Deep Learning in Python (An Example in NLP)

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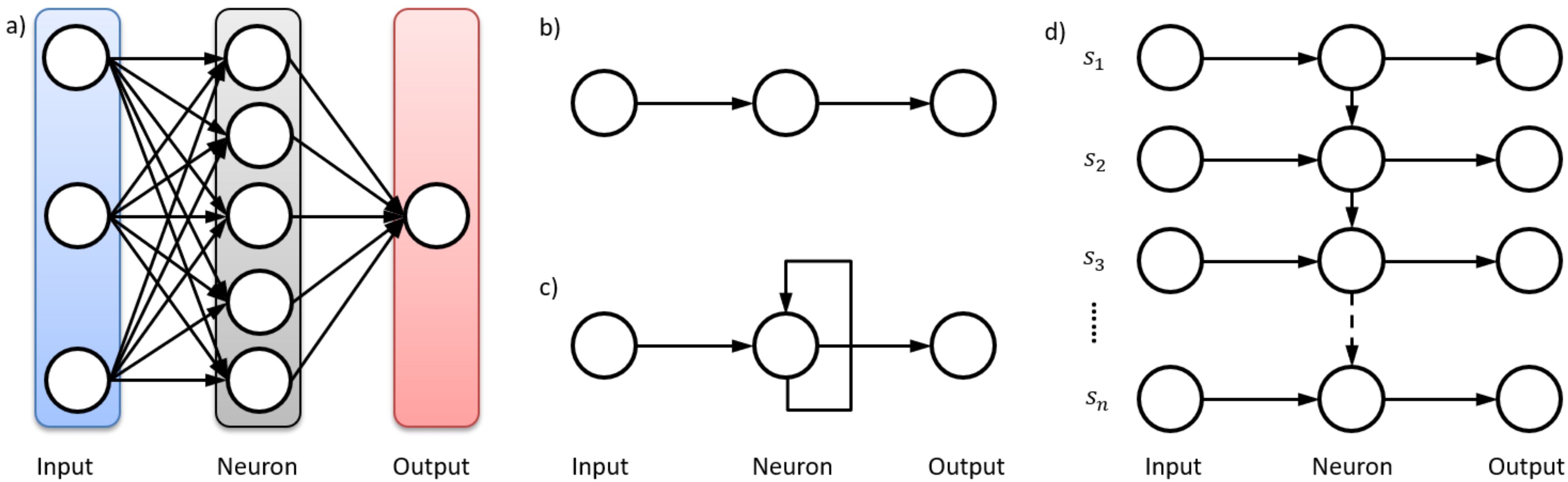
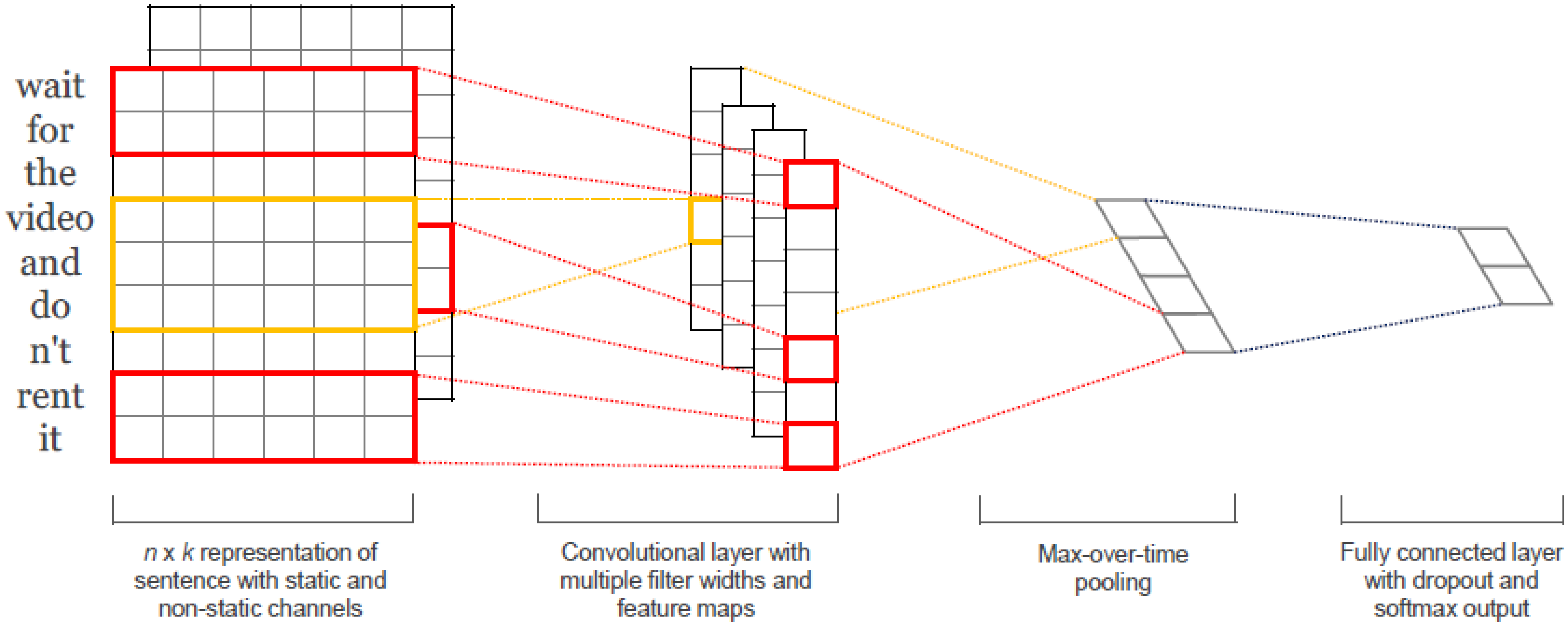
Basics on Neural Networks

- From multi-layer neural networks to recurrent neural networks



Convolutional Neural Networks



Y Kim. Convolutional neural networks for sentence classification. *In EMNLP 2014, 1746-1751*

Using GCN for Long Text Understanding

- Challenges of Long Text Understanding
  - CNN and RNN prioritize locality and sequentiality.
  - They can model local consecutive word sequences well
  - They may ignore global word co-occurrence in a corpus

- GCN can
  - Generalizing well-established neural network models like CNN that apply to regular grid structure (2-d mesh or 1-d sequence) to work on arbitrarily structured graphs
  - Can preserve global structure information of a graph in graph embeddings (node, edge, subgraph and whole graph embeddings)

Graph Convolution

- Denote $A \in \mathbb{R}^{n \times n}$ as the dependency graph G's adjacency matrix
- Graph Laplacian is $L = D - A$, where $D_{ii} = \sum_j A_{ij}$
- Let $U \in \mathbb{R}^{n \times n}$ be the matrix of eigenvectors of the normalized graph Laplacian $L_n = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U \Lambda U^T$
- Let $g_w \in \mathbb{R}^{n \times n}$ be a Fourier domain filter matrix parametrized with a scalar w as its diagonal elements (recall signal processing theory)
- The graph convolution for the 1-dimensional embedding $x \in \mathbb{R}^n$ (for n words) is

$$h = U g_w U^T x = U diag([w, \ldots, w]) U^T x = U U^T x \, diag([w, \ldots, w])$$

- Simplify using Chebyshev polynomial approximation
- $h = \left(I + D^{-\frac{1}{2}} A D^{-\frac{1}{2}}\right) x w$, after renormalization $h = \widetilde{D}^{-\frac{1}{2}} \tilde{A} \widetilde{D}^{-\frac{1}{2}} x w$
- Extend the embedding and convolved signal to d-dimensional $X \in \mathbb{R}^{n \times d}$ and $H \in \mathbb{R}^{n \times d}$

$$H = \rho\left(\widetilde{D}^{-\frac{1}{2}} \tilde{A} \widetilde{D}^{-\frac{1}{2}} X W\right)$$

Graph Convolutional Networks (GCN)

- A graph $G = (V, E)$:
  - $(v, v) \in E$ for any v
  - $X \in R^{n \times m}$: node features matrix
  - A: adjacency matrix, degree matrix $D_{ii} = \sum_j A_{jj}$
  - $\tilde{A} = \widetilde{D}^{-\frac{1}{2}} A \widetilde{D}^{-\frac{1}{2}}$: normalized symmetric adjacency matrix
  - W_j: weight matrix, trained via SGD

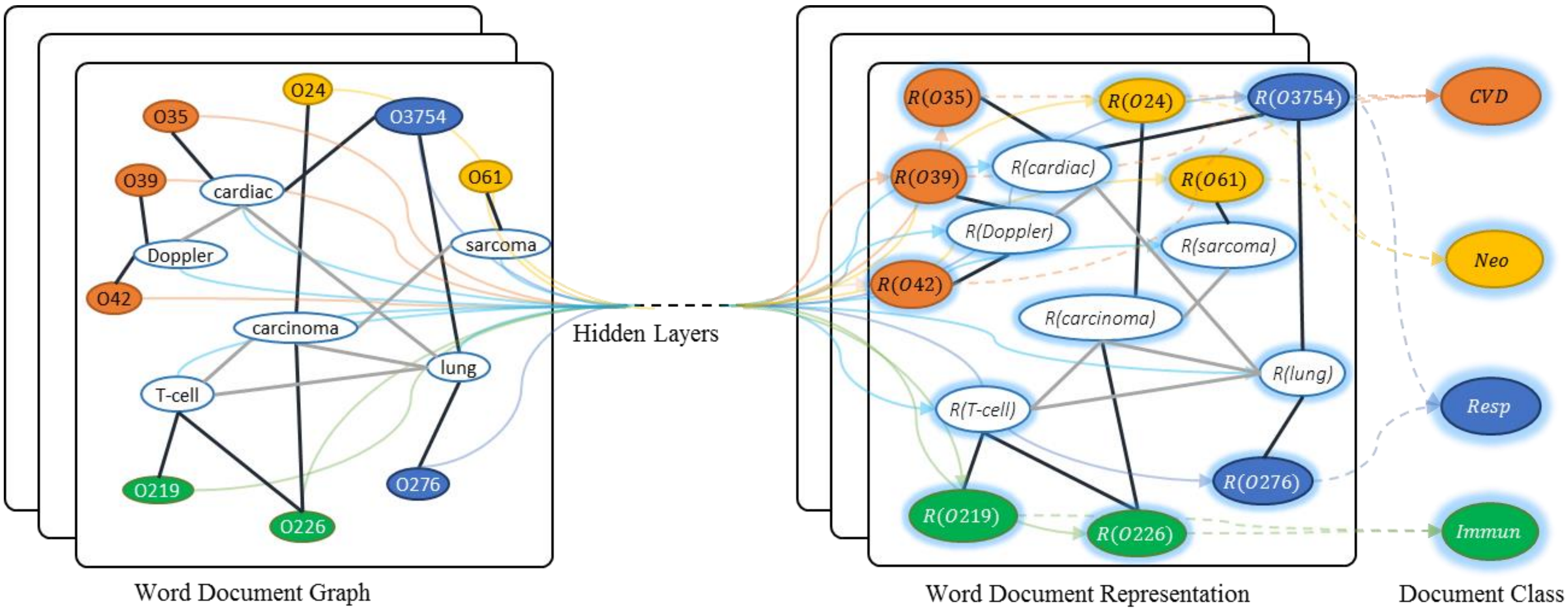
- One layer GCN:
- $L^{(1)} = \rho(\tilde{A} X W_0)$

- Stacking multiple GCN layers:
- $L^{(j+1)} = \rho(\tilde{A} L^{(j)} W_j)$

Graph Convolutional Networks (GCN)

- GCN can capture information only about immediate neighbors with one layer
- When multiple GCN layers are stacked, one can incorporate higher order neighborhoods information
  - e.g., a two-layers GCN can allow message passing among nodes that are at maximum two steps away.
- A special form of Laplacian smoothing:
  - computes the new features of a node as the weighted average of itself and its neighbors (second order neighbors for a two-layer GCN).

Text Graph Convolutional Networks (Text GCN)



L Yao, C Mao, **Y Luo***. Graph Convolutional Networks for Text Classification. *Proceedings of AAAI Conference on Artificial Intelligence 2019 Full paper.*

Text Graph Convolutional Networks (Text GCN)

- Document content and global word co-occurrence
  - Document-word edges: TF-IDF
  - Word-word edges: point-wise mutual information (PMI)

$$p(i,j) = \frac{\#W(i,j)}{\#W}$$

$$p(i) = \frac{\#W(i)}{\#W}$$

$$\mathrm{PMI}(i,j) = \log \frac{p(i,j)}{p(i)p(j)}$$

$$A_{ij} = \begin{cases} \mathrm{PMI}(i,j) & i,j \text{ are words, } \mathrm{PMI}(i,j) > 0 \\ \text{TF-IDF}_{ij} & i \text{ is document, } j \text{ is word} \\ 1 & i = j \\ 0 & \text{otherwise} \end{cases}$$

Text Graph Convolutional Networks (Text GCN)

- A simple two-layer GCN:
  - one-hot feature matrix for words and documents: $X = I$
  - 1st layer document and word embeddings: $\tilde{A}XW_0$
  - 2nd layer document and word embeddings: $\tilde{A}ReLU(\tilde{A}XW_0)W_1$
  - $\mathcal{Y}_D$ is the set of document indices that have labels and F is the dimension of the output features, which is equal to the number of classes, Y is the label indicator matrix
  - Loss function

$$Z = \mathrm{softmax}(\tilde{A}\ \mathrm{ReLU}(\tilde{A}XW_0)W_1)$$

$$\mathcal{L} = -\sum_{d \in \mathcal{Y}_D} \sum_{f=1}^{F} Y_{df} \ln Z_{df}$$

Dataset

- The Ohsumed corpus is from the MEDLINE database, which is a bibliographic database of important medical literature maintained by the National Library of Medicine
- In this tutorial, we created a subsample of the 2,762 unique diseases abstracts from 3 categories
  - C04: Neoplasms
  - C10: Nervous System Diseases
  - C14: Cardiovascular Diseases
- As we focus on single-label text classification, the documents belonging to multiple categories are excluded
- 1230 train (use 10% as validation), 1532 test

Now let's look at some code

- https://github.com/yuanluo/text_gcn_tutorial
- Run `python remove_words.py ohsumed_3`
- Run `python build_graph.py ohsumed_3`
- Run `python train.py ohsumed_3`
- Run `python tsne.py`

Results

- C04: Neoplasms
- C10: Nervous System Diseases
- C14: Cardiovascular Diseases