word2vec gradients Charlie Colley 9/29/17

$$\sigma(x) = \frac{1}{1+e^x}$$

$$\begin{split} \frac{\partial \sigma}{\partial x}(x) &= \frac{\partial}{\partial x}(\frac{e^x}{1+e^x}) = \frac{(1+e^x)e^x - e^x(e^x)}{(1+e^x)^2} = (\frac{e^x}{1+e^x})(\frac{1-e^x + e^x}{(1+e^x)}) \\ &= \sigma(x)(\frac{1+e^x}{1+e^x} - \frac{e^x}{(1+e^x)}) = \sigma(x)(1-\sigma(x)) \end{split}$$

Thus  $\frac{\partial \sigma(x)}{\partial x}(x) = \sigma(x)(1 - \sigma(x)).$ 

Objective function:

$$\underset{V_c, V_w}{\operatorname{arg max}} = \Sigma_{(w,c) \in D} \log(\sigma(\langle v_c, v_w \rangle)) + \Sigma_{(w,c)v \in D'} \log(\sigma(-\langle v_c, v_w \rangle))$$

$$\nabla_{v_c}(\langle v_c, v_w \rangle)_k = \frac{\partial}{\partial (v_c)_k} \sum_i (v_c)_i (v_w)_i = \frac{\partial}{\partial (v_c)_k} (\sum_{i \neq k} (v_c)_i (v_w)_i + (v_c)_k (v_w)_k) = (v_w)_k$$

by symmetry, the gradient  $\nabla_{v_w}\langle v_c, v_w \rangle$  is  $v_c$ . Let  $B \in \mathbb{R}^{n \times m}$ .

$$\nabla_B(\langle v_c, v_w \rangle_B)_{kl} = \frac{\partial}{\partial B_{kl}} \sum_{ij} B_{ij}(v_c)_i(v_w)_i =$$

$$\frac{\partial}{\partial B_{kl}} \left( \sum_{i,j \neq k} (v_c)_i (v_w)_i + B_{kl} (v_c)_k (v_w)_l \right) = (v_c)_l (v_w)_k = (v_c \otimes v_w)_{kl}$$

Then the gradient of  $\log(\sigma(\langle v_c, v_w \rangle))$  with respect to  $v_c$  is

$$\begin{split} \frac{\partial}{\partial (v_c)_k} (\log(\sigma(\langle v_c, v_w \rangle))) &= (\frac{1}{\sigma(\langle v_c, v_w \rangle)}) (\sigma(\langle v_c, v_w \rangle)(1 - \sigma(\langle v_c, v_w \rangle)))(v_w)_k \\ &= (1 - \sigma(\langle v_c, v_w \rangle)))(v_w)_k \end{split}$$

again by symmetry we can show that the gradient with respect to  $v_w$  is similarly  $\nabla_{v_w}(\log(\sigma(\langle v_c, v_w \rangle))) = (1 - \sigma(\langle v_c, v_w \rangle))v_c$ 

Let  $P \in \mathbb{R}^{n \times n}$  and  $U, V \in \mathbb{R}^{n \times d}$  and let  $f = \|P - UV^T\|_F^2$ 

$$\begin{split} (\nabla_U f)_{ij} &= \frac{\partial}{\partial U_{ij}} \|P - UV^T\|_F^2 = \frac{\partial}{\partial U_{ij}} (\sum_{i_1, i_2 = 1}^n (P_{i_1, i_2} - \sum_{i_3}^d U_{i_1, i_3} V_{i_3, i_2}^T)^2) \\ &= \frac{\partial}{\partial U_{ij}} ([\sum_{i_1 \neq i, i_2 = 1}^n (P_{i_1, i_2} - \sum_{i_3}^d U_{i_1, i_3} V_{i_3, i_2}^T)^2] + (P_{i, i_2} - \sum_{i_3}^d U_{i, i_3} V_{i_3, i_2}^T)^2) \\ &= \frac{\partial}{\partial U_{ij}} \sum_{i_2}^n (P_{i, i_2} - \sum_{i_3}^d U_{i, i_3} V_{i_3, i_2}^T)^2 \\ &= \sum_{i_2}^n 2(P_{i, i_2} - \sum_{i_3}^d U_{i, i_3} V_{i_3, i_2}^T) \frac{\partial}{\partial U_{ij}} (P_{i, i_2} - \sum_{i_3}^d U_{i, i_3} V_{i_3, i_2}^T) \\ &= \sum_{i_2} 2(P_{i, i_2} - \sum_{i_3}^d U_{i, i_3} V_{i_3, i_2}^T) (V_{j, i_2}^T) \\ &= \sum_{i_2} 2(P_{i, i_2} - (UV^T)_{i, i_2}) (V_{i_2, j}) = 2(PV - UV^TV)_{ij} \\ &(\nabla_V f)_{ij} = \frac{\partial}{\partial V_{ij}} \|P - UV^T\|_F^2 = \frac{\partial}{\partial V_{ij}} \|P^T - VU^T\|_F^2 \end{split}$$

Now note that by the generality of the last gradient computation we can show that  $\nabla_V f = 2(P^T U - V U^T U)$ .

Consider the function  $g = \lambda ||U||_F^2$  for  $\lambda \in \mathbb{R}$ , then the gradient with respect to U is

$$(\nabla_U g)_{ij} = \lambda \frac{\partial}{\partial U_{ij}} (\sum_{i_1, i_2 = 1}^{n, d} U_{i_1, i_2}^2) = \lambda \frac{\partial}{\partial U_{ij}} ([\sum_{i_1 \neq i, i_2 \neq j}^{n, d} U_{i_1, i_2}^2] + U_{ij}^2) = 2\lambda U_{ij}$$

Let  $P \in \mathbb{R}^{n \times n}$ ,  $U \in \mathbb{R}^{n \times d}$ , and  $B \in \mathbb{R}^{d \times d}$ . Consider the function  $f : \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times d} \times \mathbb{R}^{n \times n} \mapsto \mathbb{R}$  such that

$$f(P, U, B) = ||P - UBB^TU^T||_F^2$$

## useful gradients

$$\begin{split} &\frac{\partial}{\partial U_{ij}} (-\sum_{i_3,i_4}^{d,d} U_{i,i_3} C_{i_3,i_4} U_{i,i_4}) \\ &= -\frac{\partial}{\partial U_{ij}} (\sum_{i_3 \neq j,i_4}^{d,d} U_{i,i_3} C_{i_3,i_4} U_{i,i_4} + \sum_{i_4}^{d} U_{i,j} C_{j,i_4} U_{i,i_4}) \\ &= -\frac{\partial}{\partial U_{ij}} (\sum_{i_3 \neq j,i_4 \neq j}^{d,d} U_{i,i_3} C_{i_3,i_4} U_{i,i_4} + \sum_{i_3 \neq j}^{d} U_{i,i_3} C_{i_3,j} U_{i,j} + \sum_{i_4}^{d} U_{i,j} C_{j,i_4} U_{i,i_4}) \\ &= -\frac{\partial}{\partial U_{ij}} (\sum_{i_3 \neq j,i_4 \neq j}^{d,d} U_{i,i_3} C_{i_3,i_4} U_{i,i_4} + \sum_{i_3 \neq j}^{d} U_{i,i_3} C_{i_3,j} U_{i,j} + \sum_{i_4 \neq j}^{d} U_{i,j} C_{j,i_4} U_{i,i_4} + U_{i,j} C_{j,j} U_{i,j}) \\ &= -\frac{\partial}{\partial U_{ij}} (\sum_{i_3 \neq j}^{d} U_{i,i_3} C_{i_3,j} U_{i,j} + \sum_{i_4 \neq j}^{d} U_{i,j} C_{j,i_4} U_{i,i_4} + U_{i,j} C_{j,j} U_{i,j}) \\ &= -(\sum_{i_3 \neq j}^{d} U_{i,i_3} C_{i_3,j} + \sum_{i_4 \neq j}^{d} C_{j,i_4} U_{i,i_4} + 2 U_{i,j} C_{j,j}) \\ &= -(\sum_{i_3}^{d} U_{i,i_3} C_{i_3,j} + \sum_{i_4 \neq j}^{d} C_{j,i_4} U_{i,i_4}) = U C_{i,j} + C U_{ji}^T = U C_{i,j} + U C_{i,j}^T \end{split}$$

Letting  $C = BB^T$ 

$$\begin{split} (\nabla_{U}f)_{ij} &= \frac{\partial}{\partial U_{ij}} \|P - UBB^{T}U^{T}\|_{F}^{2} = \frac{\partial}{\partial U_{ij}} \|P - UCU^{T}\|_{F}^{2} = \frac{\partial}{\partial U_{ij}} \sum_{i_{1},i_{2}}^{n,n} (P_{i_{1},i_{2}} - (UCU^{T})_{i_{1},i_{2}})^{2} \\ &= \frac{\partial}{\partial U_{ij}} \sum_{i_{1},i_{2}}^{n,n} (P_{i_{1},i_{2}} - \sum_{i_{3}}^{d} (U_{i_{1},i_{3}}(CU^{T})_{i_{3},i_{2}})^{2} = \frac{\partial}{\partial U_{ij}} \sum_{i_{1},i_{2}}^{n,n} (P_{i_{1},i_{2}} - \sum_{i_{3},i_{4}}^{d,d} U_{i_{1},i_{3}}C_{i_{3},i_{4}}U_{i_{2},i_{4}})^{2} \\ &= \frac{\partial}{\partial U_{ij}} \sum_{i_{1},i_{2}}^{n,n} (P_{i_{1},i_{2}} - \sum_{i_{3},i_{4}}^{d,d} U_{i_{1},i_{3}}C_{i_{3},i_{4}}U_{i_{2},i_{4}})^{2} \\ &= \frac{\partial}{\partial U_{ij}} (\left[ \sum_{i_{1},i_{2}}^{n,n} (P_{i_{1},i_{2}} \sum_{i_{3},i_{4}}^{d,d} U_{i_{1},i_{3}}C_{i_{3},i_{4}}U_{i_{2},i_{4}})^{2} \right] + (P_{i,j} - \sum_{i_{3},i_{4}}^{d,d} U_{i,i_{3}}C_{i_{3},i_{4}}U_{j,i_{4}})^{2} \\ &+ \left[ \sum_{i_{2}}^{n} (P_{i,i_{2}} - \sum_{i_{3},i_{4}}^{d,d} U_{i,i_{3}}C_{i_{3},i_{4}}U_{i_{2},i_{4}})^{2} \right] + \left[ \sum_{i_{1}}^{n} \frac{\partial}{\partial U_{ij}} (P_{i_{1},i} - \sum_{i_{3},i_{4}}^{d,d} U_{i_{1},i_{3}}C_{i_{3},i_{4}}U_{i,i_{4}})^{2} \right]) \end{split}$$

Note that each terms of the sum can be computed as

$$\begin{split} &\frac{\partial}{\partial U_{ij}}((P_{i,j} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{j,i_4})^2) \\ &= -2(P_{i,j} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{j,i_4})(\frac{\partial}{\partial U_{ij}}(\left[\sum_{\substack{i_3,i_4\\i_3\neq j}}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{j,i_4}\right] + U_{i,j}\sum_{i_4}C_{j,i_4}U_{j,i_4})) \\ &= -2(P_{i,j} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{j,i_4})(\sum_{i_4}C_{j,i_4}U_{j,i_4}) = -2(P_{i,j} - (UCU^T)_{i,j})(CU^T)_{j,j}) \\ &\frac{\partial}{\partial U_{ij}}\sum_{i_2}^{n}(P_{i,i_2} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{i_2,i_4})^2 = \sum_{i_2}^{n}\frac{\partial}{\partial U_{ij}}(P_{i,i_2} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{i_2,i_4})^2 \\ &= \sum_{i_2}^{n}2(P_{i,i_2} - \sum_{i_3,i_4}^{d,d} U_{i,i_3}C_{i_3,i_4}U_{i_2,i_4})(-\sum_{i_4}C_{j,i_4}U_{i_2,i_4}) \\ &\sum_{i_1}^{n}\frac{\partial}{\partial U_{ij}}(P_{i_1,i} - \sum_{i_3,i_4}^{d,d} U_{i_1,i_3}C_{i_3,i_4}U_{i,i_4})^2 \\ &= \sum_{i_1}^{n}2(P_{i_1,i} - \sum_{i_3,i_4}^{d,d} U_{i_1,i_3}C_{i_3,i_4}U_{i,i_4})(-(UC_{i,j} + UC_{i,j}^T)) \end{split}$$

plugging these back into the original computation we get