9. Classification, Clustering, and Learning to Rank

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- Know the basics of machine learning
- Understand supervised text classification
- Know some methods for (unsupervised) text clustering
- Understand how to combine different ranking functions (and other features) in a supervised IR setting – learning to rank
- Have an idea of what neural (re-)rankers (neural L2R) look like

- Recap of Lecture #8
- Primer on Machine Learning
- Text Classification
- Text Clustering
- Learning to Rank
- Neural (Re-)Ranking

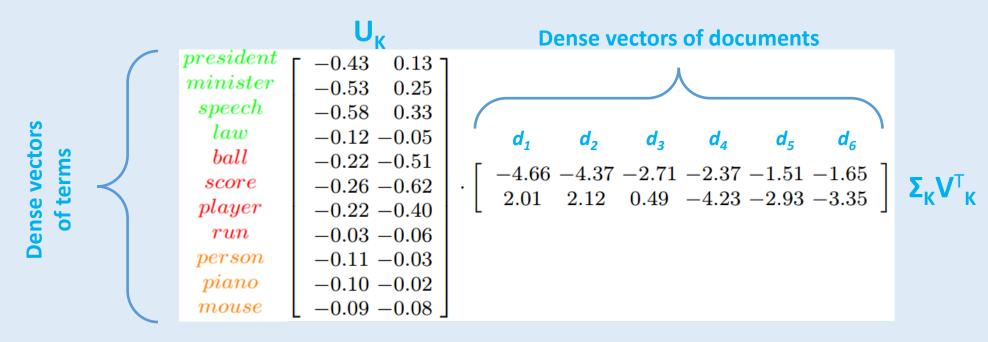
- Latent and Semantic Retrieval
 - Q: Why is term matching sometimes not good enough for retrieval?
 - Q: When should you use term-based IR models and when semantic/latent ones?
- Latent Semantic Indexing
 - Q: What Latent Semantic Indexing (LSI)?
 - Q: What is Singular Value Decomposition and how are latent topics represented?
 - Q: How do we obtain latent representations of documents and terms? How to transform the query into latent space?
- Latent Dirichlet Allocation
 - Q: What is LDA and how are latent topics represented in this probabilistic setting?
 - Q: What is the generative story that LDA assumes?
- Word embeddings for IR
 - Q: How are word embedding models different from latent topic models?
 - Q: How does CBOW model learn word embeddings?
 - Q: How to exploit word embeddings for an IR model?

■ Given a matrix A (with non-negative elements), the Singular Value Decomposition finds orthogonal matrices U and V and a rectangular diagonal matrix Σ such that:

$$A = U\Sigma V^T$$

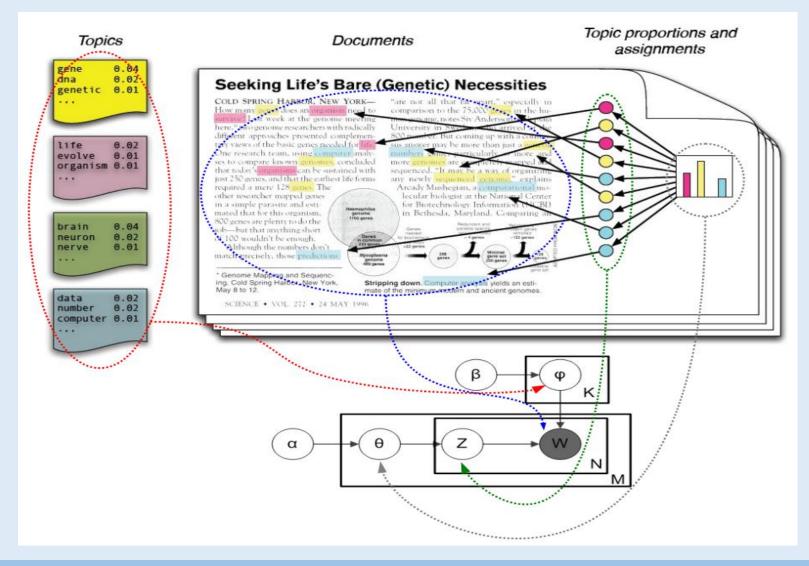
- Matrix U is of dimensions M x M
- Matrix V is of dimensions N x N
- Matrix Σ is of dimensions M x N
- U and V are orthogonal: U^TU = I, V^TV = I
- Values of the diagonal matrix ∑ are singular values of the original matrix A
- Let r be the rank of matrix A

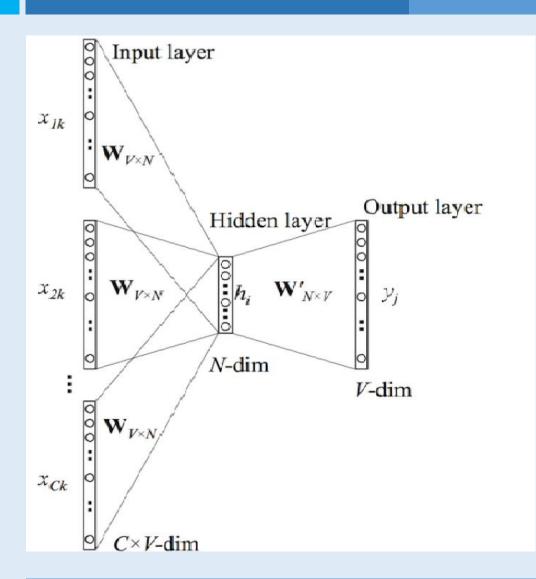
■ This leaves us with the best possible approximation of rank A_K (K = 2 in our example) of the original term-document occurrence matrix A



- \blacksquare A_K has the same dimensions as original A (M x N)
- U_K is of size M x K, and $\Sigma_K V_K^T$ of size K x N

- 1. For each topic k (k = 1, ..., K):
 - Draw parameters of a multinomial distribution φ_k (over terms) for topic k from a Dirichlet distribution $Dir_N(\beta)$
- 2. For each document d in the collection:
 - Draw parameters of a multinomial distribution of topics for the document d, θ_d , from a Dirichlet distribution $Dir_{\kappa}(\alpha)$
 - For each term position w_{dn} in the document d:
 - a) Draw a topic assignment (i.e., a concrete multinomial distribution over terms) z_{dn} from $Mult_{\kappa}(\theta_{d})$
 - b) Draw a concrete term w_{dn} from the multinomial distribution over terms of the topic zdn (drawn in a)), $Mult_N(\varphi z_{dn})$





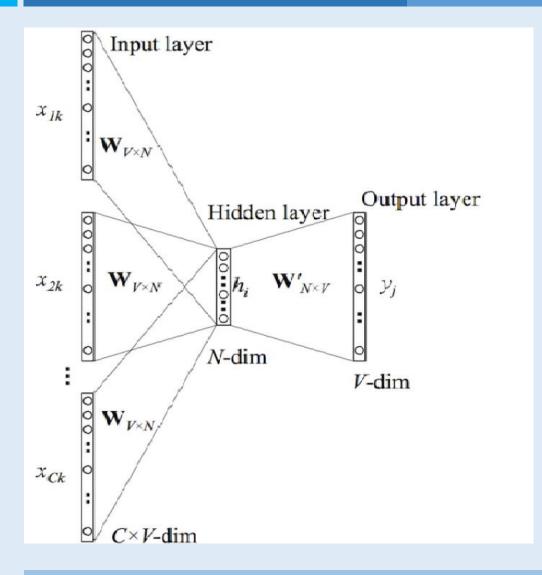
- Context consists of C words, with corresponding one-hot vectors
 - X_{1k}, X_{2k}, ..., X_{Ck}
- One-hot vectors transformed to dense vectors using input matrix W (V x N)
- Dense context vector h is obtained as:

$$h = \frac{1}{C} \mathbf{W} (\sum_{i=1}^{C} x_{ik})$$

 Dense context vector h is then multiplied with the output matrix W' (N x V)

$$y_k = softmax(h^T \mathbf{W'})$$

Continuous Bag-of-Words (CBOW)



- Output vector y needs to be as similar as possible to one-hot vector of center word
- Parameters of the model are elements of W and W'
 - Each row of W is the dense context vector of one vocabulary word
 - Each column of W' is the dense center vector of one vocabulary word
- Dense representation (embedding) of the
 i-th vocabulary term is concatenation of
 - 1. i-th row of W and
 - 2. i-th column of W'

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Why machine learning?

- For many IR and NLP tasks, it is difficult to come up with an explicit (i.e., rule-based) algorithm that solves the task efficiently
- For example
 - POS tagging difficult to devise the closed set of rules that infer the POS tag of the words from the word's context
 - Sentiment analysis complete set of rules that determine the sentiment of a reivew?
 - Named entity recognition a manually defined finite state automaton that recognizes the sequences of words that form named entities?
 - Semantic textual similarity measure the word overlap and manually determine the treshold according to which two texts are considered similar?

Why machine learning?

- The problems with devising rule-based systems for complex tasks are numerous:
 - 1. We simply need to many rules to cover all the cases
 - 2. There are many exceptions (including exceptions to exceptions!) to be handled
 - 3. We need expert knowledge (i.e., an expert to handcraft the rules)
 - 4. Rules can be difficult to
 - Design rules interact in unpredictable ways
 - Maintain adding new rules can easily break everything
 - Adopt to new domains we need to significantly modify/add rules
- IR and NLP tasks are often inherently subjective (e.g., relevance of a document for the query)
 - It is difficult to model subjectivity with rules

Why machine learning?

- It is often easier to manually label some concept than to design an explicit algorithm that captures the concept automatically
- Labeling typically does not require too much expert knowledge
- We don't care how complex or subjective the task is
 - We let the data "speak for itself" and machine learning algorithm to do the work
- If we're lucky, the labeled data might be already readily available (e.g., reviews with assigned ratings)

Machine learning basics

Supervised machine learning

- We have labeled data as input
- Supervised ML algorithms learn the mapping between input representations and output labels
- Classification: output is a discrete label (no ordering between the labels)
- Regression: output is a an integer or real value (obviously, there is ordering)

Unsupervised machine learning

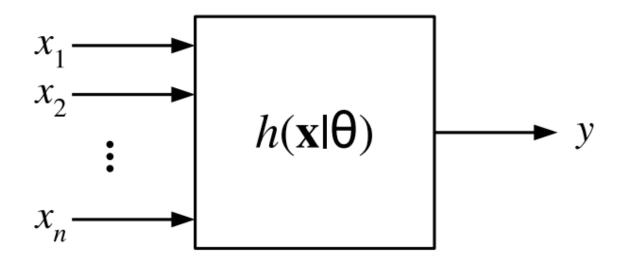
- We have no labels (i.e., we have unlabeled data) at input
- Clustering: grouping instances by the similarity of their representations
- Outlier detection: recognizing instances that are very dissimilar from all other instances in the dataset

Supervised machine learning

- Supervised machine learning models "learn" the mapping between input values and output values
- A single input to the classifier is called an **instance** or **example** (denoted "x")
 - An instance is represented as an n-dimensional feature vector

$$\mathbf{x} = (x_1, x_2, ..., x_n)$$

- The desired output is called the target label (or just label, denoted y)
- A classifier h maps an instance x to a label $y h : x \rightarrow y$
- "Learning" model has parameters θ (denoted $h(x \mid \theta)$) whose values are optimized to maximize the prediction accuracy of the output labels, given instance



- Types of classifiers in IR/NLP:
 - Binary classification: just two output labels (yes/no, 0/1)
 - Multi-class classification: each instance has one of K labels
 - Multi-label classification: an instance can have more than one label at once
 - Sequence labeling: input is a sequence of instances and the output is the sequence of labels

Supervised classification

- Training (or learning) adjustment of model parameters ⊕ so that the classification error is minimized
 - The error is computed on a labeled training set this is the training error
- The training error is minimized with an optimization method
 - ML algorithms differ in optimization criteria and optimization method they use
- We want to know how classifier works on new, unseen instances
 - This property is called **generalization** the classifier must generalize well
 - Testing error the error computed on instances not used for training
- ML models can be of different complexity
 - The more parameters the model has, the more complex it is
 - The model may be too simple of too complex for the task at hand
 - Underfitting (model too simple for the task): both training and test errors are big
 - Overfitting (model too complex for the task): training error small, test error big

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- **Text Classification** is the automated categorization of some unit text (sentence, paragraph, document) into one (or more) of predetermined labels
 - E.g., classify news stories into high-level topics: *politics*, *sport*, *culture*, *entertainment*
- Why text classification in IR?
 - Automatically assigned classes/labels provide an additional semantic layer
 - These additional semantic annotations can be exploited to rerank/filter results
 - E.g., Query: "lionel messi" (but retrieve only documents categorized as sport)
- Some popular ML algorithms for text classification:
 - Traditional: Naive Bayes classifier, Logistic regression, (linear) SVM
 - Recent: Convolutional neural networks (CNN)

Text representations

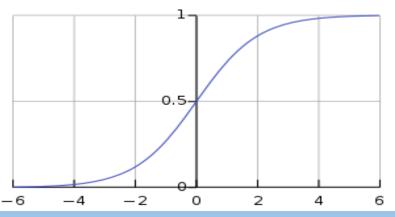
- For the majority of text classification algorithms, instances of text need to be transformed to numeric vector representations
 - Exceptions: Naive Bayes classifier and Decision Trees/Random Forests which can directly use word-based representations of text
- Numeric vector representations may be:
 - 1. Sparse each text is represented as (potentially weighted) vectors of word occurrences, the size of the vector is the size of vocabulary
 - 2. Dense each text is represented by a semantic dense vector (or by a concatenation of dense vectors of its consituent words)
- Traditional text classification models like logistic regression or SVM ignore the order of words in the text
 - I.e., they use bag-of-words representation of text
- Convolutional neural networks do take into account the order of words in the text
 - They compute abstract representations of subsequences of text

Logistic regression

- Despite its name, logistic regression is a classification algorithm
 - We will focus on binary classification logistic regression computes the probability that some instance x belongs to some class (y = 1)

$$h(\mathbf{x} \mid \boldsymbol{\theta}) = P(y = 1 \mid \mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})} = \sigma(\boldsymbol{\theta}^T \mathbf{x})$$

- Logistic regression is based on a logistic function: $\sigma(a) = 1/(1 + e^{-a})$
- The logistic function maps the input value to the output interval [0, 1]



Logistic regression

- Looking at the logistic regression formula (and the properties of log. function):
 - $h(x|\theta) > 0.5$ (i.e., instance belongs to the class) if and only if $\theta^T x > 0$
 - $h(x|\theta) < 0.5$ (i.e., instance doesn't belong to the class) if and only if $\theta^T x < 0$
- \blacksquare In order to make predictions, we need to know the parameter vector Θ
 - We learn the values of parameters by minimizing some error function for the set of training instances
 - Logistic regression minimizes the so-called cross-entropy error

$$J(\mathbf{\theta}) = -\sum_{i} y^{i} * \log(h(\mathbf{x}^{i}|\mathbf{\theta})) + (1 - y^{i}) * \log(1 - h(\mathbf{x}^{i}|\mathbf{\theta}))$$

- $J(\theta)$ is minimized (i.e., parameters θ are optimized) via numeric optimization
 - Most commonly using stochastic gradient descent (SGD)

- Convolutional neural network is a neural machine learning model that has been successfully used for text and image classification tasks
 - Unlike bag-of-words classifiers, treats text as an ordered sequence of words
 - Requires a dense representation of text as input we typically represent text as (2D) concatenation of word embeddings
- CNNs parameters are convolution filters real-valued matrices that are being used to compute the convolution with the partso of the input sequence
- The convolutional layer is followed by the max-pooling layer where only the top K largest convolution scores are taken
- The final prediction is made by the softmax regression (generalization of the logistic regression for more than two labels)

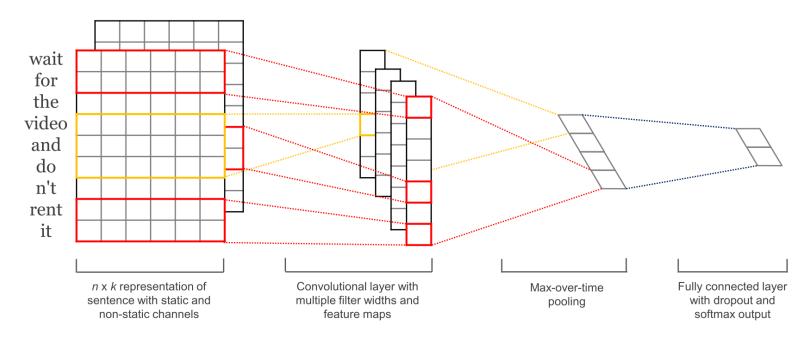


Image taken from: http://www.wildml.com/2015/11/understanding-convolutional-neural-networks-for-nlp/

 CNNs parameters (real-values of all convolution filter matrices) are learned by propagating the classification error via backpropagation algorithm

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- Cluster analysis (or, colloquially, clustering) is a multivariate statistical technique that allows automated generation of groupings in data
- Components of clustering:
 - 1. An **abstract representation** of an object using which the object is compared to other objects
 - 2. A **function** that measures the **distance or similarity** between the objects based on their abstract representations
 - 3. A **clustering algorithm** that groups the objects based on the similarities / distances computed from their representations
 - 4. (optional) Constraints with respect to cluster membership, cluster proximity, shape of the clusters, etc.

- Representations of text for clustering are typically similar as for text classification (only we lack the labels)
 - Sparse vectors (binary or weighted, e.g., using TF-IDF)
 - Dense vectors (latent or semantic representations)
 - Sometimes also more structured representations like trees or graphs
- Common distance/similarity functions
 - Euclidean distance, cosine similarity/distance, Jaccard coefficient, Kullback-Leibler divergence, tree/graph kernels for structured representations (trees/graphs)
- Clustering algorithms:
 - 1. Sequential e.g., single pass clustering
 - 2. Hierarchical e.g., agglomerative clustering, divisive clustering
 - 3. Cost-function optimization clustering e.g., K-means, mixture of Gaussians

- Why clustering in information retrieval?
 - We have already seen clustering at work in speeding up VSM retrieval (leaders)
- Cluster information retrieval model
 - Cluster hypothesis (van Rijsbergen, 1979): Documents similar in content tend to be relevant for the same queries
 - Steps:
 - 1. Collection documents are pre-clustered
 - 2. The query is matched against cluster centroids
 - 3. All documents from clusters represented by top-ranked centroids are returned (ranked)
 - Improves efficiency as the query needs not be compared with all documents
 - No comparison with documents from clusters with low-ranked centroids

Single pass clustering

- Simplest clustering algorithm
 - The number of clusters does not need to be predefined
- Algorithm:
 - 1. Start by putting the first text t_1 into the first cluster $c_1 = \{t_1\}$
 - 2. For all other texts, t_2 , ..., t_n , one by one
 - I. Measure the distance/similarity with all existing clusters c_1 , ..., c_k
 - The similarity with the cluster is avg/max of similarities with instances in cluster
 - II. Identify the cluster c_i with which the current text t_j has the largest similarity (or smallest distance)
 - III. If the similarity between t_j and c_i is above some predefined threshold λ , add the text t_j to cluster c_i
- Although single-pass clustering doesn't explicitly require it, the number of clusters is indirectly determined by the value of the threshold λ

- Arguably the most famous and widely used clustering algorithm
- Requires the number of clusters k to be predefined K clusters, $S = \{S_1, S_2, ..., S_k\}$, represented by mean vectors $\mu_1, \mu_2, ..., \mu_k$
- K-means clusters instances $(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n)$ by finding the partition S that minimizes the within-cluster distances (maximizing the within-cluster similarities):

$$rg\min_{\mathbf{S}} \sum_{i=1}^k \sum_{\mathbf{x} \in S_i} \|\mathbf{x} - oldsymbol{\mu}_i\|^2$$

- Q: How to find the optimal clusters (i.e., minimize the above sum of within-cluster distances)?
- A: Using iterative optimization

- Algorithm for learning the centroids:
 - 1. Randomly pick k mean vectors μ_1 , μ_2 , ..., μ_k in the same space (i.e., of same dimensionality) as instance vectors
 - K-means++ is an extension that more intelligently chooses the initial mean vectors
 - 2. Iterate the following two steps until convergence:
 - I. Assign each instance x_i to the cluster with the closest mean vector μ_i :

$$S_i^{(t)} = \left\{ \mathbf{x}_j : \|\mathbf{x}_j - \boldsymbol{\mu}_i^{(t)}\|^2 \le \|\mathbf{x}_j - \boldsymbol{\mu}_j^{(t)}\|^2, \forall j, 1 \le j \le k \right\}$$

- II. For each cluster, update the mean vector of a cluster
 - Set the mean vector to the mean of the instances in the cluster

$$\mu_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{\mathbf{x}_j \in S_i^{(t)}} \mathbf{x}_j$$

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Learning to Rank

- So far, each IR model was ranking the documents according to a single similarity function between the document and the query
 - VSM: cosine between the (sparse) TF-IDF vectors of the document and query
 - Latent/semantic IR: cosine between dense semantic vectors
 - Probabilistic IR: P(d, q | relevance)
 - Language modelling for IR: P(q | d)
- Idea: Combine different similarity scores as features of a supervised model

$$\vec{f}(d,q) = \begin{pmatrix} VSM_q(d) \\ P(q|d) \\ Jaccard(qterms, dterms) \end{pmatrix}$$

- Learning to rank is a supervised information retrieval paradigm that
 - Describes instances of document-query pairs (d, q) with a range of features
 - Learns (with some ML algorithm) the mapping between these features and relevance
- Three different learning-to-rank approaches:
 - 1. Point-wise approach
 - Classify a single document-query (d, q) pair for relevance
 - 2. Pair-wise approach
 - Classify, for a pair of documents, which one is more relevant for the query, i.e., whether $r(d_1, q) > r(d_2, q)$ or $r(d_1, q) < r(d_2, q)$
 - 3. List-wise approach
 - Classify the whole ranking as either correct or wrong

Learning to Rank

- Point-wise learning to rank
 - Train a supervised classifier that for a given query q classifies each document as relevant or non-relevant
 - Binary classification task: document is either relevant or non-relevant
 - Training instances:
 - Query-document pairs (q, d) with relevance annotations
- Issues with point-wise learning to rank
 - Do not care about absolute relevance, but relative order of documents by relevance
 - If pairs (q, d₁) and (q, d₂) are classified as relevant, which document to rank higher?
 - Supervised classifiers usually have confidence/probability scores assigned to predictions
 - Rank d₁ higher than d₂ if the classifier is more confident about relevance of pair (q, d₁)

37

Learning to Rank

- Pair-wise learning to rank
 - Train a supervised classifier that for a given query q and two documents d₁ and d₂ predicts which document is more relevant for the query
 - Binary classification task:
 - Class 1: "d1 more relevant than d2"
 - Class 2: "d1 less relevant than d2"
 - Training instances:
 - Triples (q, d_1, d_2) consisting of queries and document pairs
 - We may need comparison features compare d₁ and d₂ with respect to q
 - E.g., binary feature: VSM(q, d₁) > VSM(q, d₂)
 - Generating gold labels from relevance annotations:
 - For query q we have: $d_1(r)$, $d_2(nr)$, $d_3(r)$, $d_4(nr)$
 - We create the following training instances:
 - {(q, d₁, d₂), 1}, {(q, d₁, d₄), 1}, {(q, d₂, d₃), 2}, {(q, d₃, d₄), 1}

Learning to Rank

- Issues with pair-wise learning to rank
 - If we don't use comparison features (but direct similarities of d1 and d2 with q as features), the model may not generalize well for new queries!
 - We only obtain independent pair-wise decisions
 - Q: What if pair-wise decisions are mutually inconsistent?
 - E.g., (q, d1, d2) -> 1, (q, d2, d3) -> 1, (q, d1, d3) -> 2
 - We need an additional postprocessing step
 - To turn the sorted pairs into a ranking, i.e., partial ordering into global ordering
 - Inconsistencies need to be resolved
 - E.g., In a set of conflicting decisions, the one with the lowest classifier confidence is discarded
 - Another issue: we effectively treat pairs from the bottom of ranking same as those from the top of the ranking (and eval. metrics don't treat them equally!)

Learning to Rank

- List-wise ranking approach
 - Instead of learning decisions for individual documents or pairs of documents, learn to classify entire rankings as correct or wrong
 - Training instances: query and an entire ranking of documents (q, d₁, ..., d_n)
 - Binary classification task:
 - Class 1: the ranking (q, d₁, ..., d_n) is correct
 - Class 2: the ranking (q, d₁, ..., d_n) is incorrect
 - Advantage: optimization criteria for the machine learning algorithm can be the concrete IR evaluation metric we're looking to optimize
- Issues with list-wise approach
 - Entire ranking just one training instance
 - Difficult to collect many positive training instances
 - Informative features for the whole ranking are difficult to design

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Ranking Based on Neural Language Models

- We have access to enormous amounts of raw unannotated texts (at least for major languages)
- Can we somehow pre-train the encoder using raw text?
 - Yes, via language modeling! Task is to predict the word from the text based on the encoding of the surrounding context
- LM-pretraining
 - Causal (unidirectional) language modeling: **GPT (1, 2, 3, 4, ...)**
 - Masked (bidirectional) language modeling: BERT
- In retrieval
 - Use the Neural LM to encode queries and documents



Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019, January). **BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding**. *NAACL 2019*.

- **Pretraining:** Masked language modeling, MLM (and next sentence prediction, NSP)
- Encoder architecture: deep Transformer (attention-based) network
- Encoder's parameters (learned in pre-training) further updated in task-specific training (aka fine-tuning)
- After task-specific training (aka **fine-tuning**), we have a **task-specific encoder**

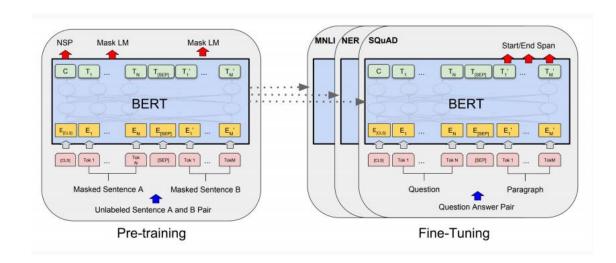


Image from [Devlin et al., NAACL 19]

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *NAACL 2019*.

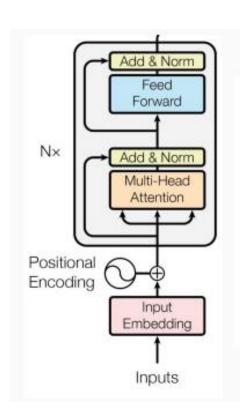
- Training instances: sentence pairs, with special tokens inserted
 - Ca. 15% of tokens masked out (replaced with [MASK] token)
 - Sequence start token [CLS] and sentence separation token [SEP]
- Pretraining: two self-supervised objectives
 - Masked language modeling, MLM (predict the masked token from the context)
 - Next sentence prediction, NSP (if sentences adjacent or not)

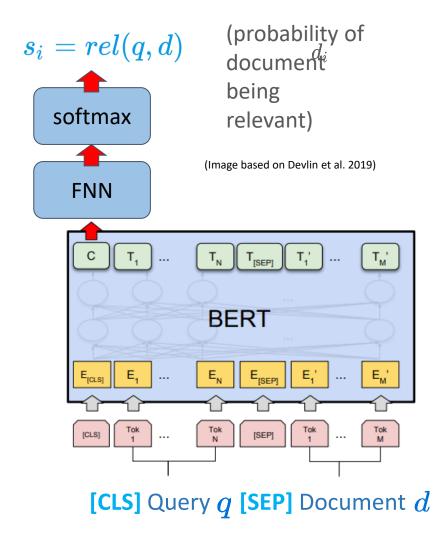
##ing likes play dog cute [SEP] he [CLS] Image from [Devlin et al., NAACL 19] Token E, ing E_[CLS] E_{play} E_[SEP] Embeddings Segment Embeddings Position Embeddings

Bidirectional Transformers for LU (BERT)

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2019, January). **BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding**. *NAACL 2019*.

- Encoder architecture: deep Transformer (attention-based) network
 - Deep architecture consisting of N transformer layers
 - Each transformer layer:
 - Multi-head attention layer
 - Feed-forward layers
 - Residual connection (representation before the layer added to the result of the layer)
 - Layer normalization
 - All parameters of the Transformer: θ_{TRANS}





BERT as a point-wise ranker (monoBERT): binary relevance classifier

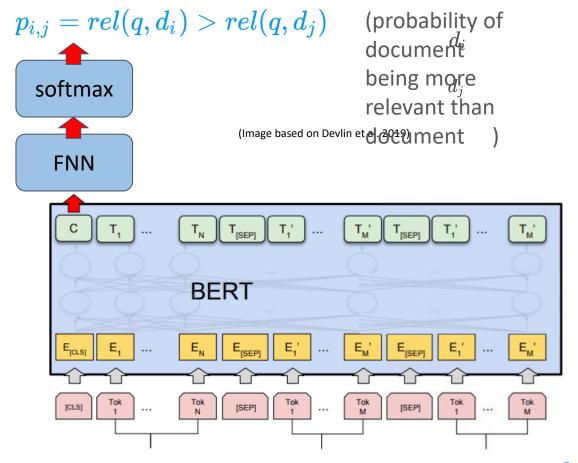
- → Feeds concatenation of guery and document to BERT
 - → Truncate query to at most 64 tokens
 - → Concatenate query with document ([SEP]-token)
 - → Truncate whole sequence to 512 tokens (max. seq. length)
- **♦**Obtain representation representation of [CLS]-token in last layer
- ◆ Feed [CLS] vector to single layered Feedforward Neural Network (FNN, binary classification model) to obtain relevance score

Optimize the following loss:

$$\mathcal{L}_{mono} = -\sum_{j \in J_{pos}} \log(s_j) - \sum_{j \in J_{neg}} \log(1-s_j)$$

J_pos/neg = set of indexes of relevant/non-relevant documents

Retrieval: Rank documents by their probability of being relevant s_j



[CLS] Query q [SEP] Document d_i [SEP] Document d_j

BERT as a pair-wise ranker (duoBERT):

- lacktriangle Truncate the query, candididate document d_i and d_j to 62, 223 and 223 tokens respectively
- **→** Concatenate query and document pair into single sequence
- igspace For a candidate list of k_1 documents, compute $k_1(k_1-1)$ probabilities

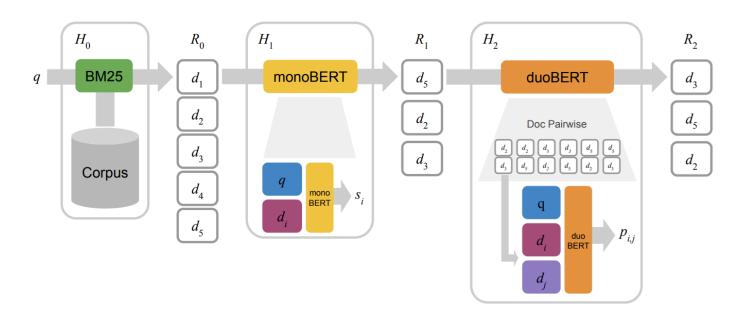
Optimize the following loss:

$$\mathcal{L}_{duo} = -\sum_{i \in J_{pos}, j \in J_{neq}} \log(p_{i,j}) - \sum_{i \in J_{neq}, j \in J_{pos}} \log(1-p_{i,j})$$

Retrieval:

Aggregate pairwise scores $p_{i,j}$ into single score s_i Set of all (other) document indexes in ranking R1: $J_i = \{0 \le j \le |R_1|, j \ne i\}$

Relevance score as **pair-wise agreement** that is more relevant than the rest of the candidates (other aggregation methods possible too, cf. paper): $s_i = \sum_{i=1}^{n} p_{i,i}$



Combining monoBERT and duoBERT into a multi-stage ranking architecture

Stage 1: Retrieve top- $k_0=1000$ documents using BM25 ($k_0=5$ in example above) \Rightarrow input to monoBERT

Stage 2: Re-rank top- $k_1=50$ documents with monoBERT ($k_1=3$ in example above) \rightarrow input to duoBERT

Stage 3: Re-rank subset with duoBERT

Summary

It's common practice to use neural rankers for re-ranking, ranking the full collection would be too slow for practical purpose

Arranging retrieval in a multi-stage pipeline allows for trading off quality against latency by controlling admission of candidates at each stage

Target Corpus Pre-training (Masked Language Modelling on document collection) before training monoBERT/duoBERT improves results

Challenges for pair-wise ranking revisited:

- 1. We only obtain independent pair-wise decisions (inconsistent ranking): Aggregate (all) possible pair-wise agreements into relevance scores
- 2. We effectively treat pairs from the bottom of ranking same as those from the top of the ranking (and eval. metrics don't treat them equally!): Neural model only re-ranks top k documents (ignore bottom of ranking)

- Know the basics of machine learning
- Understand supervised text classification
- Know some methods for (unsupervised) text clustering
- Understand how to combine different ranking functions (and other features) in a supervised IR setting – learning to rank
- Have an idea of what neural (re-)rankers (neural L2R) look like