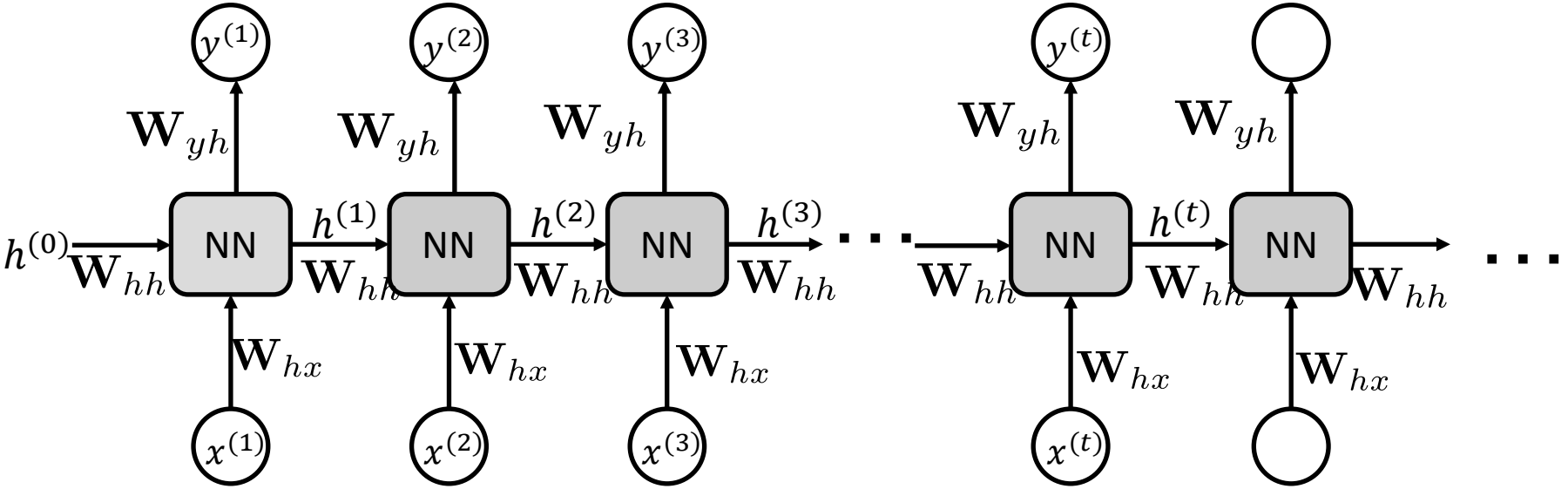
深蓝学院
shenlanxueyuan.com

图上的其他深度模型

教材：图深度学习，电子工业出版社
https://baike.baidu.com/item/图深度学习

- 图上的循环神经网络
- 图上的自编码器
- 图上的变分自编码器
- 图上的生成对抗网络

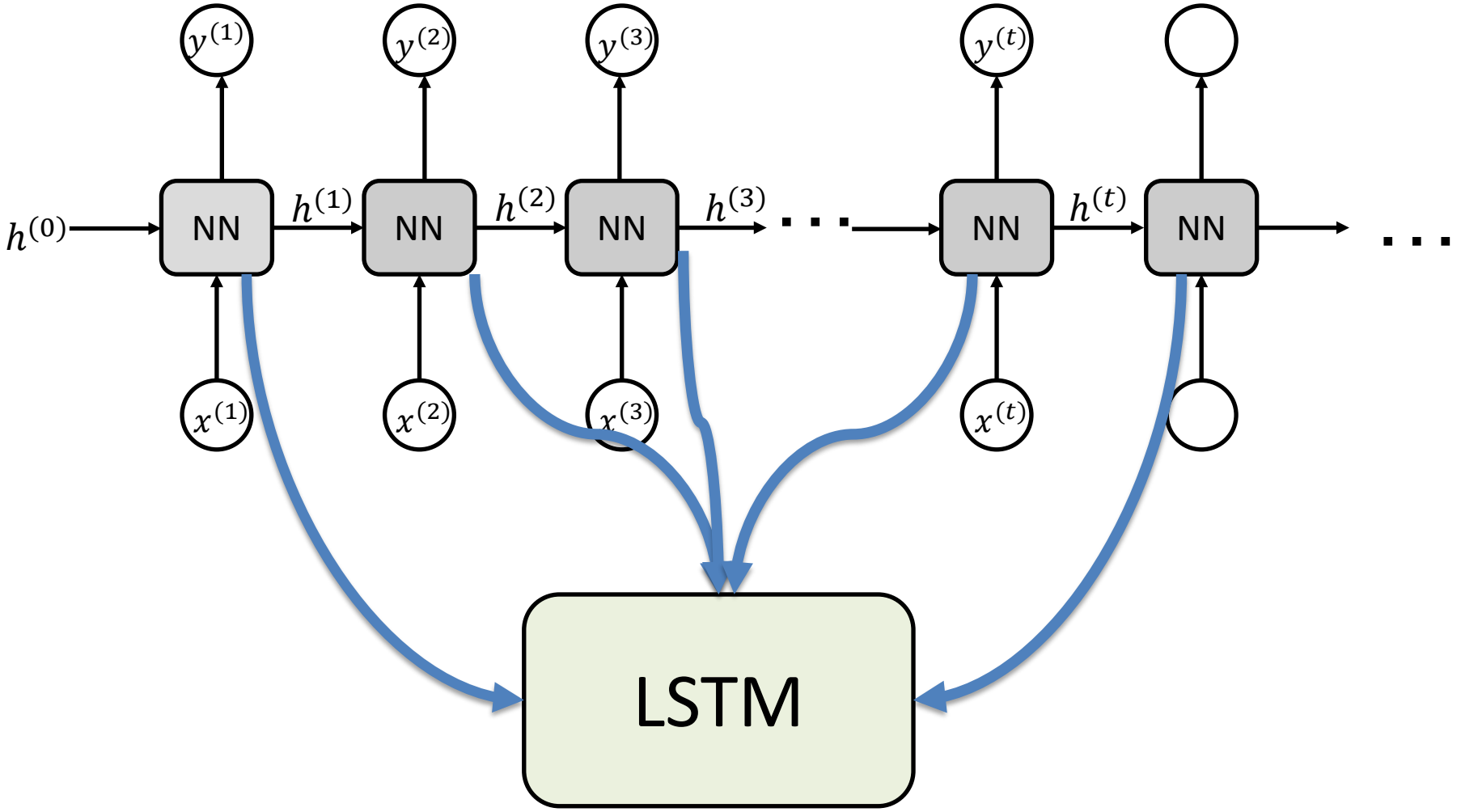
循环神经网络



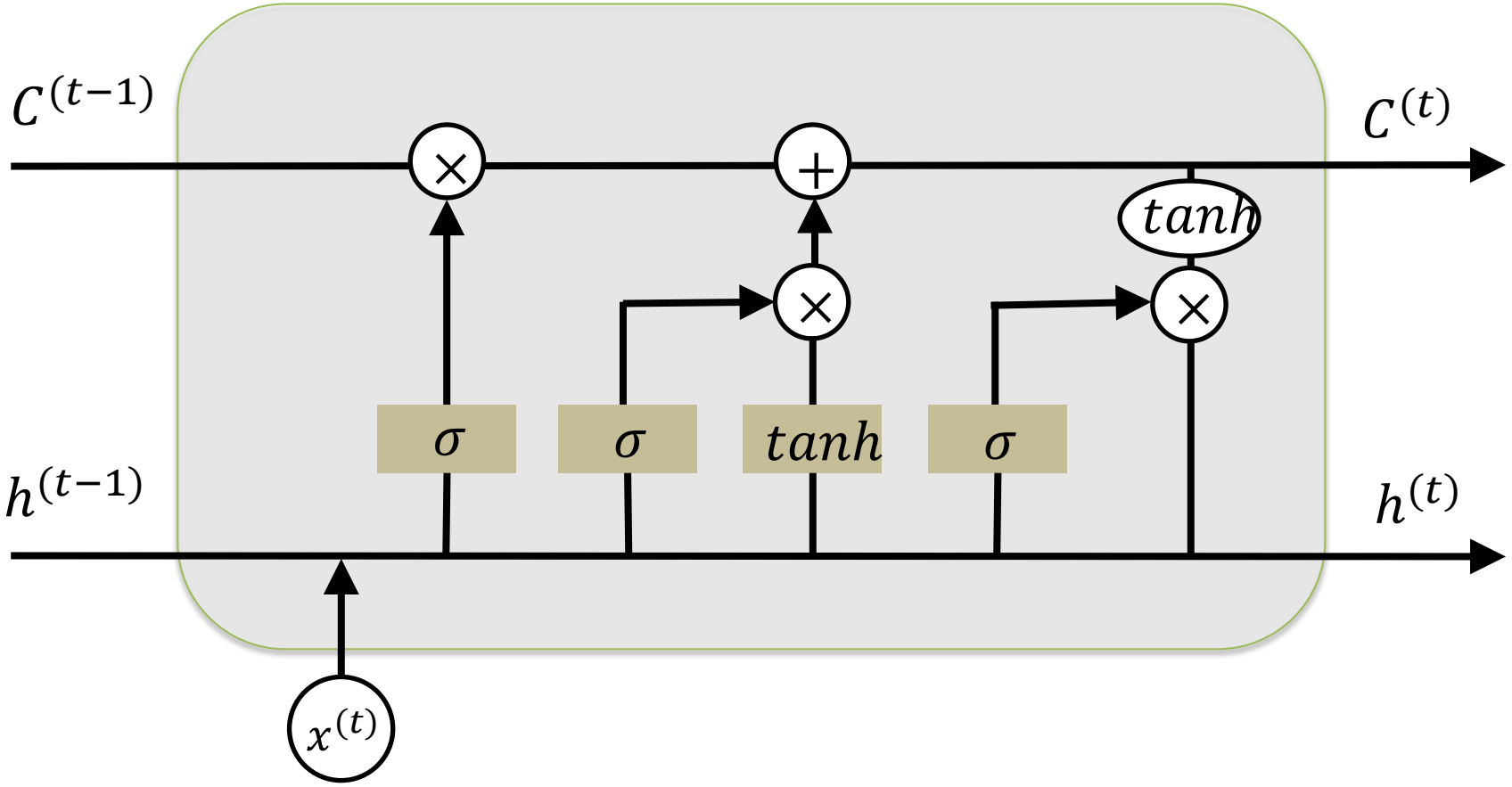
$$\boldsymbol{h}^{(i)} = \alpha_h \left(\boldsymbol{W}_{\mathrm{hh}} \cdot \boldsymbol{h}^{(i-1)} + \boldsymbol{W}_{\mathrm{hx}} \boldsymbol{x}^{(i-1)} + \boldsymbol{b}_h \right)$$

$$\boldsymbol{y}^{(i)} = \alpha_y \left(\boldsymbol{W}_{\mathrm{yh}} \boldsymbol{h}^{(i)} + \boldsymbol{b}_y \right)$$

LSTM



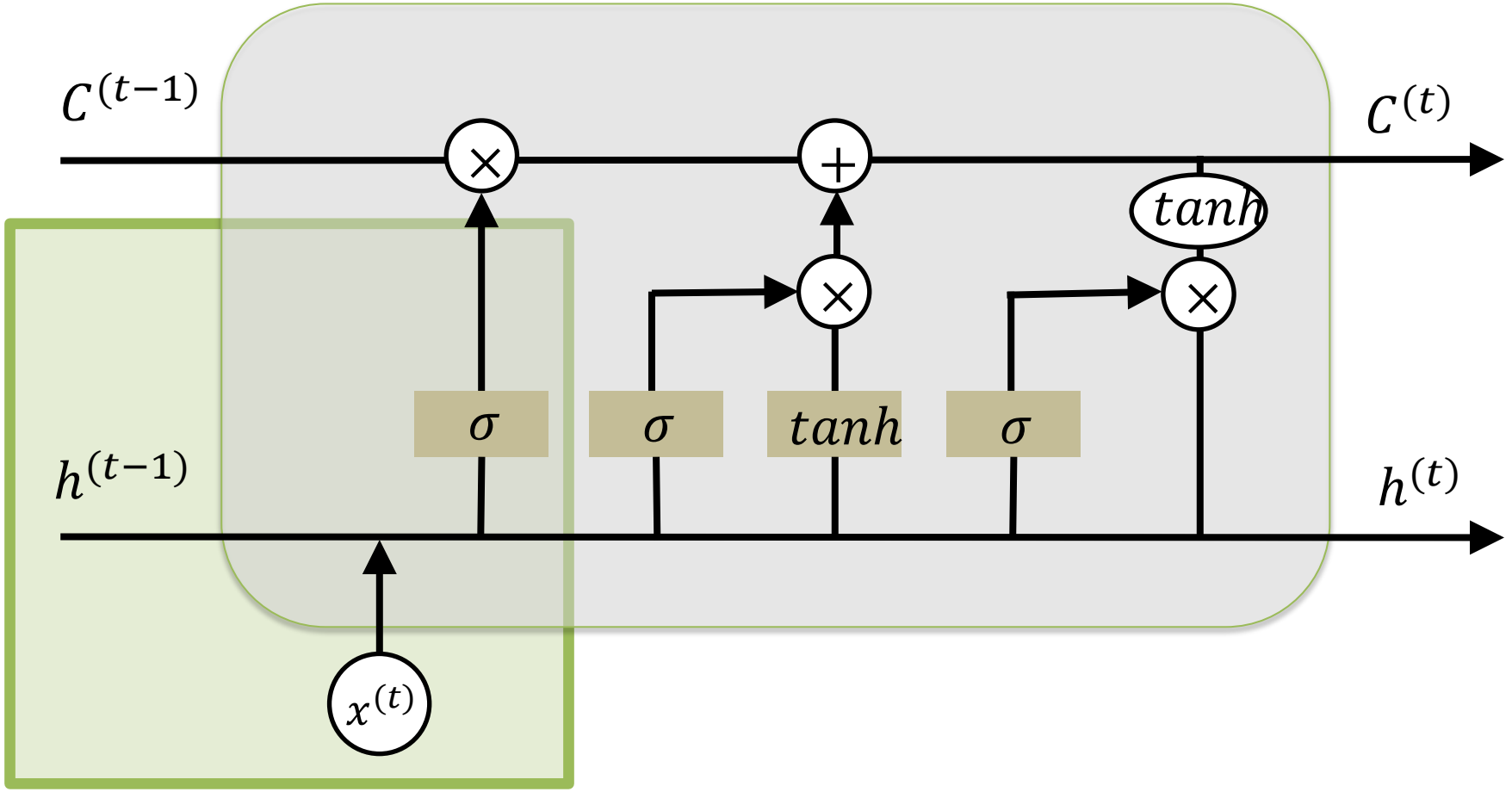
LSTM



单元状态（Cell State）： $C^{(t)}$

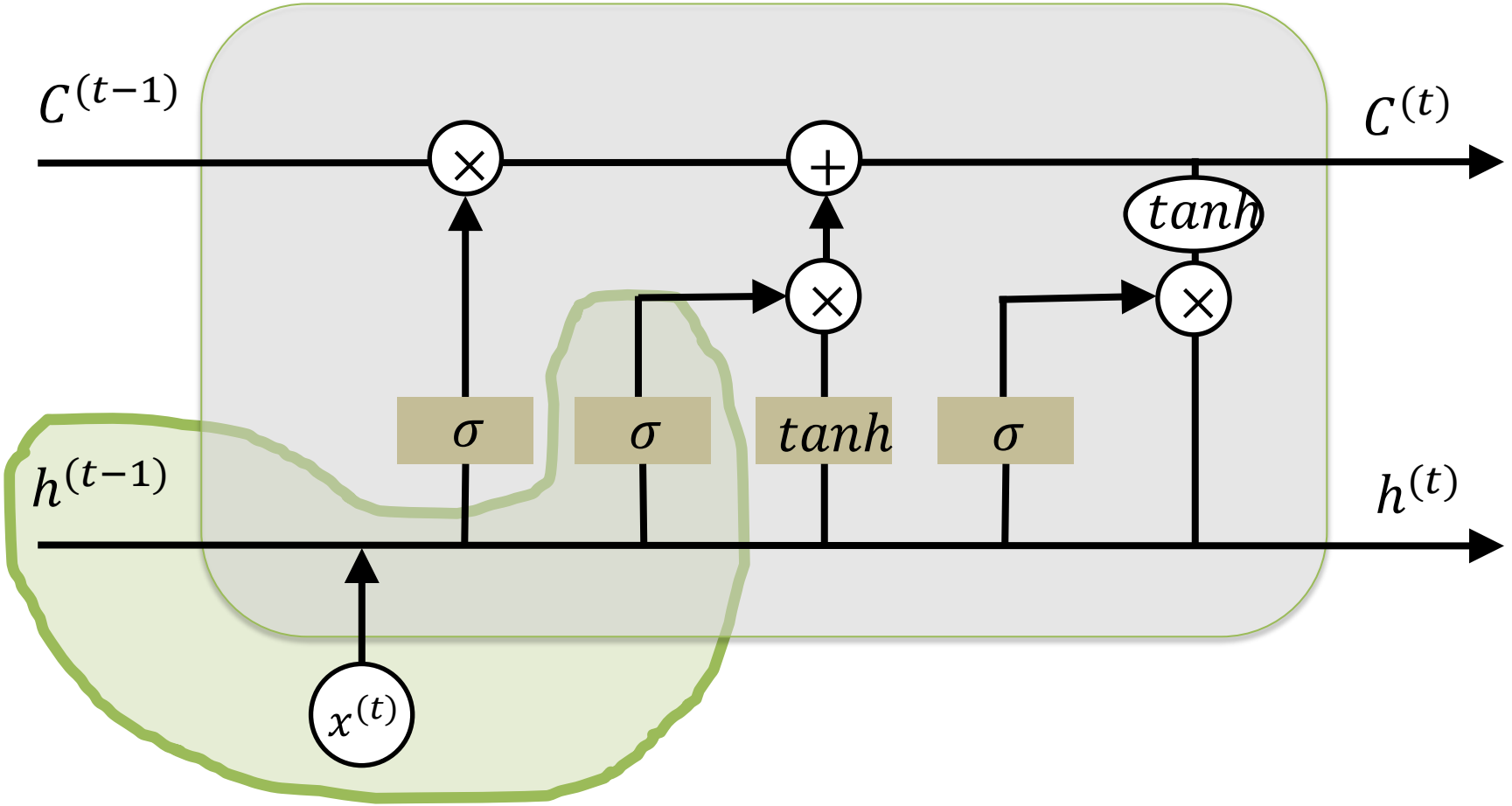
隐藏状态 (Hidden State)： $h^{(t)}$

LSTM：遗忘门



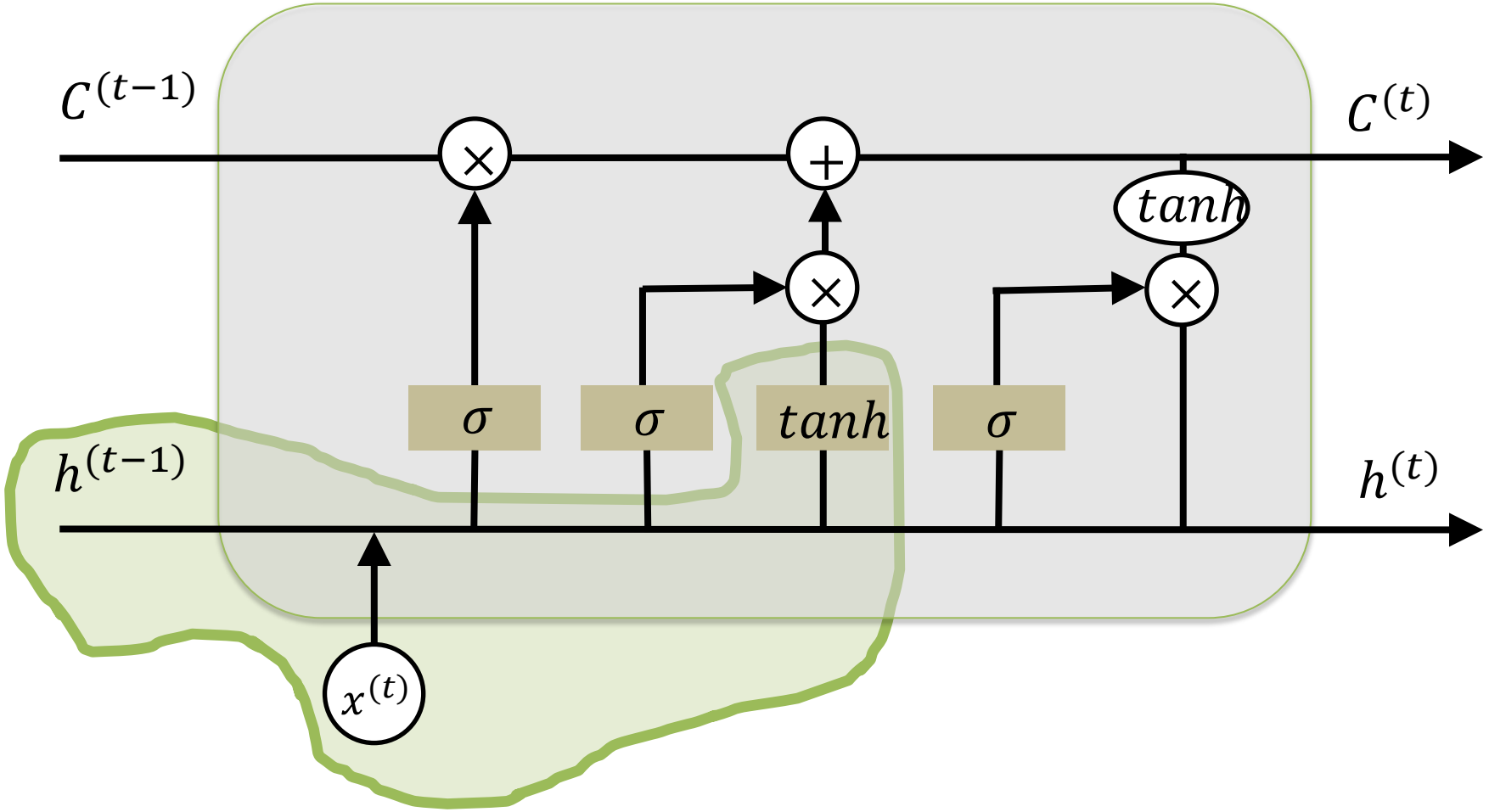
$$\boldsymbol{f}_t = \sigma\left(\boldsymbol{W}_f \cdot \boldsymbol{x}^{(t)} + \boldsymbol{U}_f \cdot \boldsymbol{h}^{(t-1)} + \boldsymbol{b}_f\right)$$

LSTM：输入门



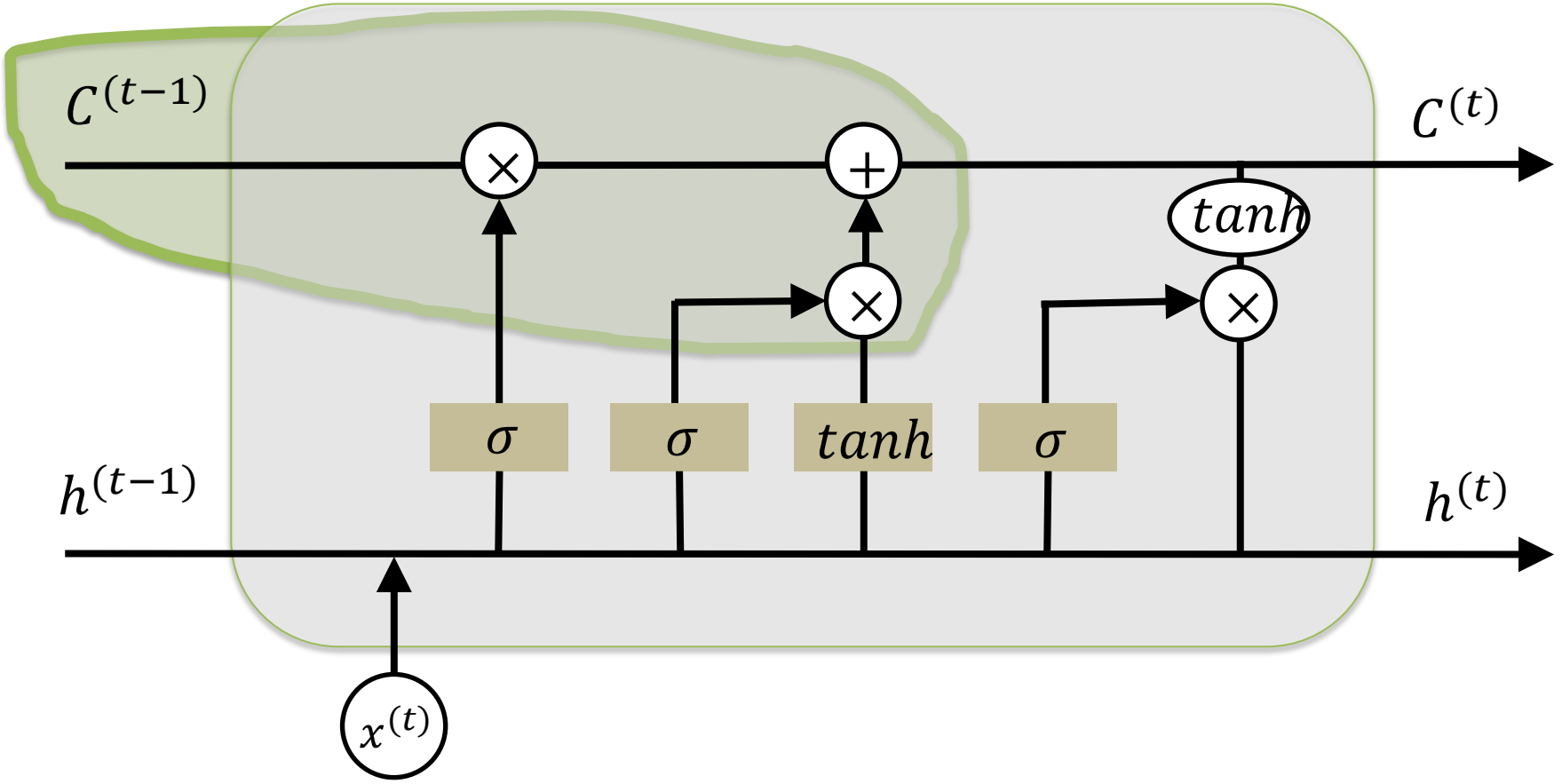
$$\boldsymbol{i}_t = \sigma\left(\boldsymbol{W}_i \cdot \boldsymbol{x}^{(t)} + \boldsymbol{U}_i \cdot \boldsymbol{h}^{(t-1)} + \boldsymbol{b}_i\right)$$

LSTM：候选值



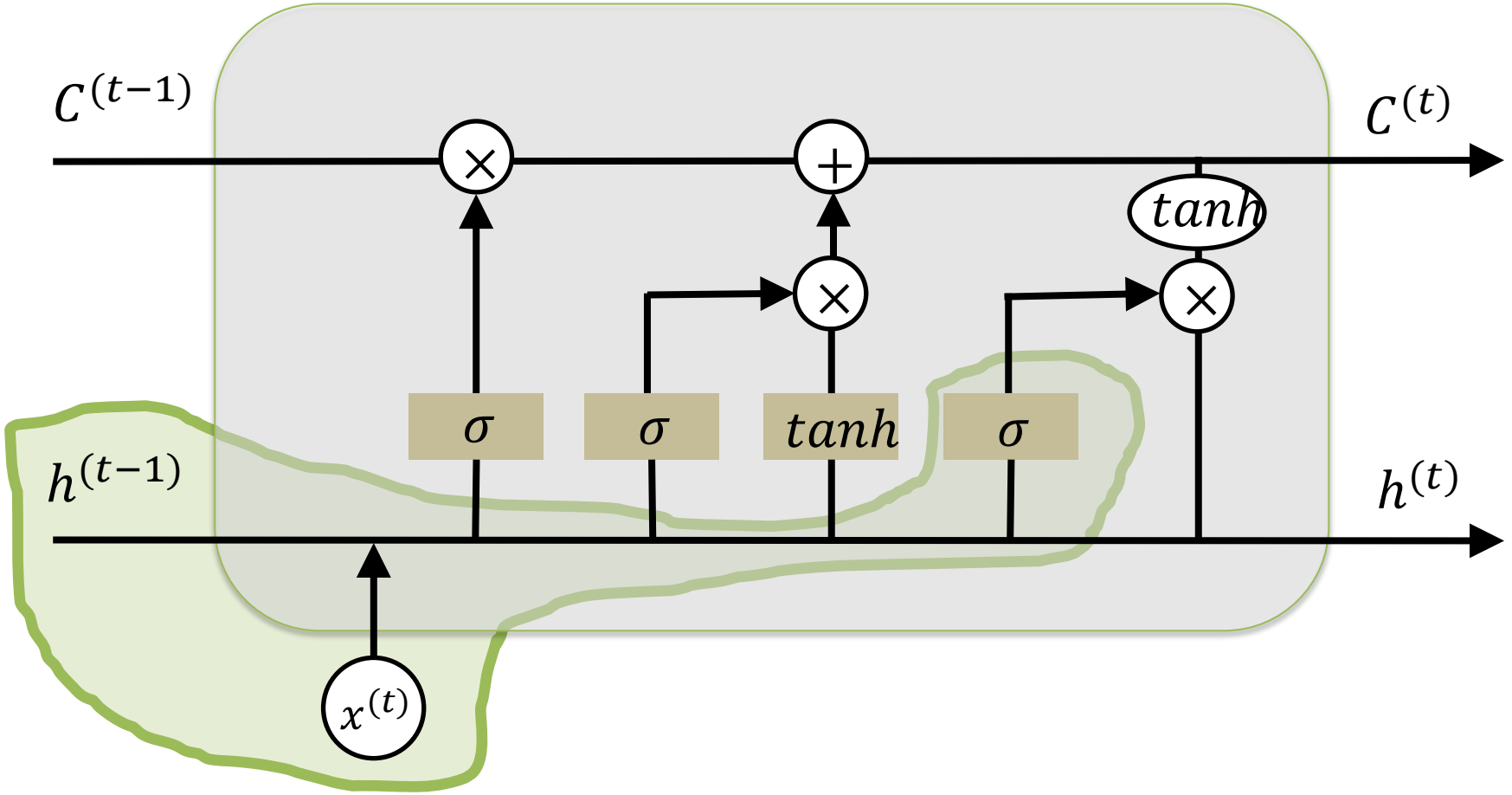
$$\tilde{C}^{(t)} = \tanh\left(\boldsymbol{W}_c \cdot \boldsymbol{x}^{(t)} + \boldsymbol{U}_c \cdot \boldsymbol{h}^{(t-1)} + \boldsymbol{b}_c\right)$$

LSTM：新的单元状态



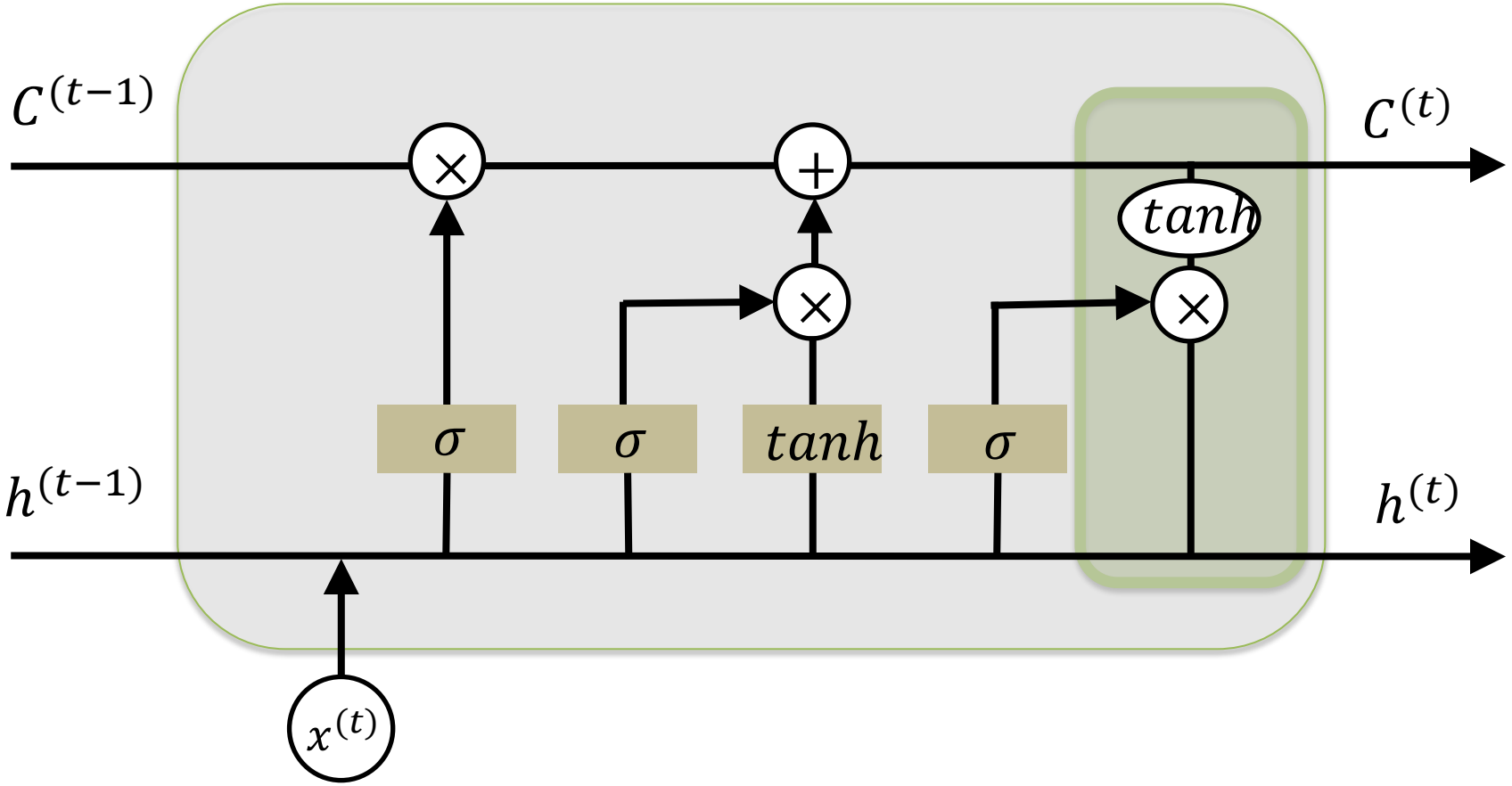
$$\boldsymbol{C}^{(t)} = \boldsymbol{f}_t \odot \boldsymbol{C}^{(t-1)} + \boldsymbol{i}_t \odot \tilde{\boldsymbol{C}}^{(t)}$$

LSTM：输出门



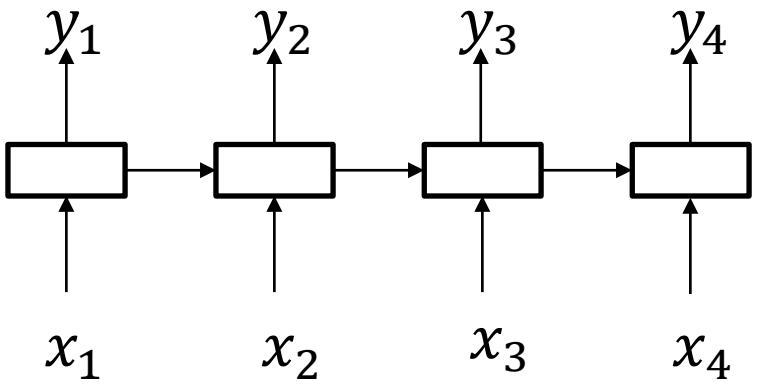
$$\boldsymbol{o}_t = \sigma\left(\boldsymbol{W}_o \cdot \boldsymbol{x}^{(t)} + \boldsymbol{U}_o \cdot \boldsymbol{h}^{(t-1)} + \boldsymbol{b}_o\right)$$

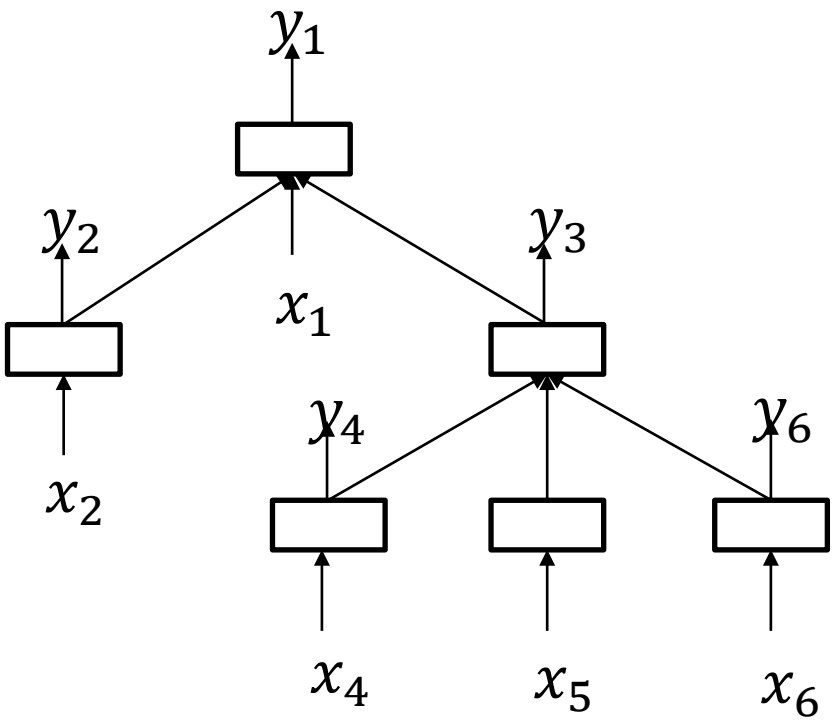
LSTM



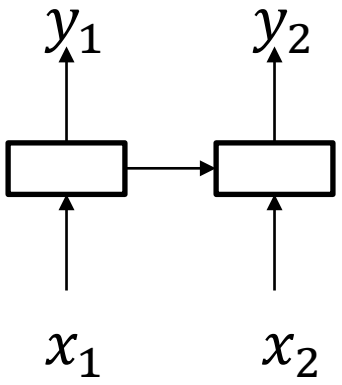
$$\boldsymbol{h}^{(t)} = \boldsymbol{o}_t \odot \tanh\left(\boldsymbol{C}^{(t)}\right)$$

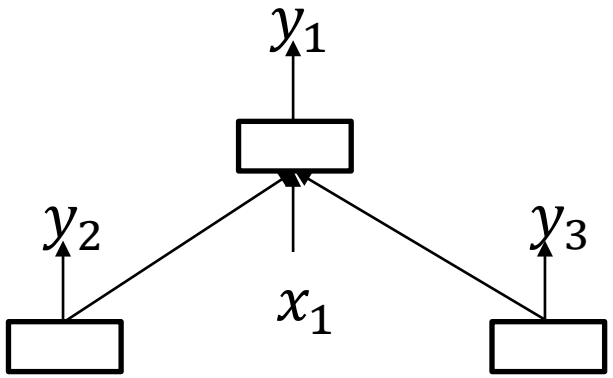
LSTM VS Tree-LSTM





LSTM VS Tree-LSTM





$$\tilde{\mathbf{h}}^{(k)} = \sum_{v_j \in \mathcal{N}_c(v_k)} \mathbf{h}^{(j)}$$

$$\mathbf{f}_{kj} = \sigma(\mathbf{W}_f \cdot \mathbf{x}^{(k)} + \mathbf{U}_f \cdot \mathbf{h}^{(j)} + \mathbf{b}_f) \quad \textbf{for } v_j \in \mathcal{N}_c(v_k)$$

$$\mathbf{i}_k = \sigma(\mathbf{W}_i \cdot \mathbf{x}^{(k)} + \mathbf{U}_i \cdot \tilde{\mathbf{h}}^{(k)} + \mathbf{b}_i)$$

$$\mathbf{o}_k = \sigma(\mathbf{W}_o \cdot \mathbf{x}^{(k)} + \mathbf{U}_o \cdot \tilde{\mathbf{h}}^{(k)} + \mathbf{b}_o)$$

$$\tilde{\mathbf{C}}^{(k)} = tanh(\mathbf{W}_c \cdot \mathbf{x}^{(k)} + \mathbf{U}_c \cdot \tilde{\mathbf{h}}^{(k)} + \mathbf{b}_c)$$

$$\mathbf{C}^{(k)} = \mathbf{i}_t \odot \tilde{\mathbf{C}}^{(k)} + \sum_{v_j \in \mathcal{N}_c(v_k)} \mathbf{f}_{kj} \odot \mathbf{C}^{(j)}$$

$$\mathbf{h}^{(k)} = \mathbf{o}_t \odot tanh(\mathbf{C}^{(k)}).$$

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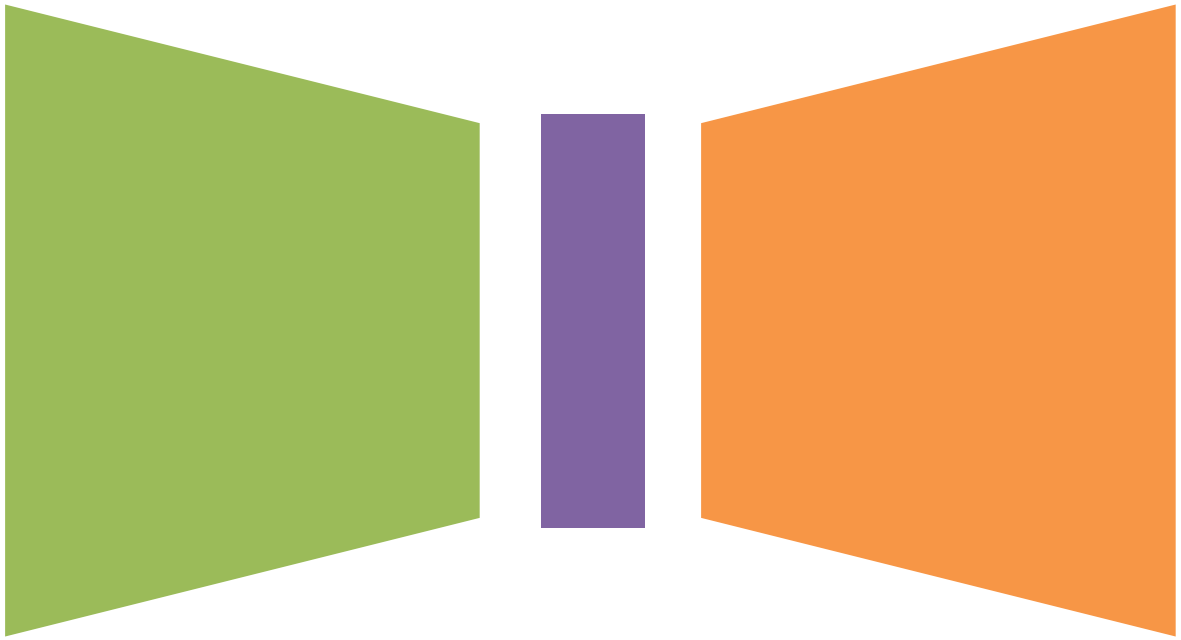
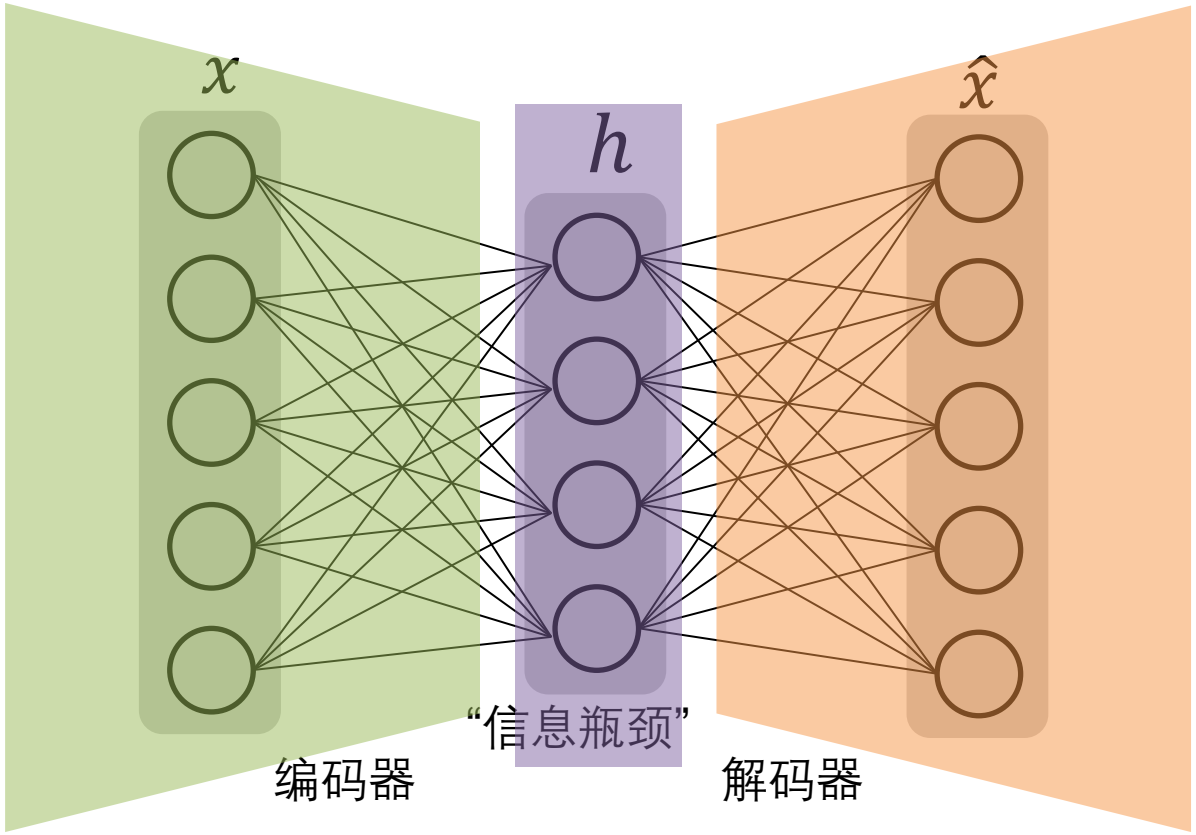
自编码器

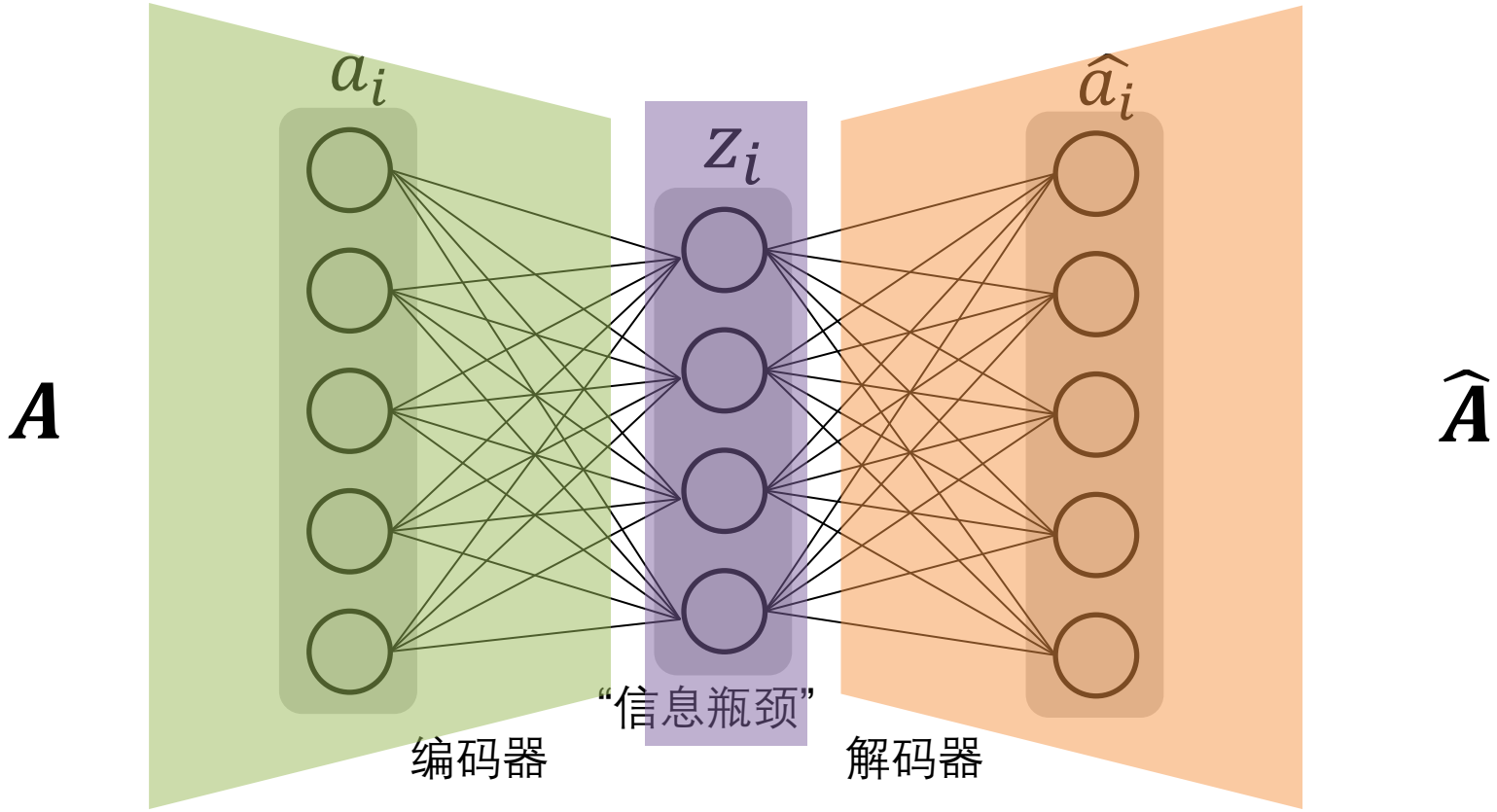


编码器　　解码器

自编码器

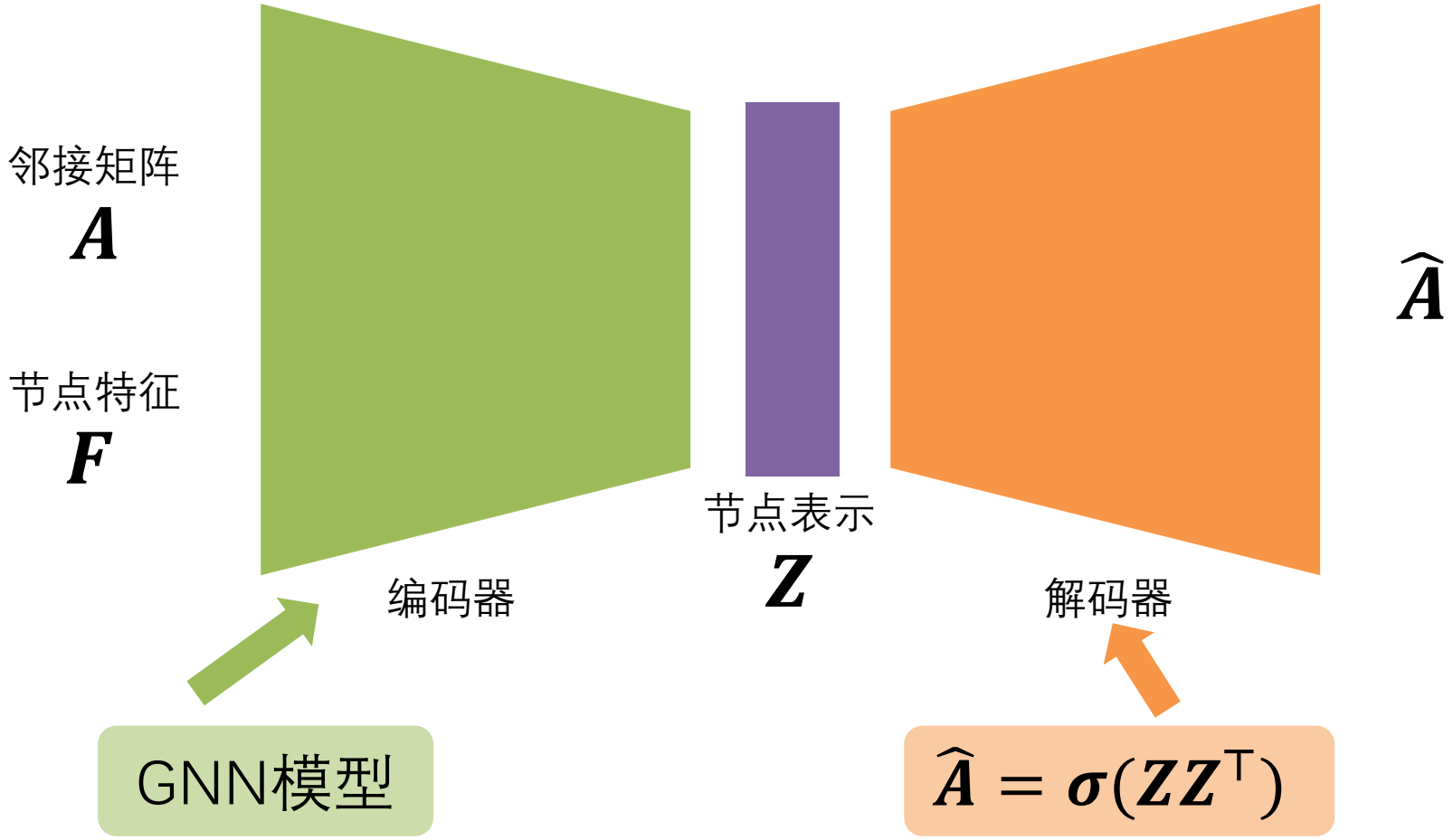


图上的自编码器



$$\sum_{v_i \in \mathcal{V}} \|\boldsymbol{a}_i - \hat{\boldsymbol{a}}_i\|_2^2 \qquad \sum_{v_i, v_j \in \mathcal{V}} \boldsymbol{A}_{i,j} \cdot \|\boldsymbol{z}_i - \boldsymbol{z}_j\|_2^2 \qquad \|\Theta_{\text{enc}}\|_2^2 + \|\Theta_{\text{dec}}\|_2^2$$

基于图神经网络的图上的自编码器



$$\mathbf{Z} = \mathrm{GNN}(\mathbf{A}, \mathbf{F})$$

- 图上的循环神经网络
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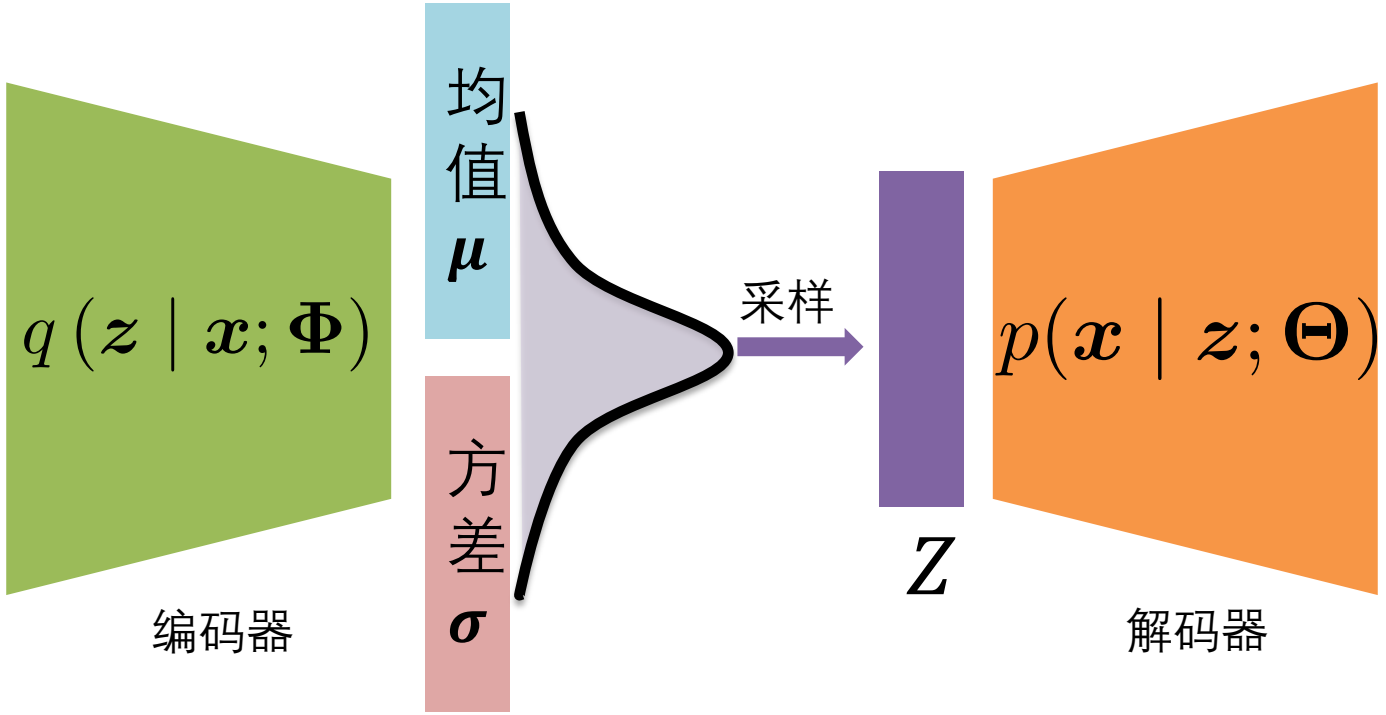
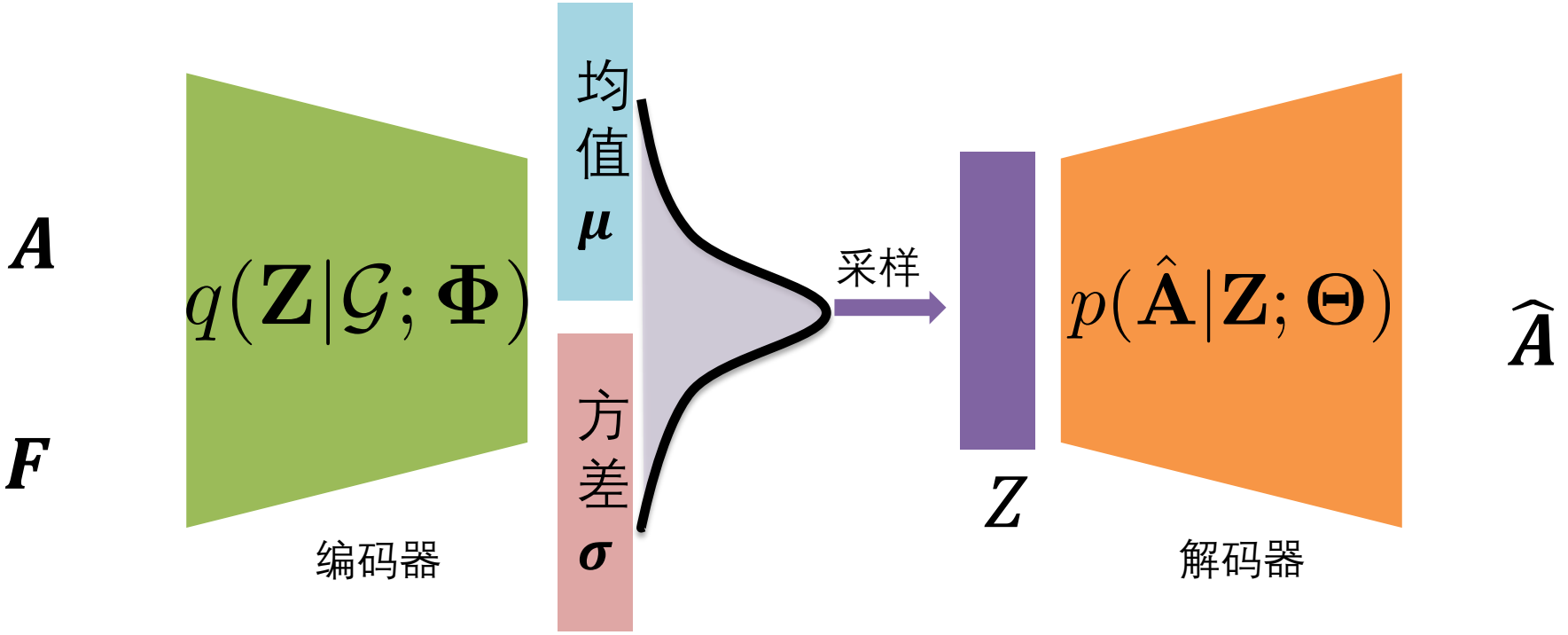
变分自编码器



$$\underbrace{\mathbb{E}_{q(z|x_i;\Phi)}[\log p(x_i \mid z; \Theta)]}_{\text{重建}}$$

用于节点表示学习的变分自编码器



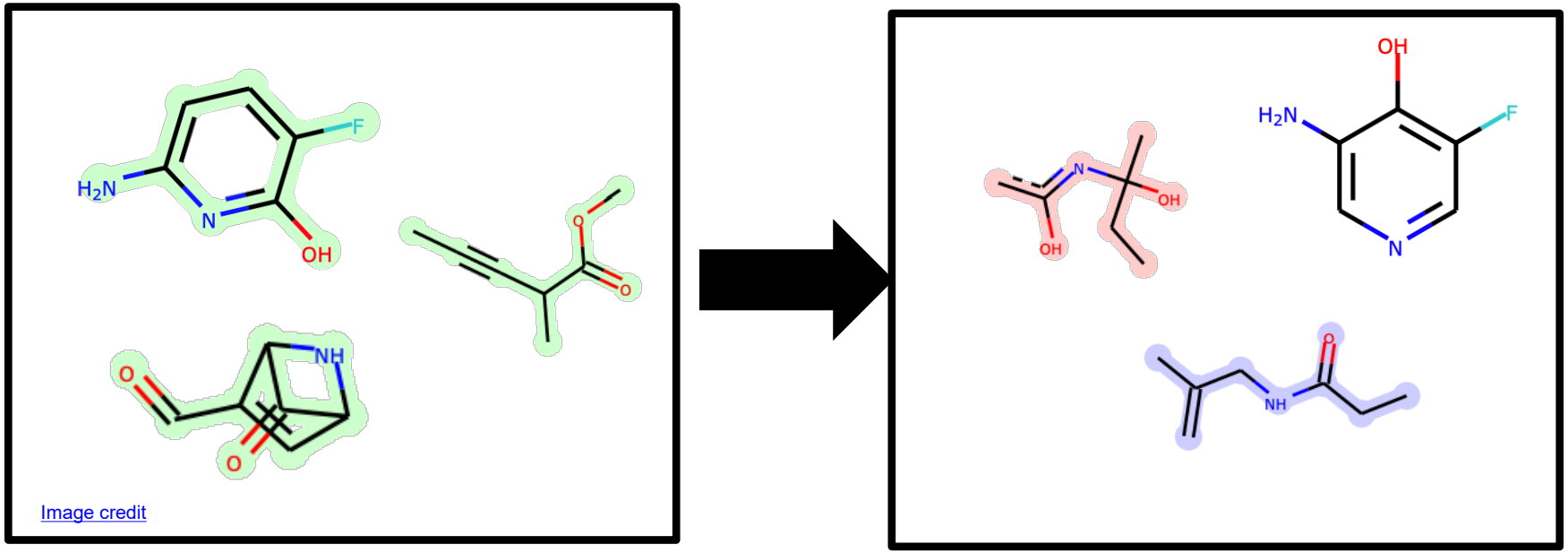
$$\boldsymbol{\mu} = \mathrm{GNN}\left(\boldsymbol{F}, \boldsymbol{A}; \boldsymbol{\Phi}_{\mu}\right)$$

$$\log \boldsymbol{\sigma} = \mathrm{GNN}\left(\boldsymbol{F}, \boldsymbol{A}; \boldsymbol{\Phi}_{\sigma}\right)$$

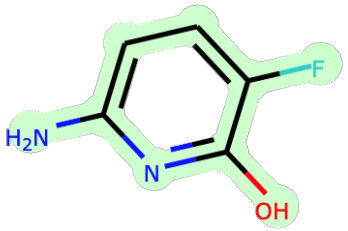
$$p\left(\boldsymbol{A}_{i,j} = 1 \mid \mathbf{z}_i, \mathbf{z}_j\right)$$

$$\sigma\left(\mathbf{z}_i^{\top} \mathbf{z}_j\right)$$

图生成



图的表示：

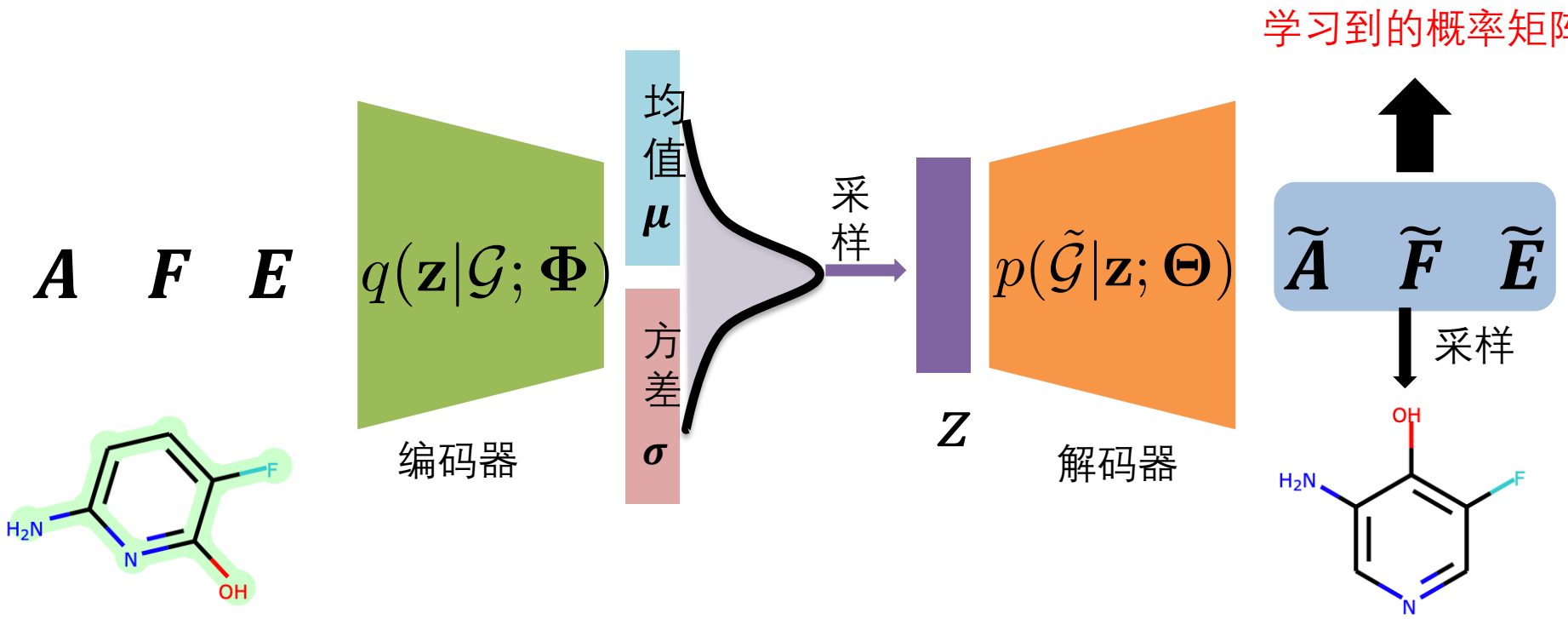


A 连接

F 节点类型

E 边类型

用于图生成的变分自编码器



$$\boldsymbol{\mu} = \text{pool}\left(\text{GNN}_{\mu}(\mathcal{G})\right)$$

$$\log \boldsymbol{\sigma} = \text{pool}\left(\text{GNN}_{\sigma}(\mathcal{G})\right)$$

$$\tilde{\mathcal{G}} = \text{MLP}(\boldsymbol{z};\boldsymbol{\Theta})$$

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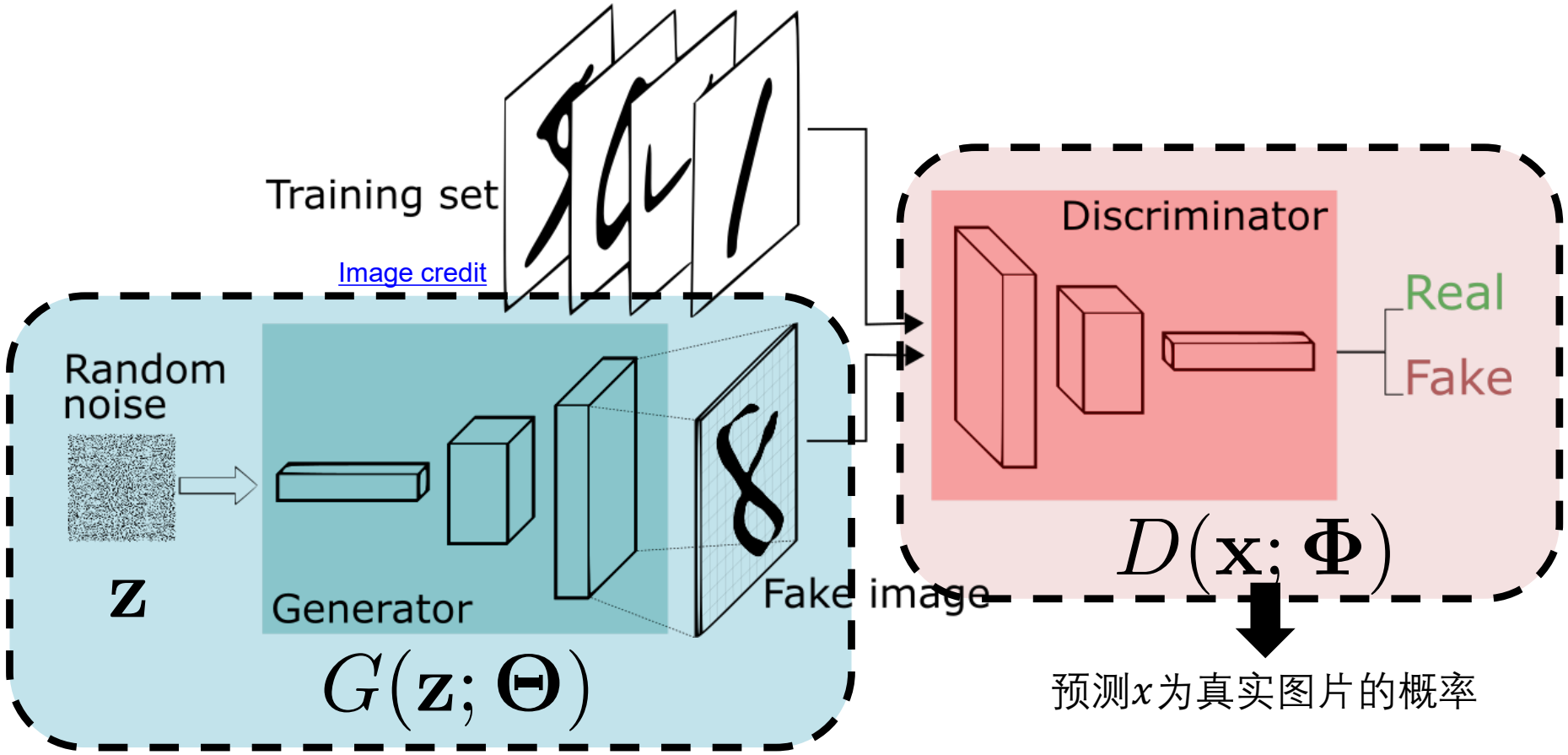
生成对抗网络 (GANs)



$$\min_{\Theta}\max_{\Phi}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x};\Phi)]+\mathbb{E}_{\boldsymbol{z}\sim p(\boldsymbol{z})}[\log(1-D(G(\boldsymbol{z};\Theta);\Phi))]$$

真实图片　　生成的图片

生成对抗网络的一些应用场景

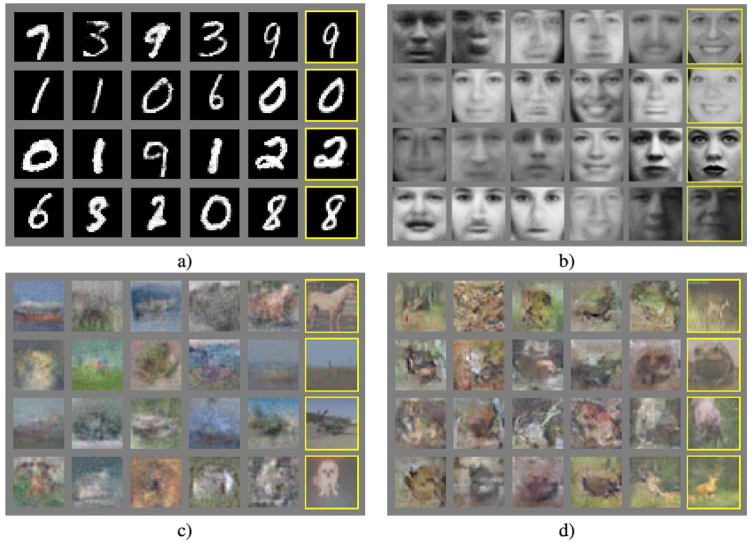


Image credit

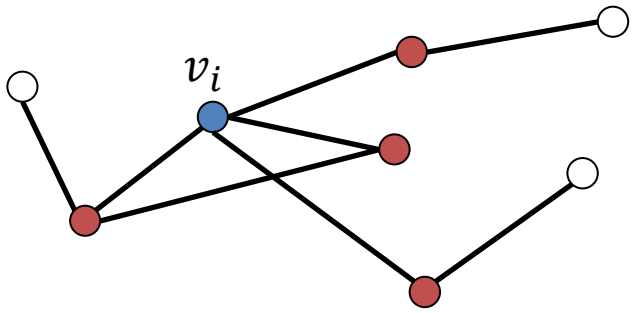
由GANs生成的图片

Image credit

基于GANs的风格转换

用于节点表示学习的生成对抗网络

Φ和 Θ 都可以作为节点表示



生成器

- 采样一个节点作为v_i的“邻居”
- 目标：使的采样出来的节点尽可能是真的邻居

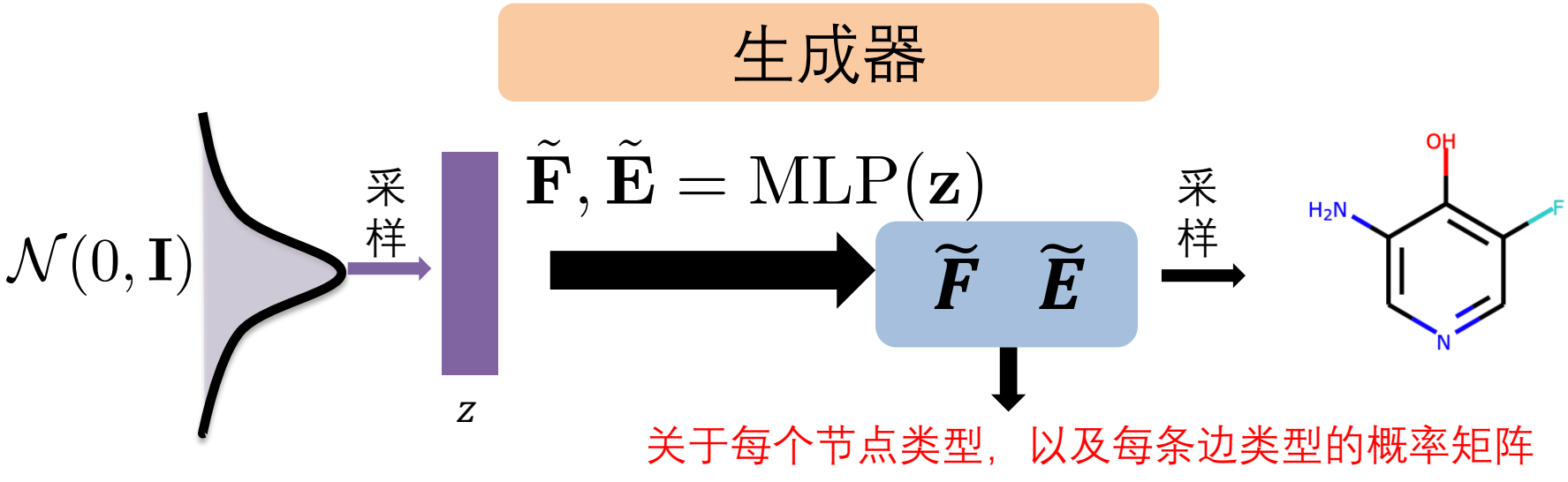
$$G\left(v_j \mid v_i; \boldsymbol{\Theta}\right) = \frac{\exp\left(\boldsymbol{\theta}_j^\top \boldsymbol{\theta}_i\right)}{\sum_{v_k \in \mathcal{V}} \exp\left(\boldsymbol{\theta}_k^\top \boldsymbol{\theta}_i\right)}$$

判别器

- 判断给定的一个节点对是否在原图中相连
- 目标：尽量区分采样出来“邻居”和原图中的真实的邻居。

$$D\left(v_j, v_i; \boldsymbol{\Phi}\right) = \frac{1}{1 + \exp\left(-\boldsymbol{\phi}_j^\top \boldsymbol{\phi}_i\right)}$$

用于图生成的生成对抗网络



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感谢聆听！

Thanks for Listening