Advanced Methods in Text Analytics Word Representations







What are representations? (1)



- Let's represent a hypothetical country called Countryland!
- What **features** should we use?
 - Area size? E.g. 400.000 km²
 - Population size? E.g. 20M
 - Continent? E.g. Europe
- Let's group those features as a single 3D feature vector
 - Countryland: (400.000; 20M; 'Central Europe')
- Features can have different types
 - Real or integer numbers, e.g. population size
 - Categorical, e.g. the continents
- We refer to that vector as a representation of 'Countryland'
- Is that useful for, say, inferring size of the economy?

What are representations? (2)



- How about the following features then?
 - GDP? E.g. 50 billion USD
 - Interest rate? E.g. 2.2%
 - Inflation rate? E.g. 7.2%
- This gives us a different representation of Countryland:
 - (50B; 2.2; 7.2)
- Manually constructing representations: feature engineering
 - Often requires expertise in the area
 - E.g. 'government debt to GDP' is a common metric in Economics
- Feature vectors: most typical form of input to machine learning (ML) methods

Can we *learn* useful representations?



- Can we learn useful features?
 - Then no more feature engineering
 - We may not even need an Economics degree to get useful features
- Yes! Deep Learning (DL) methods are useful for this.
 - But ML/DL is mostly engineering, so back to square one?
 - No! These methods are applicable to any domain, e.g. economics, applied mathematics, etc.
- The learned representations may be generally useful, e.g. word representations
 - Potentially useful for any application with text as input

Word Embeddings



- Learned vector representations of words/tokens
- Can be learned in several different ways
- Classic example: word2vec
 - Useful geometrical properties between related word vectors

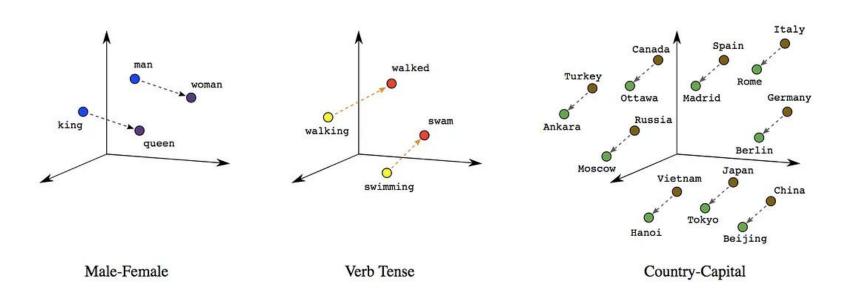


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Challenges



- Not straightforward as previous examples suggest!
 - Vector spaces with hundreds or thousands of dimensions
 - Variety in methods for learning word representations
- Thus, many challenges!
 - Here's some examples of those challenges
- Interpretability:
 - Learned features often not interpretable (real numbers)
 - Geometric properties of space not straightforward (high-dimensional space)

Cost:

- Train on terabytes of text
- Latest LLMs have trillions of parameters
- GPU memory limited
- This fixed (static) word -> vector mapping seldom used anymore
 - But still part of architectures, relevant to understand representations

Outline



1. Machine Learning Refresher

2. Deep Learning Basics

3. Word Embeddings



Machine Learning Refresher

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About this Section



 Goal: discuss basic concepts and terms that will be useful for the entire course

• Outline:

- 1. Basic Machine Learning Concepts
- 2. Probability Theory Refresher
- 3. Maximum Likelihood Estimation
- 4. Summary

What is machine learning? (1)



- Methods for developing algorithms by learning from data
 - In contrast to manually coding knowledge we already have
 - Example: flying a helicopter (how many situations must we consider?)
- Umbrella term encompassing many families of methods
 - E.g. Inductive Logic Programming, Deep Learning, etc.
- Related (umbrella) terms
 - Artificial Intelligence: solutions that show intelligent behavior
 - Data Mining: extract value from data (ML usually part of that pipeline)
- Machine learning in this course?
 - Mostly deep learning and related methods

What is machine learning? (2)



- Classic definition:
 - "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance, as measured by P, improves with experience E."

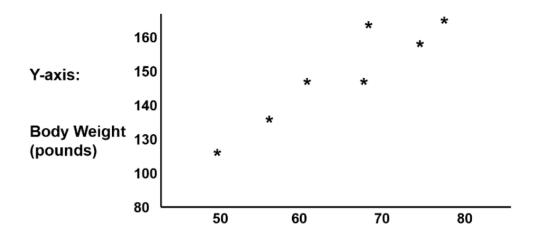
Tom Mitchell, Machine Learning, 1997

- **Experience:** data in some format
 - In our case, text (that needs to be processed so models can "read" it)
- Tasks: depends on perspective
 - ML: classification, regression, etc.
 - NLP: machine translation, question answering, etc.
- **Performance measure:** depends on task
 - E.g. F1 score for classification tasks, ROUGE scores for summarization

What is a task?



- Task: predict weight of a person (regression, supervised)
- Data: How do we represent a person?
 - Let's go with a simple 2D vector: (height, weight)
- We might see a linear relation between input and target
 - **Input:** 1D feature vector (usually denoted by **x**_i, here: height)
 - **Target:** weight (usually denoted by **y**, here: real number)



X-axis: Height (inches)

Example source

What is a model?

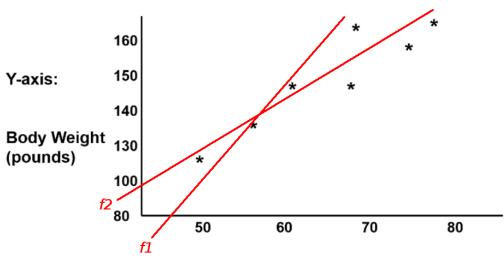


- Family of methods that we choose
 - Each comes with a set of assumptions
- E.g. based on observed data, we assume linear relation between height and weight
 - Thus, we choose a linear regression model
- Linear regression:
 - Main assumption: linear relation between inputs and output
 - Formally: learn function f(x) = y
 - Here: *f*(*height*) = *weight*
 - This model comes from statistics, studied more formally, e.g. more assumptions, ML is more "relaxed", focuses on learning (generalizing)
- How exactly do we learn a function?
 - To get there, we need to talk about parameters

What are parameters?



- We can describe the assumption in linear regression with the equation of a line:
 - y = mx + b where m is slope and b is y-intercept
 - In our case: weight = m height + b
 - Thus, we have **two parameters**: **m**, **b**
- Each value assignment of *m*, *b*: different member of linear regression family
 - Which one **fits** the data better?
 - $f_1 \text{ or } f_2$?
 - How do you know? Depends on the goal

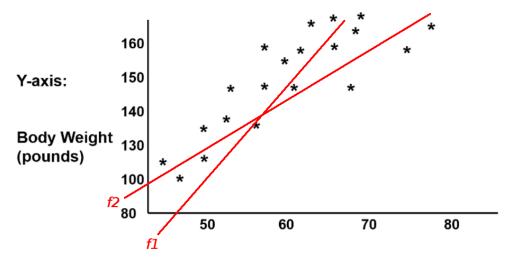


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What is generalization?



- Goal of ML: model should perform well at the task on new data
 - Not just data it was trained on
 - Thus, goal of training a model: generalize to unseen data
- For example, which function did you say fits our data best?
 - $f_1 \text{ or } f_2$?
- What if we collect more data?
 - Before, f_2 seemed best
 - With more data, f_1 is best
- How do we train for generalization?
 - We evaluate models on held-out evaluation data, represents unseen data
 - Train and eval data assumed from same distribution



How do we evaluate a model?

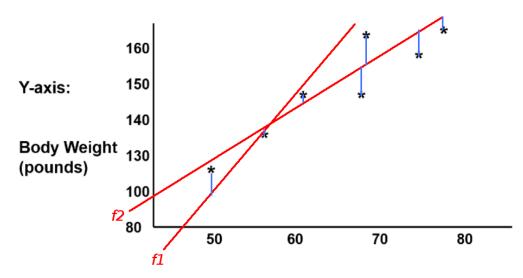


- How can we tell which member of the family is more suitable for our task?
 - We need to **select a model** from the many options
- Performance metric
 - A metric we choose to evaluate how good a model is at a task
 - For example: mean squared error (MSE)

$$ext{MSE} = rac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{Y_i}
ight)^2$$

where:

- n: # of examples
- *Y_i*: target values
- Y'_i: predicted values

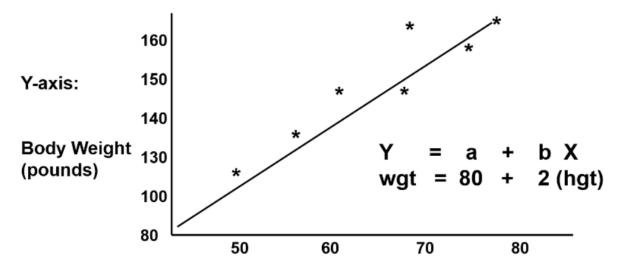


X-axis: Height (inches)

How do we use our selected model?



- Model selection: choosing a value assignment for our parameters
 - E.g. m = 80, b = 2
- To make a prediction, we make use of our selected model (function)



X-axis: Height (inches)

- Important distinction: inference vs prediction
 - Inference: use model to learn about data generation process
 - Prediction: predict specific outcomes for new input points

What are *hyper*parameters?



- Other parameters that are typically not learned
 - Instead, they are manually set by the user
 - Note that meta-learning does exist, e.g. <u>AutoML</u>
- Example in linear regression: using a bias or not
 - No bias: line passes by origin (assumes data is centered)
 - See scikit-learn's <u>documentation</u> on linear regression (fit_intercept)
- How do we choose values for hyperparameters?
 - Hyperparameter optimization methods
 - E.g. grid search, random search (<u>known</u> to be better than grid search)
 - Requires familiarity with known tricks/experience/expert knowledge
- Often involves making assumptions
 - E.g. this setting worked well in the past
 - E.g. the search space I designed benefits all models equally

What about classification?



- Logistic regression: popular model for classification
 - Main assumption: linear relation between inputs and output
- Essentially: linear regression with a logistic function
 - $y = \sigma(m x + b)$ where σ is the logistic (sigmoid) function

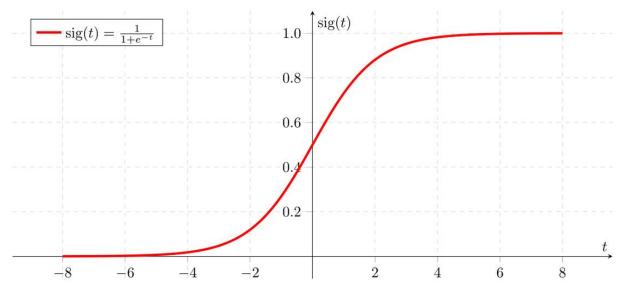


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- Logistic function maps inputs to real interval [0,1]
 - Can be interpreted as a probability distribution

How do we use logistic regression?



- **Binary** classification:
 - $P(y = 1) = \sigma(m x + b)$ --> interpreted as probability for positive class
 - $P(y = 0) = 1 \sigma(m x + b)$ --> complementary probability for negative class
- That is, we get probabilities for both positive and negative class
 - We can do some *inference*, e.g. how much more likely is one class than the other?
 - But prediction?
- Prediction: we decide on a threshold
 - $p(y = 1) \ge 0.5$, we predict positive class
 - p(y = 0) < 0.5, we predict negative class
- We get the following decision boundary
 - p(y = 1|x) = p(y = 0|x) = 0.5
- Describing tasks and models with probability theory is very common!
 - We'll do this often, so let's review the basic concepts

Probability Theory Basics

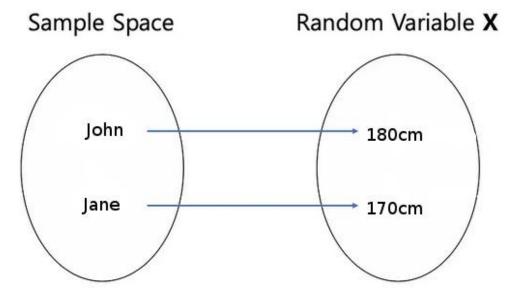


- This is a quick refresher about probability theory
- This is later useful for many things
 - Describing tasks
 - Describing models, e.g. what language models do
 - More concepts commonly used in NLP research
- Today, some basic intuitions/definitions
 - Random variables
 - Probability distributions
 - Independence of events
 - Sum rule / product rule
 - Joint distributions
 - Conditional probability
 - Conditional independence
 - Bayes rule

Random Variables



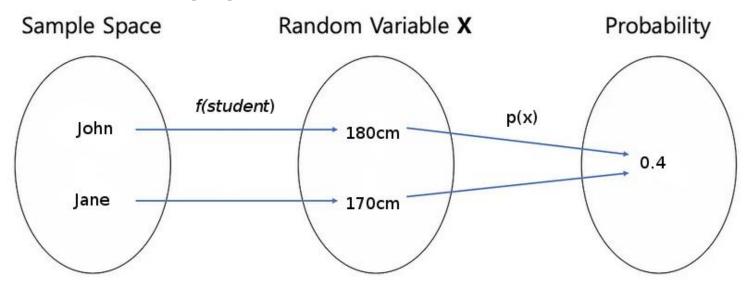
- Function between events and something relevant about the events
 - Usually designed according to something we want to model
- Example: say we are interested in average height of students
 - Event: randomly select a student
 - Event space: set of all students the course
- Random variable X: f(student) = height of student



Probability Distributions (1)



- Essentially a way to describe random variables
- Random variables: take values as a result of some random process
- Distribution of random variable: how often may each value be observed
- How does a distribution describe this?
 - A(nother) function p(X): maps set of possible values a random variable can take to interval [0,1]



Probability Distributions (2)



- Output of p for given event a: probability of observing event a
 - Written as p(X=a)
 - Example: what is the probability of observing a height of 185cm?
 - p(X = 185cm) = 0.1, i.e. probability is 10%
- **Discrete distributions:** random variable can take finite set of values
 - p usually referred to as probability mass function
- Continuous distributions: r.v. can take infinite set of values
 - p usually referred to as probability density function
- Examples:
 - Bernoulli (discrete): models output of single binary experiment
 - Gaussian (continuous): normal distribution
- Is X in our students' height example discrete or continuous?
 - Depends on how to measure height, as reals or integers

Independence of events



- Events A and B are independent when one event happening does not affect the probability of the other happening
- For example:
 - Event A: Germany wins the world cup in 2014
 - Event B: Germany loses world cup semifinal
 - Event C: The stock market crashed in 2008
 - Which of these events are dependent/independent?
- A and B are not independent
 - If Germany loses the semifinal, it cannot win the final
- A and C are independent, as well as B and C
 - Very unlikely the 2008 crash has any impact on the 2014 world cup
- Independence perhaps best understood with sum rule

Sum Rule



- Probability of union of n events happening, e.g. A OR B
 - Formally: $p(A \cup B) = p(A) + p(B) p(A \cap B)$
- For example: r.v. Y shows number in die, relevant events are:
 - A: "We observe a multiple of 3", i.e. either 3 or 6
 - **B:** "We observe a multiple of 2", i.e. either 2, 4 or 6
- Are A and B independent? No, see overlap in event spaces
- For $p(A \cup B)$ we subtract probability of overlapping events: p(Y=6)
 - p(A) = 1/6 + 1/6 = 1/3
 - $p(B) = 1/6 + 1/6 + 1/6 = \frac{1}{2}$
 - p(y = 6) = 1/6
 - $p(A \cup B) = 1/3 + \frac{1}{2} 1/6 = 0.66$
- With independent events, last term becomes zero:
 - Event A: "We observe an even number", i.e. either 2, 4 or 6
 - Event B: "We observe an uneven number", i.e. either 1, 3 or 5

Product Rule



- Probability of conjunction of n events happening, i.e. A AND B
- Formally: p(A,B) = p(A|B)p(B)
 - p(A,B) = joint distribution of A and B
 - p(A|B) = conditional distribution of A given B
- Side note:
 - All of these rules are derived from axioms of probability theory
 - For more, see probability theory literature
- Let's go over joint distributions and conditional distributions

Joint Distributions (1)



- Function $p(X_{1...n})$ from n random variables to interval [0,1]
 - Distribution of all possible combinations of those *n* random variables
- Easier to see with joint probability table
- For example, joint distribution of flipping two coins A and B:

A/B	Heads	Tails
Heads	0.1	0.2
Tails	0.3	0.4

Note that all elements in table add up to 1, i.e. a distribution

Joint Distributions (2)



- We can derive many things from a joint distribution
- A very common operation: marginalization
 - Given joint distribution of A and B, derive distribution of A or B
- For example, we get distribution of coin A by summing over all possible values of B with the sum rule:

A/B	Heads	Tails	p(A)
Heads	0.1	0.2	= 0.3
Tails	0.3	0.4	= 0.7

- New column adds up to 1, i.e. a probability distribution
 - p(A) known as marginal distribution of A
- This process is referred to as marginalizing out B
 - Normally expressed with sum rule: $p(A) = \sum_b p(A, B = b)$

Conditional Probability



- Probability of seeing event A knowing event B was already seen
- Formally, p(A|B) = p(A,B)/p(B)
- Intuitively, space of all possible events shrinks (for dependent RVs)
 - Imagine we toss a die
 - A: "We observe an even number", i.e. either 2, 4 or 6
 - B: "We observe a multiple of 3", i.e. either 3 or 6
 - After observing A, event space for B is not {3, 6}, it is {6}
- Note that p(A|B) can be derived from joint distribution p(A,B)
 - Marginalize out A to get p(B)
 - Then you have everything you need

Conditional Independence



- Two events are independent given a third event
 - Observing A tells me something about B
 - But when observing C, A no longer says anything about B
- For example:
 - Event A: knowing a person has good vocabulary
 - Event B: knowing a person's height
- Are A and B independent?
 - No, since children have limited vocabulary
- Now consider event C: knowing a person's age
 - Given C, A and B are independent, since height implies age
 - Once we have age, height gives us no new information
 - Thus, A and B are conditionally independent given C

Bayes' Rule



- Apply product rule on conditional probability
- That is, p(A|B) = p(A,B) / p(B) = p(B|A) p(A) / p(B)
 - Note that we want probability of A given B, i.e. p(A|B)
 - And to get it, we use marginal distribution of A, i.e. p(A)
 - This may seem counterintuitive
- This is typically interpreted like so:
 - p(A) known as **prior probability** distribution of event A
 - Describes what we know/believe about event A
 - p(B/A) known as likelihood
 - Given event A, what is the likelihood that we get our data
 - p(A|B) known as **posterior probability** of A
 - Interpreted as updated description of A after considering what we originally know about A (prior), as well as our data (event B)
- This interpretation gives rise to the *frequentists vs bayesian* debate
- And with this, we are done with our probability refresher!

A Probabilistic Perspective of ML



- Task: predict outcome of a coin tossed by your (unreliable) friend
 - Many factors: mass distribution, position in fingers, friction, etc.
 - Difficult to *model* physically
- Let's use a probabilistic model
 - Abstracts away complications of physical model
- **Probability:** uncertainty of some *random* event, e.g. coin toss
 - In practice: *relative frequency of observations* about the event
 - **Event in this case:** seeing heads when tossing the coin
- Simple Model: Bernoulli distribution
 - Intuition: it models outcome of single binary experiment
 - Formally: $p(k|\Theta) = \Theta^k (1-\Theta)^{1-k}$ where k in $\{0,1\}$ is possible outcomes
 - O is the only parameter of model: probability of seeing heads
- How do we get a value for this parameter so we can use our model?
 - We could estimate this parameter
 - We could blindly guess, or we could use data for that estimation!

Training Models: Parameter Estimation



- Say your friend allows you to observe ten tosses
 - You observe 3 out the 10 are heads
- You can estimate the value of Θ from this data
 - $\Theta = 3/10 = 0.3$ chance of seeing heads in a single toss
- We just counted relative frequencies
 - Training example: a single coin toss, i.e. y_i in {heads, tails}
 - Training data: 10 coin tosses
 - Relevant observations: we observe heads
- With a value estimated for parameter Θ, we can make predictions!
 - Our model has been trained and is ready to be used on unseen data
- Thus, learning a function means estimating its parameters
 - We don't know the parameters of a model
 - Instead, we have data and use it to estimate those parameters
- Let's look at a common framework for parameter estimation

Maximum Likelihood Estimation (1)



- Common approach for parameter estimation
 - Otherwise known as MLE
- Finds model that maximizes likelihood of observed data
 - But what does likelihood mean?
- Our model for the coin toss:
 - $p(k|\Theta) = \Theta^k (1-\Theta)^{1-k}$ is a function of k with Θ fixed (how we predict with it)
 - Let's *instead see it as* function of Θ with fixed k, i.e. $L(\Theta \mid k) = \Theta^k (1-\Theta)^{1-k}$
 - That is, a function of parameters given fixed data (assumed during training)
- We call $L(\Theta/k)$ the likelihood function
 - It is not a probability distribution
 - Instead, we use it to find distributions that fit observed data
- How do we use the likelihood function during training?
 - We want distribution with highest (max) probability to our data
 - Assumption: set of observed data is most likely sample among all data

Maximum Likelihood Estimation (2)



- Formally, we want $\Theta = max_{\Theta}L(\Theta/k)$
 - Equivalently, we want $\Theta = argmax_{\Theta} log p(k|\Theta)$
- First, we make a common assumption: examples are i.i.d.
 - This stands for independent and identically distributed
 - Examples are independent, belong to same distribution
- Then, we apply this assumption to our coin toss setting
 - Our model for a single example: $p(k|\Theta) = \Theta^k (1-\Theta)^{1-k}$
 - The **joint probability of N observed examples** is then given by:

$$P(D) = P(y_1, y_2, ..., y_N)$$

$$= P(y_1)P(y_2)...P(y_N)$$

$$= P(head)^k P(tail)^{N-k}$$

$$= \theta^k (1 - \theta)^{N-k}.$$

Here we used the i.i.d. assumption from line 1 to line 2

Maximum Likelihood Estimation (3)



- Finally, to find this maximum value, we:
 - Compute the first derivative
 - Set it to zero
 - Extract a value for Θ

$$\begin{split} \frac{\partial \log P(D)}{\partial \theta} &= \frac{\partial \left(\log \theta^{k} (1 - \theta)^{N - k} \right)}{\partial \theta} \\ &= \frac{\partial \left(k \log \theta + (N - k) \log(1 - \theta) \right)}{\partial \theta} \\ &= \frac{k}{\theta} - \frac{N - k}{1 - \theta} = 0 \\ &\Rightarrow \hat{\theta} = \frac{k}{N}, \end{split}$$

- We obtained relative frequencies, as we had done already!
 - In practice, MLE often does not have a closed-form solution
 - Instead, we rely on numerical methods
- MLE related to many aspects of ML: cross entropy, MAP, etc.

Empirical Risk Minimization



- This is a general training approach
- Main goal: estimate how a model will work in practice by averaging a loss function $L(x_i, y_i)$ on a training set
 - Here x_i is a training example and y_i its corresponding label
- Formally:

$$R_{ ext{emp}}(h) = rac{1}{n} \sum_{i=1}^n L(h(x_i), y_i).$$

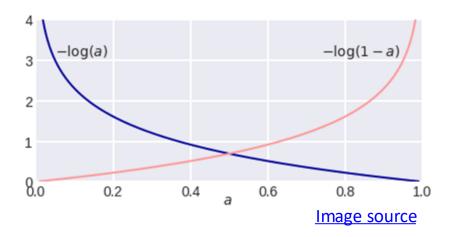
- Note the training set is of size n here
- This is the most common training approach in ML/DL/NLP.
 - But what is a loss function, exactly?

What are loss functions?



- Functions that tell us how a model performs during training
 - Being a cost/loss, we want to minimize it
- Desiderata:
 - Low loss: when model prediction matches given label
 - The closer, the lower the loss/cost
 - High loss: when model prediction does not match label
 - The farther, the higher the loss/cost
- Example: log loss
 - Here a is model prediction
 - Note the desired behavior
 - Works with probabilistic models only

$$-\begin{cases} \log a_i, & y_i = 1, \\ \log(1-a_i), & y_i = 0. \end{cases}$$



Let's design a training objective



- Combine empirical risk minimization with log loss
 - Assume binary classification
- We have:
 - $J = -1/N \sum_{n} [y_i \log(p_i) + (1 y_i) \log (1 p_i)]$ where N is size of training and p_i is prediction for example i
- Note the following:
 - Labels act as indicator factors
 - Log loss means bad model predictions get punished
 - We negate the entire expression so we can minimize it
- Thus, this is an optimization problem
 - This one can be shown to be a form of maximum likelihood estimation
- Training objectives: very important in NLP
 - E.g. masked vs autoregressive language have different, manually designed, training objectives

Summary: ML Refresher



- Goal: learn models that perform a task well on unseen data
- Task: from some input to some output
 - Regression: real-valued output
 - Classification: categorical output
- Model: abstract, often simplified version of a task
 - Comes with set of assumptions, e.g. linearity
- **Evaluation:** given predictions, compute relevant metric
- Training: parameter estimation
 - Objective functions (more not covered in *refresher*, e.g. regularization)
- All of these concepts are common in advanced NLP!
 - E.g. LLMs are models with trillions of parameters
 - Different LLMs train on different objective functions for different tasks
 - Empirical risk minimization and MLE used during training
 - They are evaluated on various metrics relevant to various tasks



Deep Learning Basics

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About this Section



- Goal: discuss basic concepts and terms that will be useful for the entire course
- Outline:
 - 1. Basic Deep Learning Concepts
 - 2. Backpropagation
 - 3. Language Models with Feed-forward Neural Networks

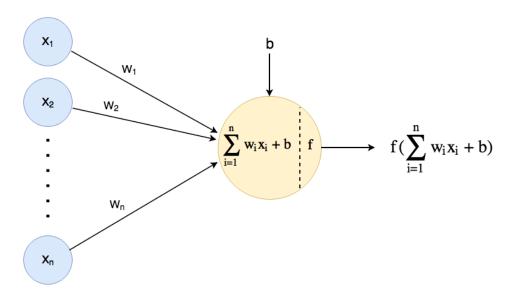
Mathematical Notation



- Scalars: a, b
- Vectors: x, y (by default column vectors, i.e. size is n x 1)
- Matrices: X, Y
- Scalar product: ax
- Dot product: $\mathbf{x}^{\mathsf{T}}\mathbf{w}$ (transpose because \mathbf{x} is column vector)
- Matrix-vector product: Xy
- Matrix-matrix product: XY

What is an artificial neuron?



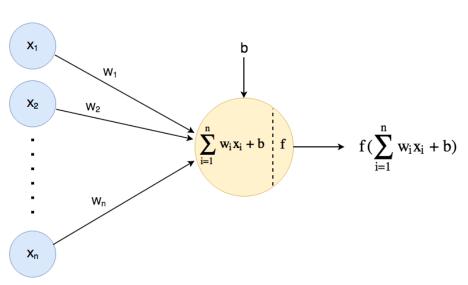


- Input is n-dimensional vector x
- Features x_i multiplied with weights w_i , their products then added
 - What common operation is this?
 - A bias is optional, but almost always there, adds lots of flexibility to model
- Then an *activation function f* is applied to the result
- Different activation functions determine different artificial neurons

Types of Artificial Neurons



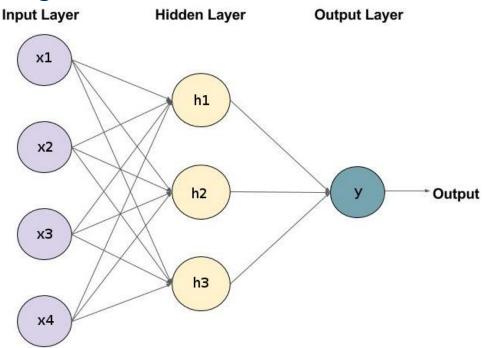
- They are mainly distinguished by their activation functions, e.g.
 - Linear neuron: f(x) = x
 - **Logistic neuron:** $f(x) = \sigma(x)$ (sigmoid function)
- What model do we obtain with a linear neuron?
 - Linear regression
- And with a logistic neuron?
 - Logistic regression
- More types:
 - **Tanh:** maps to [-1,1]
 - ReLu: f(x) = max(0,x)
 - Etc.
- By adjusting weights:
 - We learn functions!



Feed-forward Neural Networks



- Let's do some feature learning!
 - We use hidden layers
 - Input to h_i : x (our data)
 - h_i : learned values
 - Input to *y*: *h* (learned!)
- If y is linear neuron:
 - Linear regression with learned features
- If *y* is logistic neuron:
 - Logistic regression with learned features

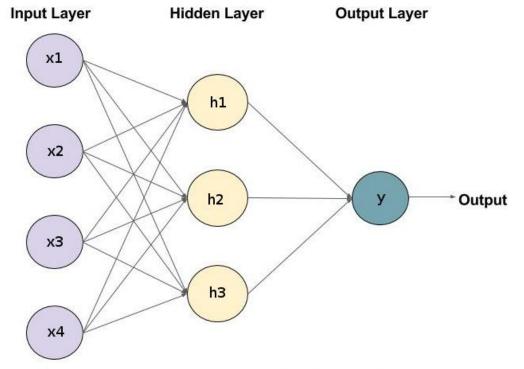


- Thus, FNNs are a framework for *designing* functions (*algebraic circuits*)
 - Information flows forward (but also backward during training, more later)
 - Main restriction: no loops! Computations seen as directed acyclic graphs

Operations in FNNs



- Example so far: fully-connected neural network (useful intuition)
- What does it compute?
- **x**: n x 1 input vector
- h: m x 1 hidden representation
- h_k has $n w_i$, together: \mathbf{w}_k
- Let \mathbf{W}_1 be $n \times m$ matrix
 - m columns, each a w_i
- Then $\mathbf{h} = \mathbf{W}_1^T \mathbf{x}$ if h_k linear
 - $\mathbf{h} = f(\mathbf{W}_1^T \mathbf{x})$ w. activ. f
 - $\mathbf{h} = f(\mathbf{W}_1^T \mathbf{x} + \mathbf{b})$ w. bias

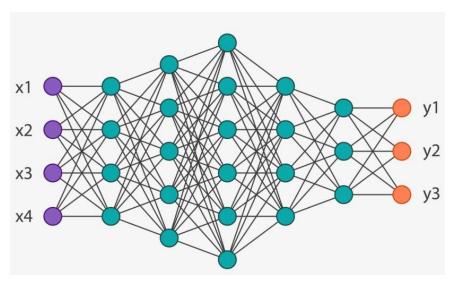


- Similarly: $y = f(\mathbf{W}_2^T \mathbf{h} + b)$ where \mathbf{W}_2 is $m \times 1$, constructed as \mathbf{W}_1
 - Note network $y = W_3^T x + b$ exists with $W_3 = W_1 W_{2}$, i.e. no hidden layers
 - Why do we always use hidden layers then?

Why use Deep Networks?



- When is a network deep?
 - Not well defined
 - Some say >4 hidden layers
 - Others say >2
- More important: why?
- Universality theorem
 - Formalities about FNN limits to approximate functions
 - One takeaway: no depth needed

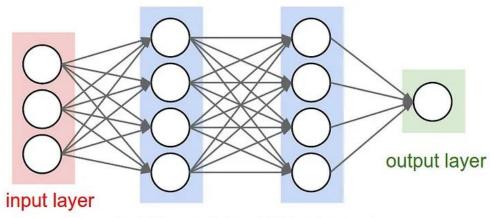


- Why use depth then? Hidden representations!
 - Each hidden layer is a learned feature vector, hierarchical features
 - Component for designing networks: number and size of hidden layers
 - Smaller layers force models to learn compact but useful representations
 - More/larger hidden layers: more freedom, more parameters, difficult to train
- More parameters -> stronger model, may overfit, requires lots of data

FNNs for Regression



- Let's design a fully-connected network for regression
- **Input:** *n*-dimensional *x*
- Output: real number *y*
- So, how many input units?
 - What type of units?
- How many output units?
 - What type of units?
- How many hidden layers?
 - What size/type of units?



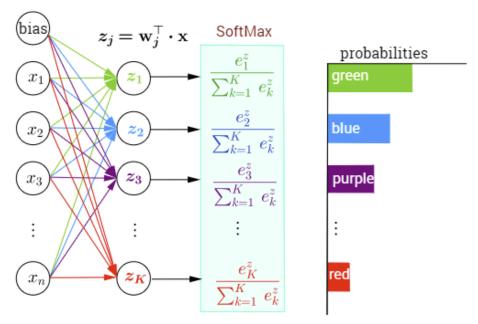
hidden layer 1 hidden layer 2

- How to ensure this number of output units? Linear layer!
 - Project down to the size that you need
 - Remember: $y = W_k^T h + b$ where W_k is $m \times n$ matrix
 - \mathbf{W}_{k}^{T} projects n dimensional vector to m dimensional vector space
- Linear transformation are everywhere in Deep Learning!

FNNs for Classification



- Let's design a fully-connected network for classification
- **Input:** *n*-dimensional **x**
- Output: one of *K* classes
- So, how many input units?
 - What type of units?
- How many output units?
 - How do we ensure that?
 - What type of units?
- How to get predictions?
 - Softmax layer



- Softmax function: turns given vector into probability vector
- **x** is a probability vector if $x_i \in [0,1]$ for all i and $\Sigma_i x_i = 1$ (see first tutorial)
- Softmax *layer*: linear layer for projection + softmax function
 - Input: vector of logits; Output: probability vector for inference/prediction

Information Flow



- "Feed-forward neural networks: information flows forward"
 - Oversimplified! Important information flows backward during training
 - This influences design, inspired creation of important components
 - E.g. LSTMs, residual units, etc.
- Training often done with gradient-based optimizers
 - E.g. SGD, Adagrad, etc. (briefly discussed in first tutorial)
 - Gradient information tells us how to update model parameters!

Forward pass

Compute function we are learning

Backward pass

- Compute gradient information to learn parameters
- How to compute gradients of functions computed by FNNs? Backpropagation!

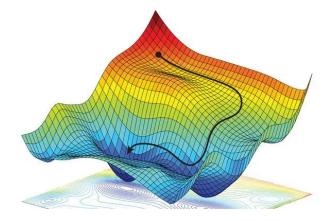


Image source

Backpropagation (1)

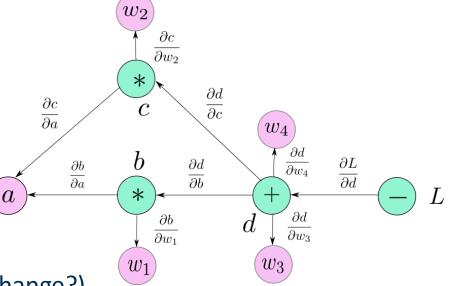


- What is a derivative?
 - Let y = f(h)
 - dy/dh asks: how much does y change when h changes?
- A gradient is a multidimensional derivative
 - Let **h** be n-dimensional vector and y = f(h) a function from R^n to R
 - $\partial y/\partial h = (\partial y/\partial h_1, \partial y/\partial h_2, ..., \partial y/\partial h_n)$ is gradient of y w.r.t. \mathbf{x}
 - I.e. the gradient of y w.r.t. h is also an n-dimensional (row) vector
 - Geometrically, gradient vector is direction of the largest change of y
- What rate of change are we interested in during training?
 - How much does loss *L* change when model parameters *O* change?
 - I.e. ∂*L/*∂**Ø**
- What if L is output of a compound parameterized function (FNN)?
 - E.g. L = f(y) where $\mathbf{y} = g(\mathbf{h}/\mathbf{\Theta}_2)$, $\mathbf{h} = z(\mathbf{x}/\mathbf{\Theta}_1)$ (z is 1st layer, g is 2nd, f is loss)
 - Here $\partial y/\partial h$ is a Jacobian $(m \times n \text{ matrix where } m \text{ is size of } y, n \text{ size of } h)$
 - Same for $\partial h/\partial x$

Backpropagation (2)



- We propagate the change/error back using the chain rule!
- Recall chain rule
 - Let y = g(h) and $h = f(\Theta)$
 - $\partial y/\partial \Theta = \partial y/\partial h \cdot \partial h/\partial \Theta$
- Take this computation graph
 - **Internal nodes:** operations
 - **Leaves:** learnable weights w_i , input a
- Here L = d label, $d = w_3b + w_4c$
- We want $\partial L/\partial w_4$ (which rate of change?)
- Chain rule: $\partial L/\partial w_4 = \partial L/\partial d \cdot \partial d/\partial w_4$
- Similarly, $\partial L/\partial w_2 = \partial L/\partial d \cdot \partial d/\partial c \cdot \partial c/\partial w_2$ where $c = w_2 a$
 - Note that $\partial L/\partial d$ is useful for both $\partial L/\partial w_4$ and $\partial L/\partial w_2$
 - Reusing gradients is common during backpropagation



Backpropagation (3)



- Perhaps more important, take $\partial L/\partial w_2 = \partial L/\partial d \cdot \partial d/\partial c \cdot \partial c/\partial w_2$
 - Here, gradient $\partial c/\partial w_2$ is multiplied by factor $\partial L/\partial d \cdot \partial d/\partial c$
 - $\partial L/\partial d$ comes from passing gradient through minus operator in L
 - $\partial d/\partial c$ comes from passing gradient through plus operator in d
- Thus, operations have impact on their "input" gradients!
 - Important to consider when designing networks
 - E.g. plus operator has no effect on gradient
 - Concat operator splits gradient into two
- E.g. if either $\partial d/\partial c$ or $\partial L/\partial d$ are close to zero, $\partial L/\partial w_2$ will be small
 - In other words, we get little info about how to change w_2 to improve L
 - Generally, small gradients = slow/difficult to learn
- Many challenges in *training* deep networks, e.g. vanishing gradients
 - Inspired solutions like LSTMs, residual connections (used in transformers)
- Let's look at a FNN for a practical NLP use case!

Language Modeling Recap



- Predict the next word:
 - "Every Thursday there is a Schneckenhof ..."
- This suggests:
 - Some words are more likely to appear than others given some context
- Probabilistically:
 - p(meeting|"Every Thursday there is a Schneckenhof")
- Generally: $p(w_{n+1}/w_1, w_2, ..., w_n)$
 - Conditional probability of w_{n+1} given joint distribution of $w_1, w_2, ..., w_n$
 - w_i are words/tokens in some fixed vocabulary V the model can process
- Such models can predict entire sequences with probability chain rule
 - $p(w_1, w_2, ..., w_n) = p(w_1)p(w_2/w_1) p(w_3/w_1, w_2)... p(w_n/w_1, w_2, ..., w_{n-1})$
- Useful in many NLP settings, e.g. machine translation
 - A good language model should identify more common phrases
 - p(This sentence makes sense) < p(Makes sense this sentence does)

Language Modeling with FNNs (1)



- Bengio et al. (2003) proposed a FNN that simultaneously learns:
 - 1. "Distributed representations of words"
 - "Probability function of word sequences expressed in terms of these representations"
- Size of word vectors (30, 60, 100) much smaller than vocabulary (17K)
- Intuition: similar words have similar feature vectors
- Thus, training sentence *The cat is walking in the bedroom* can be generalized to, e.g.:
 - A dog is walking in a room
 - The cat is running in a room
 - A dog is walking in a bedroom
 - The dog is walking in the room
- How did they implement such a model?
 - A feed-forward neural network
 - Not the first time it was done, but the first time at that scale

Language Modeling with FNNs (2)



- How did they model $p(w_m/w_1, w_2..., w_{m-1})$?
 - A mapping C between every word w_i ∈ V to a m-dimensional vector w_i
 Today known as an embedding layer.
 Given w_i, get row i in embedding matrix C (V rows, each a vector w_i)
 - 1. Function g that maps input sequence of word vectors to a probability vector of size |V|, i-th component is probability of i-th word being next
- Embeddings are parameters that are learned
- Function g uses these embeddings plus additional parameters $oldsymbol{\omega}$
 - $p(w_i/w_1, w_2..., w_{m-1}) = g(i, w_1, w_2..., w_{m-1}/\omega)$ where *i* is index of word w_i
- Overall, they learned function f, a composition of C and g, with a FNN
 - $f(i, w_1, w_2, ..., w_{m-1}) = g(i, C(w_1), C(w_2), ..., C(w_{m-1}) | \Theta)$
 - All model parameters are $\Theta = (C, \omega)$
- It's easy to see what C might look like, but what does g look like?
 - In other words, what did their network architecture look like?

Language Modeling with FNNs (3)



 1^{st} : Get word vectors \mathbf{w}_i

2nd: Concatenate vectors to

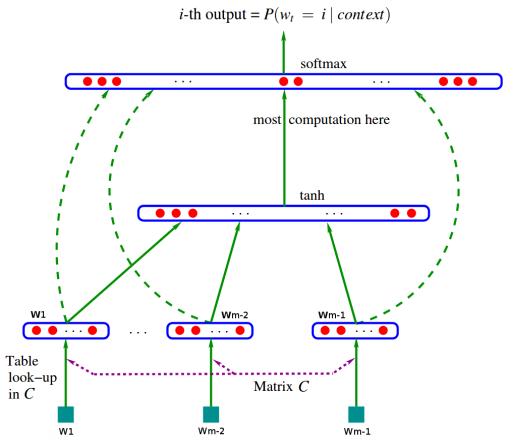
form x

3rd: Hidden layer (matrix *H* transform. + *tanh* activ.)

4th: Optional linear layer w. matrix **W** from input to softmax layer (dashed lines)

5th: Softmax layer (matrix *U* transform. + softmax)

Overall: input to softmax



- y = b + Wx + Utanh(d + Hx) where b,d are biases
- Then **O** = (**b**, **d**, **W**, **U**, **H**, **C**)

Language Modeling with FNNs (4)



- How did they train?
 - They estimated **O** that maximized likelihood of training data (i.e. **MLE**)
- Specifically:
 - $L = 1/T \sum_{m} log f(w_1, w_2..., w_{m-1}; \Theta) + R(\Theta)$
 - Here, T is number of words in training corpus
- Note a few things:
 - They average loss over the training set (empirical risk)
 - Penalizing term $R(\Theta)$ is regularization (weight decay on C, W, H, U)
- They trained in a self-supervised manner
 - I.e. yes, there are labels, but no manual labeling required
 - Instead, they used sequences of length m in the training corpus
 - For each sequence, first *m-1* words are input, word *m* is target
- Many of these components still in use today!
 - Softmax layer, MLE, empirical risk, self-supervision

Summary: DL Basics



- FNNs: framework for constructing parameterized real-valued functions
 - We design and learn these functions (algebraic circuits)
- Information flows in both directions on these circuits
 - Forward pass: model expressivity
 - Backward pass: model "learnability"
- Backpropagation: training deep networks, chain rule
- Important: we can learn useful features with deep models!
 - Hidden layers interpreted as *learned representations*
 - Learned representations useful in other settings, i.e. transfer learning
 - E.g. style transfer, pre-training word representations
- Language modeling with FNNs by Bengio et al. (2003)
 - Established many modeling and training components still used today
- Later in the course, other types of FNNs relevant for NLP
 - RNNs, transformers



Word Embeddings

Dr. Daniel Ruffinelli - FSS 2025

About this Section



- Goal: introduce concepts and methods about static word embeddings
- Outline:
 - 1. Sparse vs Dense Word Representations
 - 2. Word2Vec
 - 3. Properties of Word Vectors
 - 4. Evaluation of Word Vectors

What do we want to represent? (1)



- Words? I.e. strings of symbols such as cat or dog?
 - No, those are representations themselves!
 - What do they represent?

Meaning!

- We map strings such as cat or dog to concepts (or senses)
- We refer to this mapping as meaning, what those words refer to
- Is meaning a 1-to-1 mapping?
 - No, words can have many meanings (remember ambiguity?)
- How do we, humans, handle word ambiguity? Context!
 - "I work at a bank."
 - What's more likely? A financial institution or by the river?
 - Again, context. Does the person work in Frankfurt? Are they fishermen?
- So, we want to represent the relation between words and senses!

What do we want to represent? (2)



- What do we want from such representations? Ideally usefulness, e.g.
 - Tell us if words have similar meanings, e.g. cat and dog
 - Tell us if words are antonyms, e.g. hot and cold
 - Tell us if they have positive or negative connotations, e.g. happy or sad
- "Generally, a model of word meaning should allows us to draw inferences to address meaning-related tasks like question answering." Jurafsky and Martin, 2023
- Perhaps we should represent senses, then, not words!
 - Use something like WordNet, expert-crafted database of senses
- Databases like WordNet have not worked well in practice
 - Missing nuance, "good" is synonym of "proficient" only in some cases
 - New meanings missing, e.g. genius, wicked, wizard
- In practice, dealing with word representations works better
 - We focus on their relation to meaning (based on context)
 - We don't commit to a given representation of sense

Sparse Word Representations



- Traditional approach: sparse word vectors
- Example: one-hot vectors
 - Given vocabulary V, represent each word with vector of size |V| using one-hot encoding
- For example, given *V* = {cat, dog, airplane}
 - $V_{cat} = [1, 0, 0]$
 - $V_{dog} = [0, 1, 0]$
 - $V_{airplane} = [0, 0, 1]$
- Problem 1: /V/ can be very large
 - Recall Bengio's work from 2003: |V| = 17K
- Problem 2: No natural notion of similarity from such vectors
 - They are all equally different, e.g. with a dot product
 - But cat and dog are more similar to each other than to airplane
- Generally, difficult to draw inferences from such representations
 - Let's look at another approach that addresses these issues

Distributed Representations



- Idea from deep learning community (Geoffrey Hinton in 1986)
- Sparse representations:
 - Each representational component maps to single represented object
 - E.g. each feature in vector corresponds to one word
- Distributed (or dense) representations:
 - Many-to-many relation between representational components and represented objects
 - E.g. each word is represented with a set of (distributed) features
- PROs: model has freedom to use features "at will" during learning
- **CONs:** Less interpretable than, e.g. one-hot encoding
 - Given V, we know what word is represented by [0, 1, 0]
 - But what word is this? [0.23, 0.447, 0.02]
- Using vectors to represent words also has a history in linguistics
 - Osgood et al. (1957) represented words with 3-dimensional vectors
 - Each dimension encoded known useful (non-learned) features

Distributional Semantics (1)



- Idea from linguistics (Joos, 1950; Harris, 1954; Firth, 1957)
- Not the same concept!
 - Distributed representations != distributional semantics
 - In NLP, the latter can be seen as a special case of the former
- Let's guess what the word foobar means
 - 1. Foobar is often played in teams of 7.
 - 2. A *foobar* match is divided into 3 thirds of 25 minutes each, called runs.
 - 3. A *foobar* match is won by scoring 10 points.
- What would you guess the word foobar refers to? Why?
 - A type of food?
 - A sport?
 - A country?
- Distributional hypothesis:
 - "A word is characterized by the company that it keeps." (Firth, 1957)

Distributional Semantics (2)



- Put differently:
 - We define the meaning of a word by its distribution in a language
 - I.e. by its neighboring words, grammatical environment
- Words whose neighboring words are similar, have similar meanings.
- We can use this idea to build useful vector representations of words!
- For example: co-occurrence matrices
 - Given defined context, e.g. a document, a sentence, a word window
 - Construct matrix C of size V x V where V is given vocabulary
 - Rows in matrix are words, columns are also words
 - m_{ii} denotes number of times word *i* appears in same *context* as word *j* (so, sparse)
- Co-occurrence matrices useful in many applications
 - E.g. latent semantic analysis (LSA) --> singular value decomposition of C
 - Extracts vector representations from (truncated) left-singular vectors
 - Similar count-based methods covered in basic Text Analytics course
- Word embeddings: distributional hypothesis to learn dense vectors

Word Embeddings



- Idea: to embed higher dimensional vectors into lower dimensional vector space such that (some of) the relative properties of the higher dimensional space are kept
 - Hence, embedding --> (relatively) low-dimensional vector representation
 - Low-dimensional compared to, e.g. /V/
 - Size typically between 50 and 1000 dimensions
 - Vectors are dense (distributed) representations
- Historically important approach: word2vec (Mikolov et al. 2013)
 - Training based on distributional semantics
 - Done in the context of deep learning (though this model is not deep)
- Intuition:
 - Instead of counting words for co-occurrence, let's train a classifier to predict whether two words are likely to appear in the same context.
- Two approaches proposed for learning such a classifier
 - Skip-gram and continuous bag of words (CBOW) (we focus on <u>skip-gram</u>)

The Skip-Gram Algorithm



- Algorithm for learning dense word vectors
- Basic steps
 - 1. Treat target words and neighboring context words as **positive examples**
 - 2. Randomly sample other words in vocabulary to get negative examples
 - 3. Train a classifier to predict whether two given words appear together
 - 4. Use learned weights as word embeddings
- Why negative examples?
 - In some tasks, negative examples often needed to avoid trivial solutions
 - E.g. push all vectors to same point, thus all vectors similar
 - If training objective is poorly designed, such a solution may "reach objective"
- Let's have a look at:
 - 1. The task
 - 2. The model
 - 3. The training objective

Skip-Gram: The Task



- Say we have the sentence:
 - ... known as [ramen, a Japanese dish that] has recently become...

 c_1 c_2 w c_3 c_4

- Here, w denotes **center word** and c_i denotes **context words**
 - I.e. context window is plus/minus a few words in this case
 - More context --> usually more useful, not always, more later
 - E.g. plus/minus 1 gives us [a; ???; dish]
 - Plus/minus 2 gives us [ramen; a; ???; dish; that] (assumes no punctuation)
- Task: given tuple (w,c), predict if c appears in context of w or not
 - So, binary classification
- Probabilistically, P(True|w,c)
 - Similarly, P(False|w,c) = 1 P(True|w,c)
- How can we model these probabilities?

Skip-Gram: The Model (1)



- How to get probability P(True | w,c)?
 - Key idea: based on similarity of corresponding word embeddings
 - I.e. a word c is likely to occur near a target word w if their corresponding embeddings e_c and e_w are similar
 - Probabilistically, w and c are independent given their embeddings e_c , e_w
 - Let $\Theta = [e_{1, \dots, e_{|V|}}]$. We have $P(True | w, c, \Theta)$ (Θ often omitted for brevity)
- How can we represent that similarity?
 - Skip-gram went with **dot product**, i.e. $e_c^T e_w$
- But didn't we need a probability?
 - Ok, then $P(True | w,c) = \sigma(e_c^T e_w)$ where σ is the **sigmoid function**
 - Similarly, $P(False | w, c) = 1 \sigma(e_c^T e_w) = \sigma(-e_c^T e_w)$
 - The last equality results from a property of the logistic function
- This is the probability of word c being in context of word w.
 - What if I want to provide more context? More context is better, right?

Skip-Gram: The Model (2)



- How do we compute $P(True | w, c_{1:1})$ where L is size of context window?
 - Assumption: context words are independent of each other
 - Computing joint distribution of words in context becomes much simpler
- Thus, we have

$$P(True \mid w, c_{1:L}) = \prod_{i \in L} \sigma(e_i^T e_w) = \sum_{i \in L} \log \sigma(e_i^T e_w).$$

- How is this model parameterized?
 - It actually learns two representations for each word
 - One for words as targets, one for words as context (just one vocabulary V)
 - Thus, parameterized by matrices W and C, both of size $|V| \times d$ where d is a hyperparameter (embedding size)
 - In other words, $\Theta = [W, C]$
- How was this model trained?

Skip-Gram: The Training Objective (1)



- As with Bengio's LM from 2003: self-supervision
- Given text corpus (i.e. large sequence of text)
 - Iterate over sequences of size $n = L^2 + 1$ (L is size of context window)
 - For each sequence, set center word as target, other words as context

• For example:

1. ... [known as ramen, a Japanese] dish that has recently become...

 c_1 c_2 w c_3 c_4

2. ... known [as ramen, a Japanese dish] that has recently become...

 C_1 C_2 W C_3 C_4

3. ... known as [ramen, a Japanese dish that] has recently become...

 C_1 C_2 W C_3 C_4

- Thus, for sequences 1, 2 and 3, you get positive examples (w,c):
 - 1. (ramen, known), (ramen, as), (ramen, a), (ramen, Japanese)
 - 2. (a, as), (a, ramen), (a, Japanese), (a, dish)
 - 3. (Japanese, ramen), (Japanese, a), (Japanese, dish), (Japanese, that)

Skip-Gram: The Training Objective (2)



- We also need negative examples!
- Given w, we randomly sample words from V as candidates for c
 - For example: (ramen, ostrich), (ramen, the), (ramen, Alaska), ...
 - They generated *k* (hyperparameter) negative examples per positive
- Then, given (w,c_{pos}) , corresponding $(w,c_{neg~i})$, and cross entropy (CE), we have:

$$L_{CE} = -\log \left[P(+|w, c_{pos}) \prod_{i=1}^{k} P(-|w, c_{neg_i}) \right]$$

$$= -\left[\log P(+|w, c_{pos}) + \sum_{i=1}^{k} \log P(-|w, c_{neg_i}) \right]$$

$$= -\left[\log P(+|w, c_{pos}) + \sum_{i=1}^{k} \log \left(1 - P(+|w, c_{neg_i}) \right) \right]$$

$$= -\left[\log \sigma(c_{pos} \cdot w) + \sum_{i=1}^{k} \log \sigma(-c_{neg_i} \cdot w) \right]$$

- Generally, they applied empirical risk over all training examples
 - Since this is negative log likelihood (NLL), they did MLE of the training set

Task vs Goal



- **Task:** *P(True|w,c)*
 - What do we use that task for?
 - Real-world uses?
- Goal: learn word embeddings!
 - Task designed to force model to capture properties (distributional semantics)
 - Original task was different, $P(w_{t+i}/w_t)$
- Other models have tasks and goals
 - E.g. GPT-style LLMs are autoregressive language models
 - BERT-style models are masked language models
- Sometimes we want to use the model to make predictions
 - Other times, we just want their learned weights

Other Types of Static Embeddings



- Word2vec is useful model for intuition/learning about embeddings
 - It was also successful and is historically important
 - But there are other ways of learning word embeddings
 - These are often used in practice as well
- **GloVe:** stands for Global Vectors (Pennington et al., 2014)
 - Combines count-based models with methods like word2vec
 - Constructs co-occurrence matrix
 - Learns matrix factorization with least squares objective
 - Covered in basic Text Analytics course
- fasttext: addresses problem of unknown words in word2vec
 - That is, new words in test that were not present in training
 - For this, they used representations based on subwords
 - Also covered in basic Text Analytics course
- Static embeddings have some nice and useful properties!
 - At the time, they were quite impressive!

Properties of Word Embeddings (1)

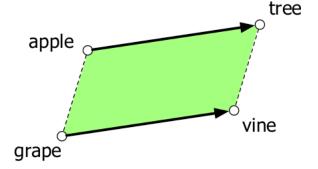


- Size of context window is important! (Levy and Goldberg, 2014)
 - It affects the representations we learn!
- Smaller sizes tend to provide more static embeddings
 - Depends on immediate neighborhood
 - Similarity tends to be based on same parts of speech
- E.g. what is similar to Hogwarts with small context window?
 - Other fictional schools, e.g. Sunnydale (from Buffy the Vampire Slayer)
- Larger sizes tend to focus on similarity based on topic
 - So words with same part of speech not necessarily related
- E.g. what is similar to Hogwarts with larger context window?
 - Dumbledore, Malfoy, half-blood
- This was observed for skip-gram
 - Different methods may differ in such properties
 - But it is safe to assume the context window has an impact

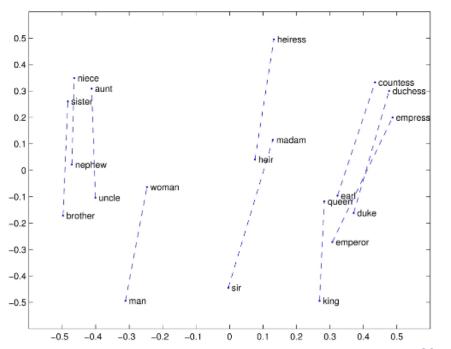
Properties of Word Embeddings (2)



- They capture relational similarity
 - Parallelogram model from cognitive science



- Example from GloVe
 - Skip-gram known to capture this
 - It's not as smooth all the time



Evaluating Word Embeddings



- Intrinsic evaluation:
 - Correlation between similarities of representations with expert-given similarity scores
- Examples:
 - WordSim353 (2002): 353 noun pairs, e.g. (plane, car)
 - SimLex-999 (2015): more difficult, e.g. (cup, mug)
- Another approach: analogy task (e.g. man + woman king = queen)
 - Word2vec used this in their original work
- Most important evaluation: extrinsic!
 - I.e. using the representations in NLP downstream tasks and see if performance improves

Summary: Word Embeddings



- Vector representations of words
- **Sparse vs dense** (distributed) representations
 - PROs and CONs to each
 - Different methods to learn them (each a different task)
- Distributional semantics
 - Important principle
 - Commonly used to learn word embeddings, language models
 - Spoiler: also used when training LLMs
- Classic way to learn dense word representations: word2vec
 - Specifically, the skip-gram task, model and training objective
 - Resulting learned representations have nice properties
- In the future, other tasks for other goals
 - E.g. masked and autoregressive language models

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