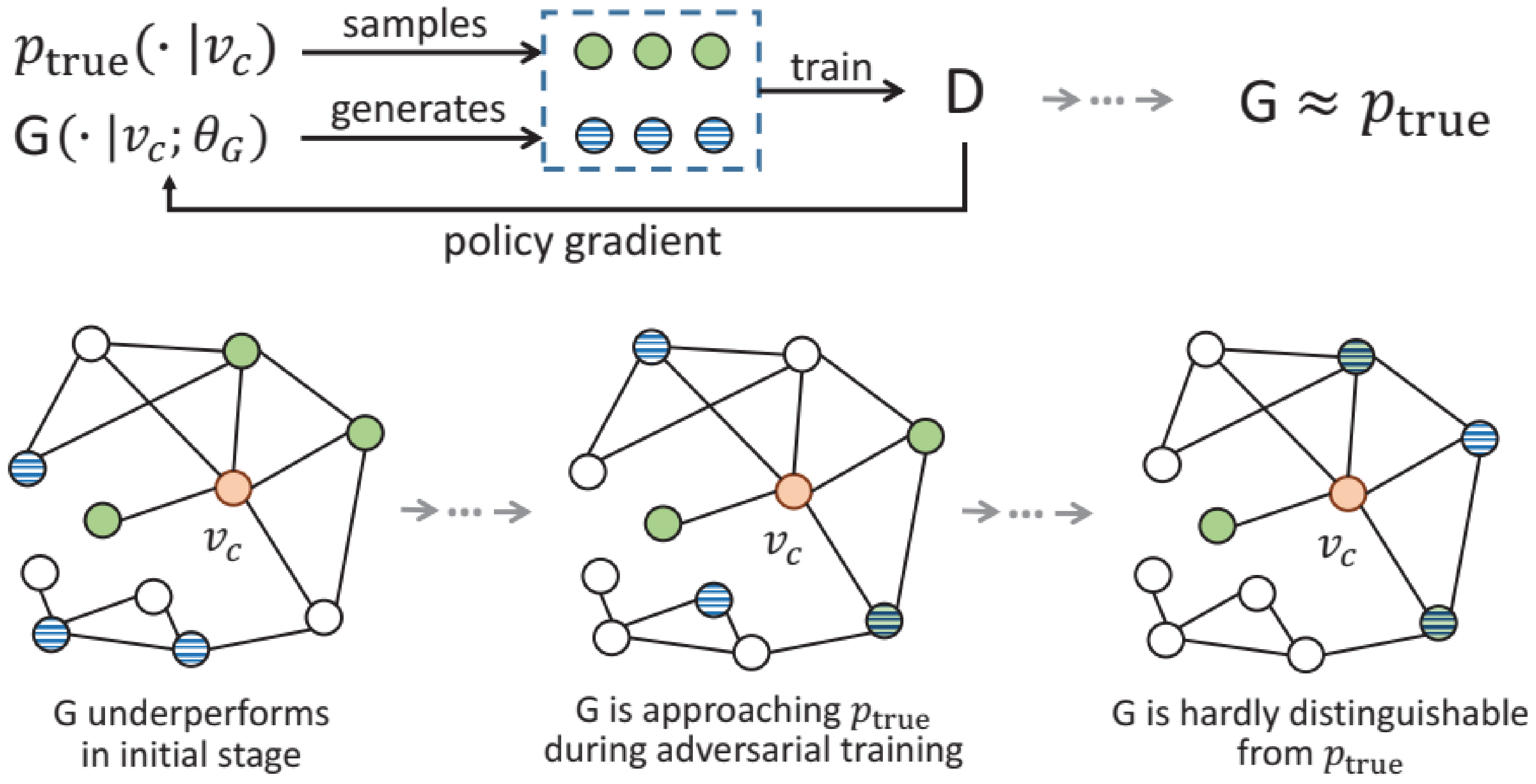
Optimization of G

$$\min_{\theta_G}\max_{\theta_D} V(G,D) = \sum_{c=1}^{V}\Big(\mathbb{E}_{v\sim p_{\mathrm{true}}(\cdot|v_c)}\big[\log D(v,v_c;\theta_D)\big]+$$
$$\mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\log\left(1-D(v,v_c;\theta_D)\right)\big]\Big) \tag{1}$$

- Gradient of $V(G,D)$ w.r.t θ_G (policy gradient):

$$\begin{aligned}
&\nabla_{\theta_G} V(G,D)\\
=&\nabla_{\theta_G}\sum_{c=1}^{V}\mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\log\left(1-D(v,v_c;\theta_D)\right)\big]\\
=&\sum_{c=1}^{V}\sum_{i=1}^{N}\nabla_{\theta_G} G(v_i|v_c;\theta_G)\log\left(1-D(v_i,v_c;\theta_D)\right)\\
=&\sum_{c=1}^{V}\sum_{i=1}^{N} G(v_i|v_c;\theta_G)\nabla_{\theta_G}\log G(v_i|v_c;\theta_G)\log\left(1-D(v_i,v_c;\theta_D)\right)\\
=&\sum_{c=1}^{V}\mathbb{E}_{v\sim G(\cdot|v_c;\theta_G)}\big[\nabla_{\theta_G}\log G(v|v_c;\theta_G)\log\left(1-D(v,v_c;\theta_D)\right)\big].
\end{aligned} \tag{4}$$

graphGAN



[GitHub - liutongyang/GraphGAN-pytorch: (Still in coding)A pytorch implementation of GraphGAN (Graph Representation Learning with Generative Adversarial Nets) from hwwang55]

[如何进行优化：论文解读-GraphGan_哔哩哔哩_bilibili]

Graph Generative Adversarial Networks for Sparse Data Generation in High Energy Physics

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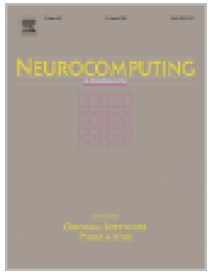

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Molecular generative Graph Neural Networks for Drug Discovery

Pietro Bongini [a] [b], Monica Bianchini [a], Franco Scarselli [a]

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