

for conventional VAE.

Assume x_i for data, $P(x)$ is the data distribution

$$\text{find } z \rightarrow P(x) = \int f(z, \theta) P(z) dz$$

{ Same
similar $\rightarrow$ increase variance $\rightarrow$ Use $P(x|z; \theta)$ to
dissimilar substitute $f(z, \theta)$

$$P(x|z; \theta) = N(x|f(z; \theta), b^2 * I)$$

$$\begin{cases} u = f(z; \theta) \\ b = \sqrt{b^2 * I} \end{cases}$$

For JT VAE $\rightarrow$ x to be represented by graph matrix

$$G(V, E) = X$$

$$V_i = \begin{bmatrix} \text{node} \\ \text{Info} \end{bmatrix} \begin{bmatrix} \text{Node} \\ \text{features} \end{bmatrix} \rightarrow x_u.$$

x_{uv} to be the edge feature matrix $\rightarrow$ bond type

$$V_{u,v}^{(t)} = \tau \left(W_1^g W_u + W_2^g x_{uv} + W_3^g \sum_{w \in N(u) \setminus v} V_w^{(t-1)} \right)$$

τ is the activation function.

$N(u) \setminus v$ Neighbors of node v except v

After T steps $\rightarrow$ Aggregate all messages as latent vector of each vertex u .

$$h_u = \tau C U_1^g X_u + \sum_{v \in N(u)} U_2^g D_{uv}^{(T)}$$

The final graph representation $h_G = \frac{\sum h_i}{|V|}$

$$U_G = W_u * h_G + b_u$$

$$\log G_G = W_G * h_G + b_G$$

Sample Σ from standard distribution $N(0, I)$

$$\Sigma \sim N(0, I)$$

Sample Z_G from Latent space $N(U_G, G_G)$

$$Z_G = U_G + G_G \odot \Sigma, \quad G_G = \exp\left(\frac{\log G_G}{2}\right)$$

$\searrow$ element wise multiplication

For Tree encoder

G R U $\rightarrow$ Gated Recurrent Unit

$$S_{ij} = \sum_{k \in N(i) \setminus j} m_{kj} \rightarrow \text{Aggregated messages}$$

Updated Gates:

$$z_{ij} = \sigma(CW^z x_i + U^z S_{ij} + b^z)$$

Determine how much information to be incorporate.

Reset Gates:

$$r_{ki} = \sigma(CW^r x_i + U^r m_{ki} + b^r)$$

control how much information is contributed by each incoming message m_{ki} from neighboring nodes $N(i) \setminus j$

So candidate message:

$$\tilde{m}_{ij} = \tanh(CW x_i + U \sum_{k \in N(i) \setminus j} (r_{ki} \odot m_{ki}))$$

So, Final message.

$$m_{ij} = \underbrace{(1 - z_{ij})}_{\substack{\uparrow \\ \text{retained info}}} \odot \underbrace{s_{ij}}_{\substack{\downarrow \\ \text{origin info}}} + z_{ij} \odot \underbrace{\tilde{m}_{ki}}_{\substack{\uparrow \\ \text{weighted} \\ \text{new info}}}$$

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