word2vec 优化方式推导

一. Negative Sampling (负采样)

选择一个正样本和K个负样本，训练 $(K+1)$ 个二分类器.

1. CBOW 的公式推导

假设中心词为 w，周围词为 $context(w)$，负样本集 $NEG(w)$

定义 Indicator Function. $I^{w}(\tilde{w}) = \begin{cases} 1, & \tilde{w}=w \\ 0, & \tilde{w}\neq w \end{cases}$

用来表示词对 $[context(w), \tilde{w}]$ 的标签，$context(w) = \dfrac{\sum_{-m\le j\le m}^{j\ne 0} u_{j+w}}{2j}$ (周围词平均向量) $= \vec{x}_w$

似然函数 likelihood ~~$p(\tilde{w}|context(w))$~~

$$= \prod_{\tilde{w}\in\{w\}\cup NEG(w)} p(\tilde{w}|context(w)) \quad ①$$，令目标词 $\tilde{w}$ 的词向量为 $\theta^{\tilde{w}}$

其中 $p(\tilde{w}|context(w)) = \begin{cases} \sigma(\vec{x}_w^{T}\cdot\theta^{\tilde{w}}), & I^{w}(\tilde{w})=1 \\ 1-\sigma(\vec{x}_w^{T}\cdot\theta^{\tilde{w}}), & I^{w}(\tilde{w})=0 \end{cases}$

$$\therefore ①式 = \sigma(\vec{x}_w^{T}\cdot\theta^{w})\cdot\prod_{\tilde{w}\in NEG(w)}\left(1-\sigma(\vec{x}_w^{T}\cdot\theta^{\tilde{w}})\right) = g(w)$$

给定语料库C，我们的目标 $\max\prod_{w\in C} g(w) \Leftrightarrow \max\log\prod_{w\in C} g(w)$

$$\Rightarrow \max\sum_{w\in C}\left[\log\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{w}) + \sum_{\tilde{w}\in NEG(w)}\log\sigma(-\vec{x}_w^{T}\cdot\theta^{\tilde{w}})\right] \quad (1-\sigma(x)=\sigma(-x))$$

令 $L(w,\tilde{w}) = I^{w}(\tilde{w})\log\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}) + (1-I^{w}(\tilde{w}))\log(1-\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}))$ ②

代表每个训练样本的 log-likelihood，使用梯度上升法

$$\frac{\partial L}{\partial\theta^{\tilde{w}}} = I^{w}(\tilde{w})(1-\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}))\cdot\vec{x}_w + (1-I^{w}(\tilde{w}))(-\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}))\cdot\vec{x}_w$$

$$= (I^{w}(\tilde{w}) - I^{w}(\tilde{w})\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}))\cdot\vec{x}_w + (I^{w}(\tilde{w})\sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}) - \sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}}))\cdot\vec{x}_w$$

$$= [I^{w}(\tilde{w}) - \sigma(\vec{x}_w^{T}\cdot\vec{\theta}^{\tilde{w}})]\cdot\vec{x}_w$$

$\sigma'(x) = \sigma(x)(1-\sigma(x))$

$(\log\sigma(x))' = 1-\sigma(x)$

$[\log(1-\sigma(x))]' = -\sigma(x)$

由于θ^w和X_w^T在②式中对称，

$\frac{\partial L}{\partial \theta^{\tilde{w}}}$换成$\frac{\partial L}{\partial X_w^T} = [I^w(\tilde{w}) - \sigma(\vec{X}_w^T \cdot \vec{\theta}^{\tilde{w}})] \cdot \vec{\theta}^{\tilde{w}}$

对于K+1个样本，可使用下述公式更新梯度

$$\theta^{\tilde{w}} : \theta^{\tilde{w}} + \eta [I^w(\tilde{w}) - \sigma(\vec{X}_w^T \cdot \vec{\theta}^{\tilde{w}})] \cdot \vec{X}_w$$

$$X_w : X_w + \sum_{\tilde{w} \in \{w\} \cup NEG(w)} \eta [I^w(\tilde{w}) - \sigma(\vec{X}_w^T \cdot \vec{\theta}^{\tilde{w}})] \cdot \vec{\theta}^{\tilde{w}}$$

2. skipgram 公式推导

似然函数 $\Rightarrow \prod_{w \in C} \prod_{u \in context(w)} \prod_{\tilde{w} \in \{u\} \cup NEG(u)} P(\tilde{w}|w)$

其中 $p(\tilde{w}|w) = \begin{cases} \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}}), & I^w(\tilde{w}) = 1 \\ 1 - \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}}), & I^w(\tilde{w}) = 0 \end{cases}$

$$Log\text{-}likelihood = \sum_{w \in C} \sum_{u \in context(w)} \sum_{\tilde{w} \dots} [I(\tilde{w}) \log \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}}) + (1 - I(\tilde{w})) \log (1 - \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}}))]$$

由于公式与一(1)一样，我们可以得到

$$\frac{\partial L}{\partial u_{\tilde{w}}} = [I^w(\tilde{w}) - \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}})] \cdot \vec{V}_w$$

$$\vec{u}_{\tilde{w}} : \vec{u}_{\tilde{w}} + \eta \frac{\partial L}{\partial u_{\tilde{w}}}$$

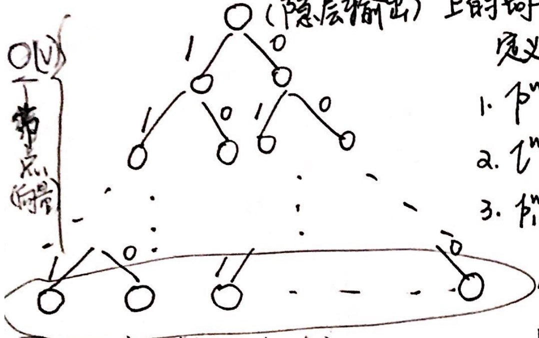
同理： $\frac{\partial L}{\partial V_w} = [I^w(\tilde{w}) - \sigma(\vec{V}_w^T \cdot \vec{u}_{\tilde{w}})] \cdot \vec{u}_{\tilde{w}}$

对于K+1个样本：

$$\vec{V}_w : \vec{V}_w + \sum_{\tilde{w} \in \{u\} \cup NEG\{u\}} \eta \frac{\partial L}{\partial V_w^T}$$

二. Hierarchical Softmax (层次softmax) (哈夫曼树)

叶子结点代表的是词典中的所有词$|V|$，通往目标词的路径上的结点(隐层输出)上的向量是我们要优化的。



单词节点(没有向量)

定义:

1. p^w: 根结点到单词结点(叶子结点)的路径
2. l^w: 路径p^w中结点的个数
3. $p_1^w, p_2^w, \dots, p_{l^w}^w$: 路径上的点，$p_1^w$根结点，$p_{l^w}^w$: w结点
4. $d_2^w, d_3^w, \dots d_{l^w}^w \in \{0,1\}$: 词$w$的哈夫曼编码，由$(l^w-1)$位二进制编码构成
5. $\theta_1^w, \theta_2^w, \dots \theta_{l^w-1}^w$ 对应p^w中非叶子节点的向量

1. CBOW的公式推导

$$\max \prod_{w\in C}\prod_{j=2}^{l^w} p(d_j^w \mid x_w, \theta_{j-1}^w) \quad ①$$

(x_w为隐层输出)

$$\vec{x_w} = \frac{\sum context(w)}{|context(w)|}$$

，有

$$p = \begin{cases} \sigma(\vec{x_w}^T \cdot \theta_{j-1}^w), & d_j^w = 0 \quad \text{向右走} \\ 1-\sigma(\vec{x_w}^T \cdot \theta_{j-1}^w), & d_j^w = 1 \quad \text{向左走} \end{cases}$$

对数似然 ⇒

$$\log ① = \sum_{w\in C}\sum_{j=2}^{l^w}\left((1-d_j^w)\log\sigma(\vec{x_w}^T\cdot\theta_{j-1}^w) + d_j^w\log(1-\sigma(\vec{x_w}^T\cdot\theta_{j-1}^w))\right)$$

$$= L(j,w)$$

对于每个样本

$$\frac{\partial L(j,w)}{\partial \theta_{j-1}^w} = (1-d_j^w)(1-\sigma(x_w^T\cdot\theta_{j-1}^w))\cdot x_w + d_j^w(-\sigma(x_w^T\cdot\theta_{j-1}^w))\cdot x_w$$

$$= (1-d_j^w-\sigma(x_w^T\cdot\theta_{j-1}^w))\cdot x_w$$

$$\theta_{j-1}^w := \theta_{j-1}^w + \eta\frac{\partial L}{\partial \theta_{j-1}^w}$$

对称性 ⇒

$$\frac{\partial L}{\partial x_w} = (1-\sigma(x_w^T\theta_{j-1}^w) - d_j^w)\cdot\theta_{j-1}^w$$

根据 x_w 来更新 V_w ⇒ $V_m := V_m + \eta\sum_{j=2}^{l^w}\frac{\partial L}{\partial x_w}$

2. skipgram 的公式推导

非常类似CBOW，多了一个遍历 context(w)

$$\max \prod_{w \in C} \prod_{u \in context(w)} \prod_{j=2}^{l^w} p(d_j^w \mid x_w, \theta_{j-1}^w)$$ （x_w 隐层输出）

对数似然 ~~L(w,u,j)~~ $L = \sum_{w \in C} \sum_{u \in context(w)} \sum_{j=2}^{l^w} \log p(d_j^w \mid x_w, \theta_{j-1}^w)$

$$= \sum \sum \sum \underbrace{(1-d_j^w)\log\sigma(x_w^T \cdot \theta_{j-1}^w) + d_j^w \log(1-\sigma(x_w^T \cdot \theta_{j-1}^w))}_{L(w,j)}$$

参考上节: $\frac{\partial L}{\partial \theta_{j-1}^w} = \left(1-d_j^w-\sigma(x_w^T \cdot \theta_{j-1}^w)\right) \cdot x_w$

$$\theta_{j-1}^w : \theta_{j-1}^w + \eta \frac{\partial L}{\partial \theta_{j-1}^w}$$

$$\frac{\partial L}{\partial x_w} = \left(1-d_j^w-\sigma(x_w^T \cdot \theta_{j-1}^w)\right) \cdot \theta_{j-1}^w$$

$$x_w : x_w + \eta \sum_{u \in context(w)} \sum_{j=2}^{l^w} \frac{\partial L}{\partial x_w}$$