CSCI 567: Machine Learning

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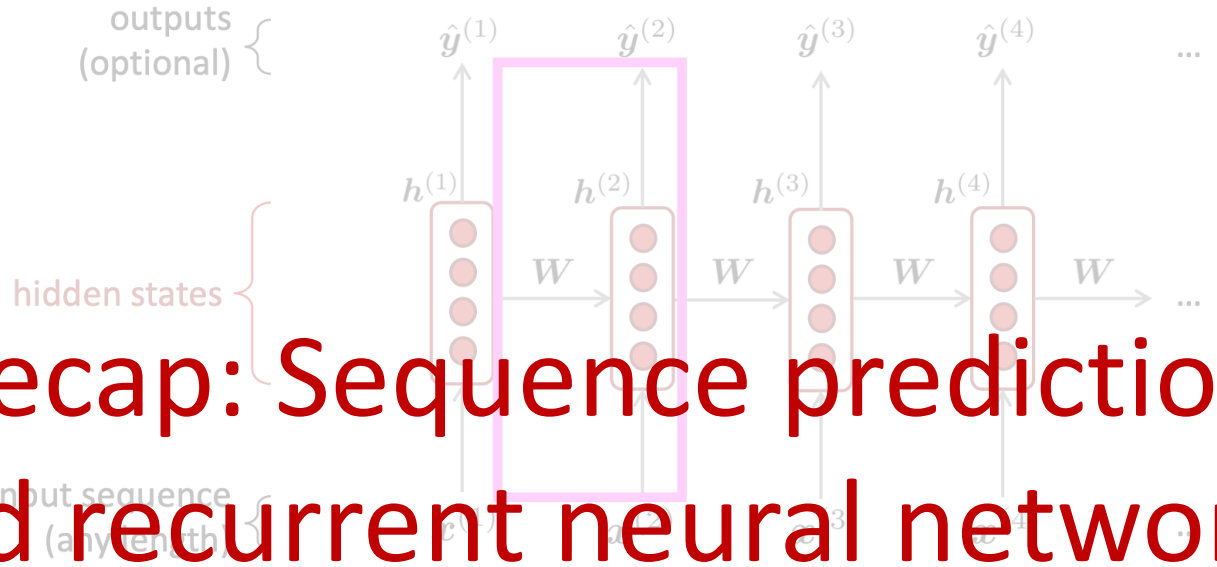
Lecture 9, March 22

USC University of Southern California

Administrivia

- HW3 due in less than 1 week
- Peer mentoring sessions on Monday, Tuesday & Wednesday next week

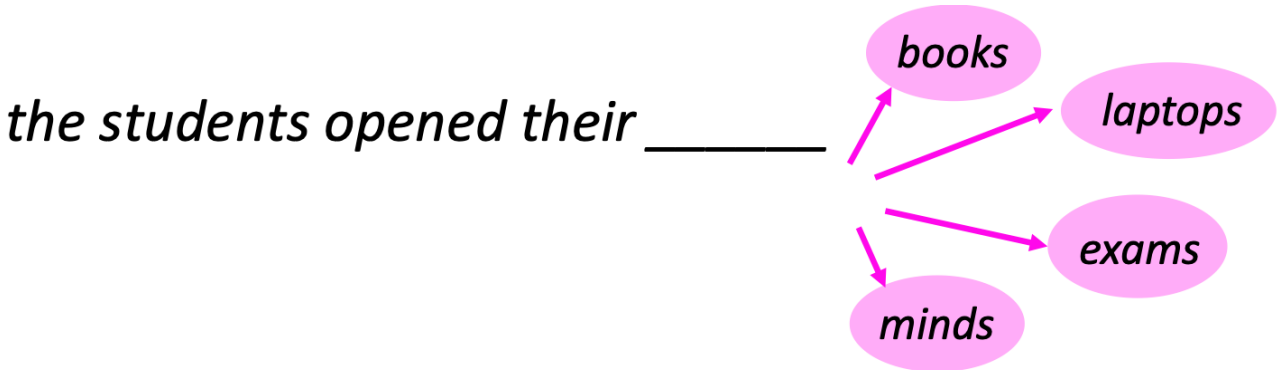
- Today's plan:
  - Attention & Transformers, Decision trees



Recap: Sequence prediction and recurrent neural networks

Language modelling

Language modelling is the task of predicting what word comes next:



More formally, let X_i be the random variable for the i-th word in the sentence, and let x_i be the value taken by the random variable. Then the goal is to compute

$$P(X_{t+1}|X_t = x_t, \ldots, X_1 = x_1).$$

A system that does this is known as a **Language Model.**

Slide adapted from CS224n by Chris Manning (Lecture 5)

n-gram language model: A type of Markov model

A **Markov model or Markov chain** is a sequence of random variables with the **Markov property**: a sequence of random variables $X_1, X_2, \cdots$ s.t.

$$P(X_{t+1} \mid X_{1:t}) = P(X_{t+1} \mid X_t) \qquad \text{(Markov property)}$$

i.e. *the next state only depends on the most recent state* (notation $X_{1:t}$ denotes the sequence $X_1, \ldots, X_t$). This is a *bigram model*.

We will consider the following setting:

- All X_t's take value from the same discrete set $\{1, \ldots, S\}$
- $P(X_{t+1} = s' \mid X_t = s) = a_{s,s'}$, known as transition probability
- $P(X_1 = s) = \pi_s$
- $(\{\pi_s\}, \{a_{s,s'}\}) = (\boldsymbol{\pi}, \boldsymbol{A})$ are parameters of the model

Higher-order Markov models

Is the Markov assumption reasonable? Not so in many cases, such as for language modeling.

Higher order Markov chains make it a bit more reasonable, e.g.

$$P(X_{t+1} \mid X_t, \ldots, X_1) = P(X_{t+1} \mid X_t, X_{t-1}) \qquad \textbf{(second-order Markov assumption)}$$

i.e. the current word only depends on the last two words. This is a *trigram model*, since we need statistics of three words at a time to learn. In general, we can consider a n-th Markov model (or a *$(n+1)$-gram model)*:

$$P(X_{t+1} \mid X_t, \ldots, X_1) = P(X_{t+1} \mid X_t, X_{t-1}, \ldots, X_{t-n+2}) \quad \textbf{(n-th order Markov assumption)}$$

Learning higher order Markov chains is similar, but more expensive.

$$\begin{aligned} P(X_{t+1} = x_{t+1} \mid X_t = x_t, \ldots, X_1 = x_1) &= P(X_{t+1} = x_{t+1} \mid X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_{t-n+2} = x_{t-n+2}) \\ &= \frac{P(X_{t+1} = x_{t+1}, X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_{t-n+2} = x_{t-n+2})}{P(X_t = x_t, X_{t-1} = x_{t-1}, \ldots, X_{t-n+2} = x_{t-n+2})} \\ &\approx \frac{\text{count}(x_{t-n+2}, \ldots, x_{t-1}, x_t, x_{t+1}) \text{ in the data}}{\text{count}(x_{t-n+2}, \ldots, x_{t-1}, x_t) \text{ in the data}} \end{aligned}$$

Generating text with a n-gram Language Model

You can also use a Language Model to generate text

today the price of gold per ton , while production of shoe lasts and shoe industry , the bank intervened just after it considered and rejected an imf demand to rebuild depleted european stocks , sept 30 end primary 76 cts a share .

Surprisingly grammatical!

…but **incoherent.** We need to consider more than three words at a time if we want to model language well.

However, larger n increases model size and requires too much data to learn

Slide adapted from CS224n by Chris Manning (Lecture 5)

A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \text{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

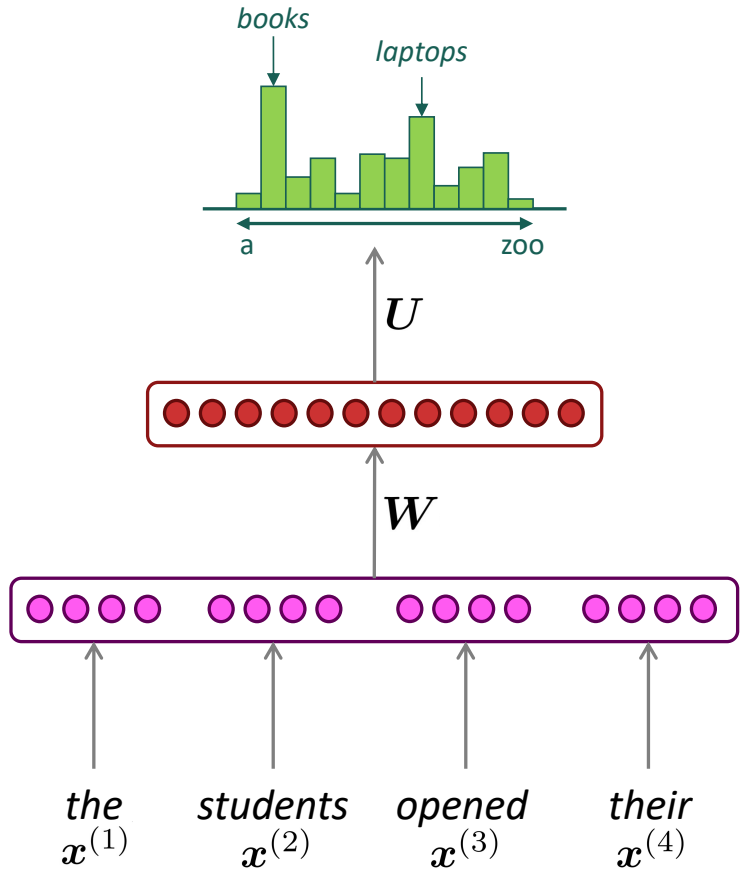
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$



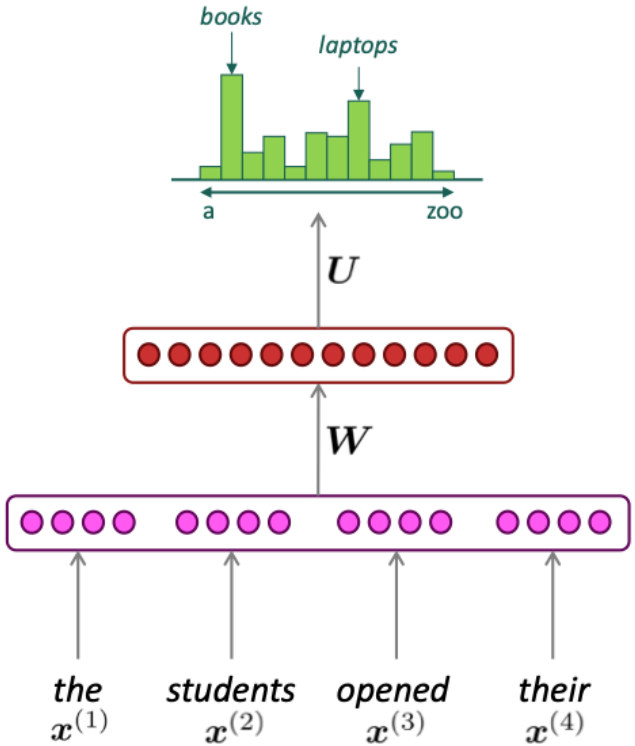
Slide adapted from CS224n by Chris Manning (Lecture 5)

The problem with this architecture

- Uses a fixed window, which can be too small.
- Enlarging this window will enlarge the size of the weight matrix $\boldsymbol{W}$.
- The inputs $\boldsymbol{x}^{(1)}$ and $\boldsymbol{x}^{(2)}$ are multiplied by completely different weights in $\boldsymbol{W}$.
  No symmetry in how inputs are processed!

As with CNNs for images before, we need an architecture which has similar symmetries as the data.

In this case, ***can we have an architecture that can process any input length?***



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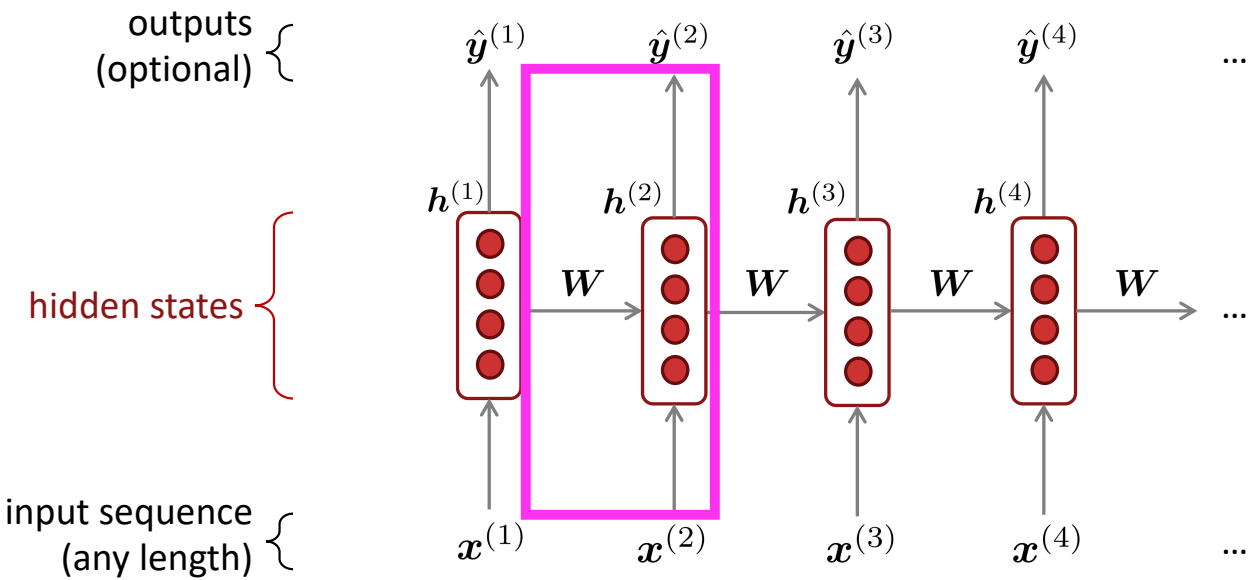
Recurrent Neural Networks (RNN)

A family of neural architectures

Core idea: Apply the same weights W *repeatedly*



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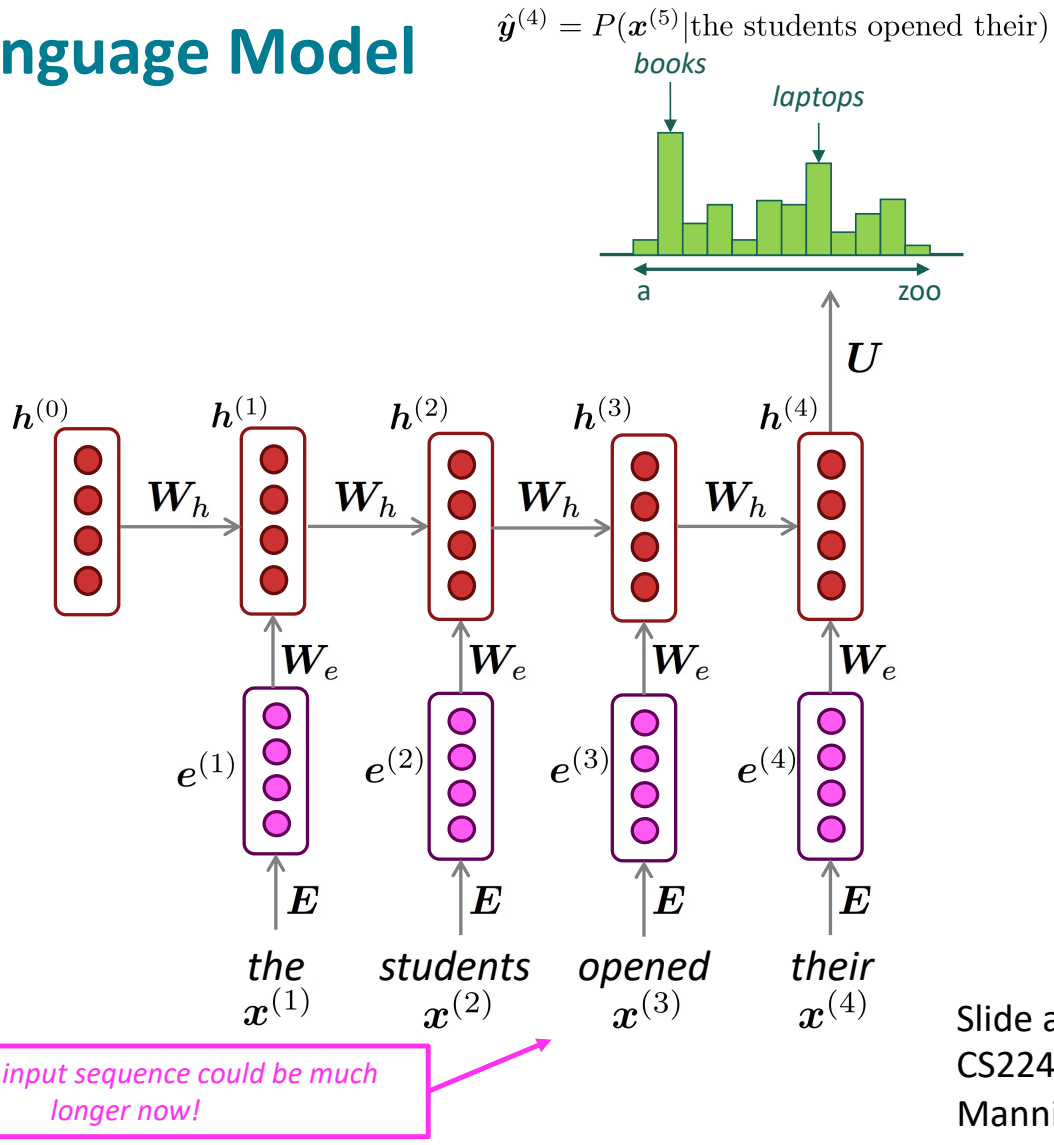
A Simple RNN Language Model



output distribution

$$\hat{\boldsymbol{y}}^{(t)} = \text{softmax}\left(\boldsymbol{U}\boldsymbol{h}^{(t)} + \boldsymbol{b}_2\right) \in \mathbb{R}^{|V|}$$

hidden states

$$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h\boldsymbol{h}^{(t-1)} + \boldsymbol{W}_e\boldsymbol{e}^{(t)} + \boldsymbol{b}_1\right)$$

$\boldsymbol{h}^{(0)}$ is the initial hidden state

word embeddings

$$\boldsymbol{e}^{(t)} = \boldsymbol{E}\boldsymbol{x}^{(t)}$$

words / one-hot vectors

$$\boldsymbol{x}^{(t)} \in \mathbb{R}^{|V|}$$

***Note**: this input sequence could be much longer now!*

Slide adapted from CS224n by Chris Manning (Lecture 5)

Training an RNN Language Model

- Get a big corpus of text which is a sequence of words $x^{(1)}, \ldots, x^{(T)}$
- Feed into RNN-LM; compute output distribution $\hat{\boldsymbol{y}}^{(t)}$ for *every step t*.
  - i.e. predict probability dist of *every word*, given words so far

- Loss function on step *t* is cross-entropy between predicted probability distribution $\hat{\boldsymbol{y}}^{(t)}$, and the true next word $\boldsymbol{y}^{(t)}$ (one-hot for $\boldsymbol{x}^{(t+1)}$):

$$J^{(t)}(\theta) = CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}) = -\sum_{w \in V} \boldsymbol{y}_w^{(t)} \log \hat{\boldsymbol{y}}_w^{(t)} = -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

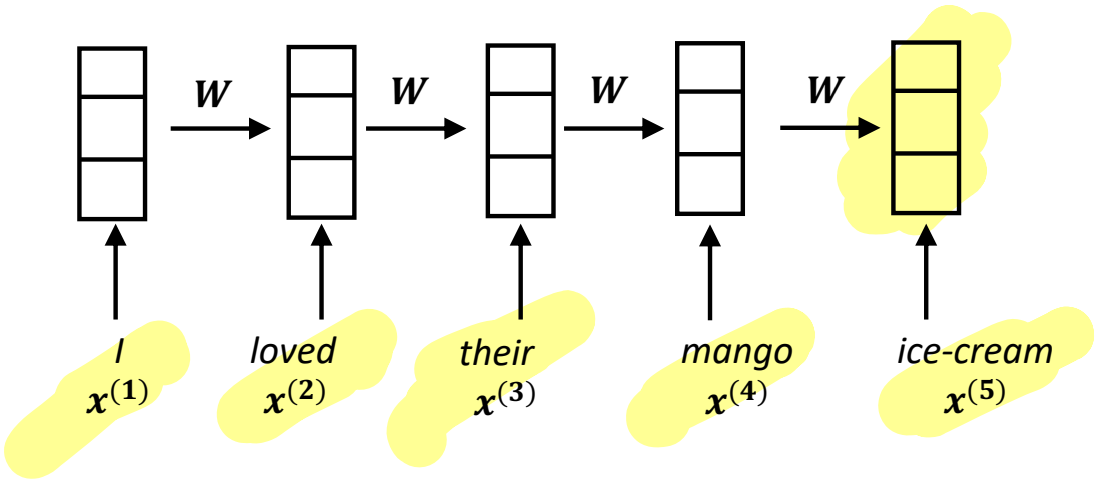
- Average this to get overall loss for entire training set:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} J^{(t)}(\theta) = \frac{1}{T} \sum_{t=1}^{T} -\log \hat{\boldsymbol{y}}_{\boldsymbol{x}_{t+1}}^{(t)}$$

Slide adapted from CS224n by Chris Manning (Lecture 5)


Gender-specific term
Name
She
He
Layer: 5
The girl and the boy walked home . She
Later , Alice came up to Bob . She
Attention: Recap

The problem with recurrence



1. Must always compress all necessary information into one hidden state representation

2. Cannot capture long-range dependencies in input ("vanishing gradients problem")

Inputs from sufficiently far away do not contribute to hidden state representation:

Suppose $\boldsymbol{W} = \begin{pmatrix} 0.8 & 0.2 \\ -0.6 & 0.9 \end{pmatrix}$

Then $\boldsymbol{W}^5 = \begin{pmatrix} -0.31 & 0.35 \\ -1.06 & -0.13 \end{pmatrix}$, $\boldsymbol{W}^{10} = \begin{pmatrix} -0.28 & -0.16 \\ 0.47 & -0.36 \end{pmatrix}$, $\boldsymbol{W}^{50} = \begin{pmatrix} 0.01 & 0.00 \\ -0.01 & 0.01 \end{pmatrix}$

A solution: Attention

Attention Is All You Need

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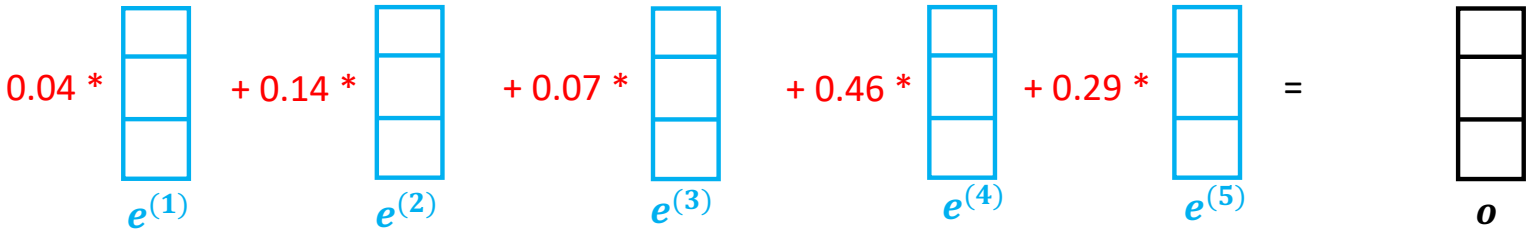
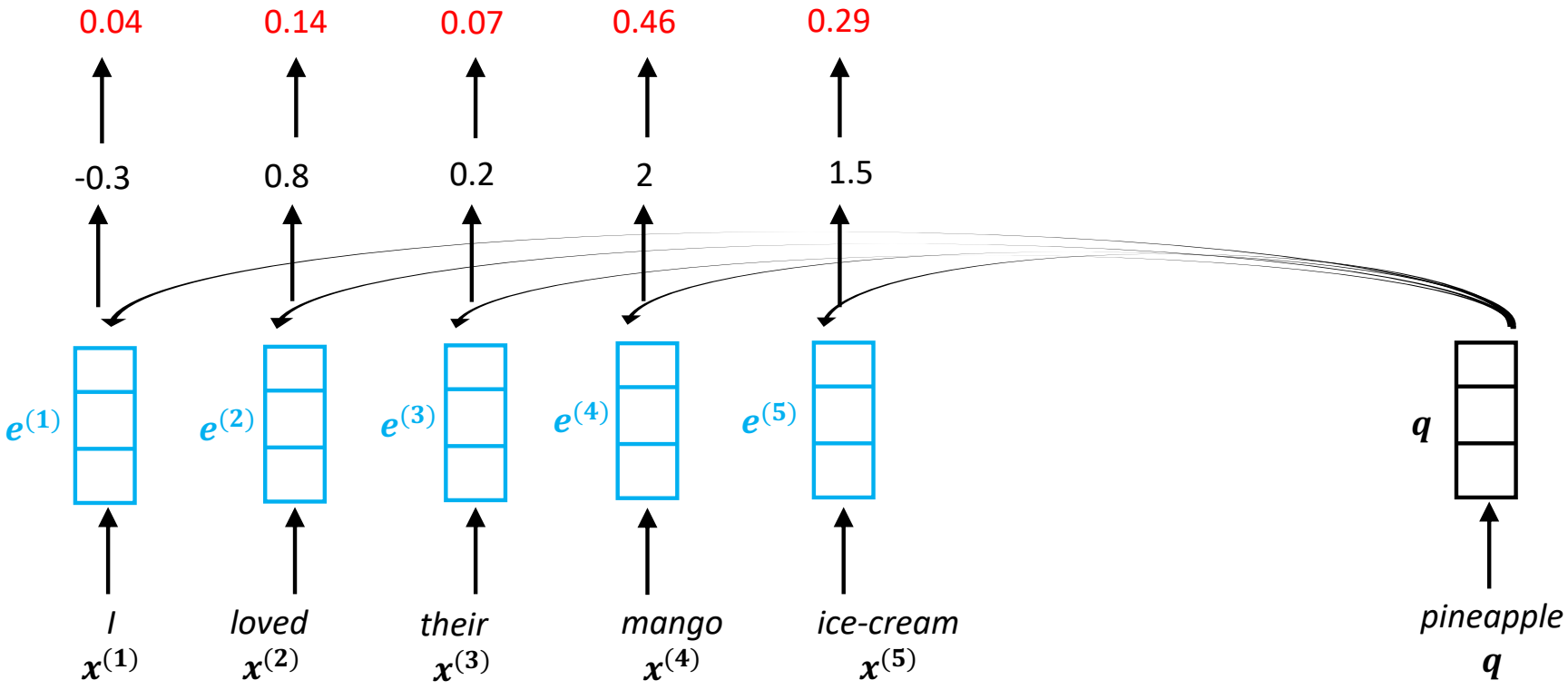
Abstract

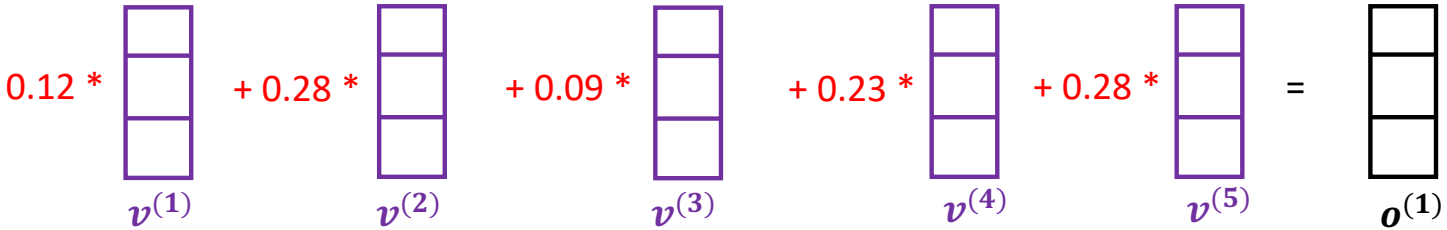
The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.0 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature.

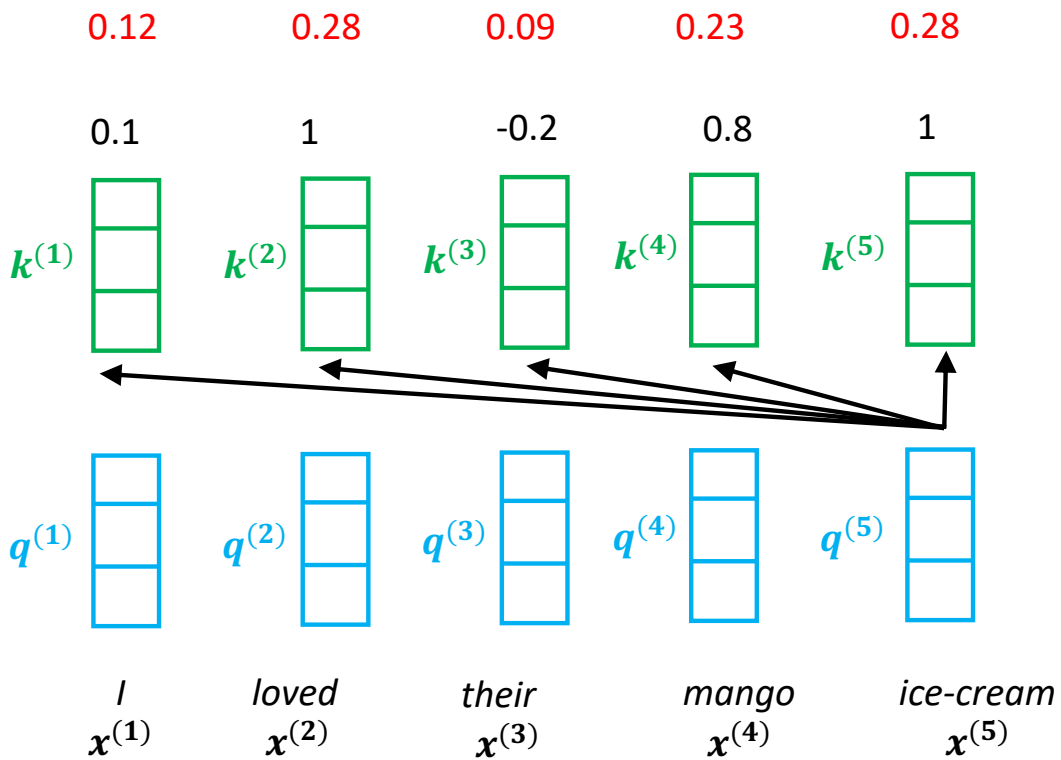
Attention: Weighted averaging





Self-attention





Self-attention in matrix form

1. Transform each word embedding with weight matrices $\boldsymbol{Q}$, $\boldsymbol{K}$, $\boldsymbol{V}$, each in $\mathbb{R}^{d \times d}$

$$\begin{aligned} \boldsymbol{q}_i &= \boldsymbol{Q}\boldsymbol{x}_i \quad \text{(queries)} \\ \boldsymbol{k}_i &= \boldsymbol{K}\boldsymbol{x}_i \quad \text{(keys)} \\ \boldsymbol{v}_i &= \boldsymbol{V}\boldsymbol{x}_i \quad \text{(values)} \end{aligned}$$

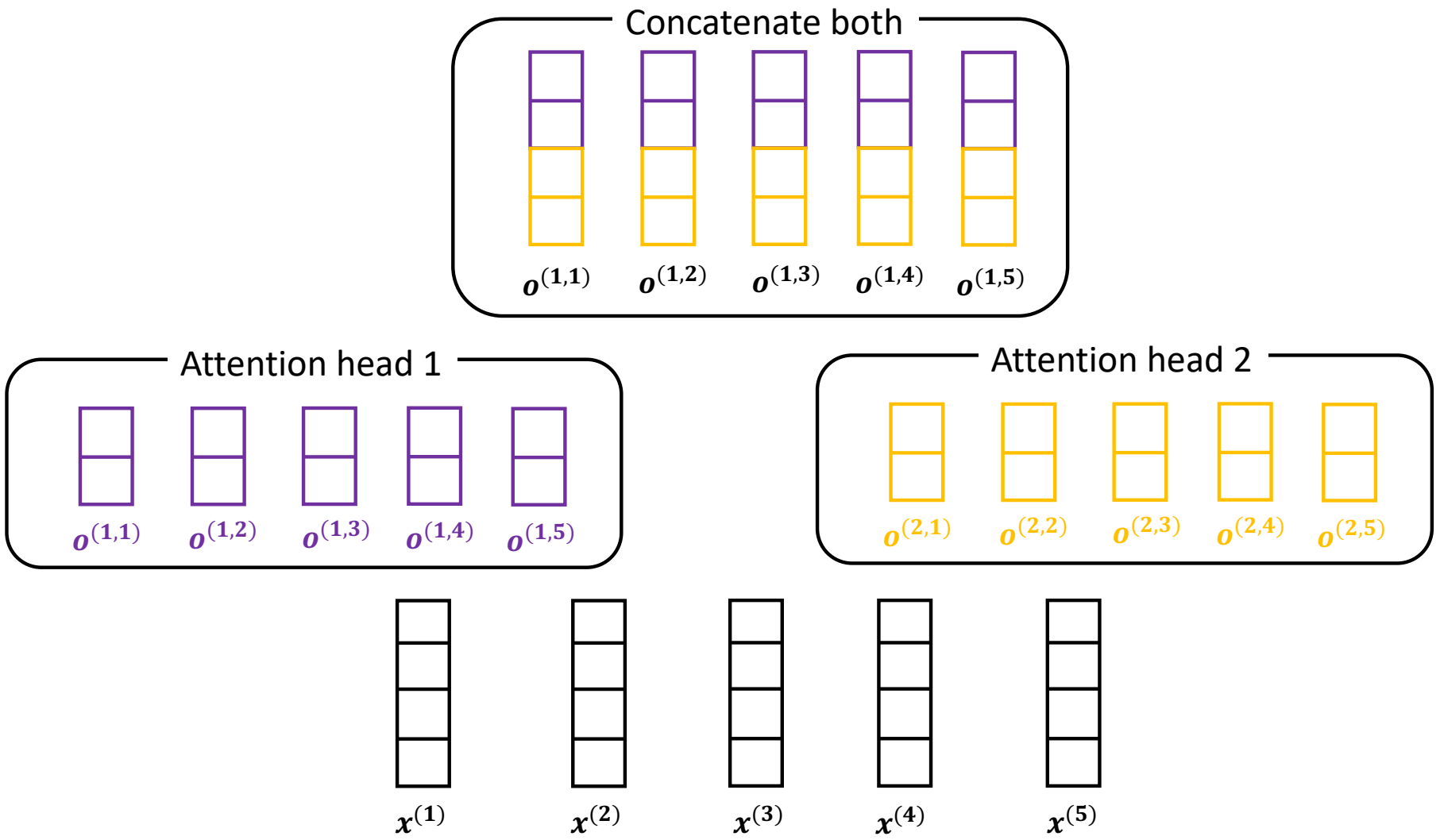
2. Compute pairwise similarities between keys and queries; normalize with softmax

$$\begin{aligned} \alpha_{ij} &= \boldsymbol{q}_i^\top \boldsymbol{k}_j \\ w_{ij} &= \frac{\exp(\alpha_{ij})}{\sum_{j'} \exp(\alpha_{ij'})} \end{aligned}$$

3. Compute output for each word as weighted sum of values

$$\boldsymbol{o}_i = \sum_j w_{ij} \boldsymbol{v}_j$$

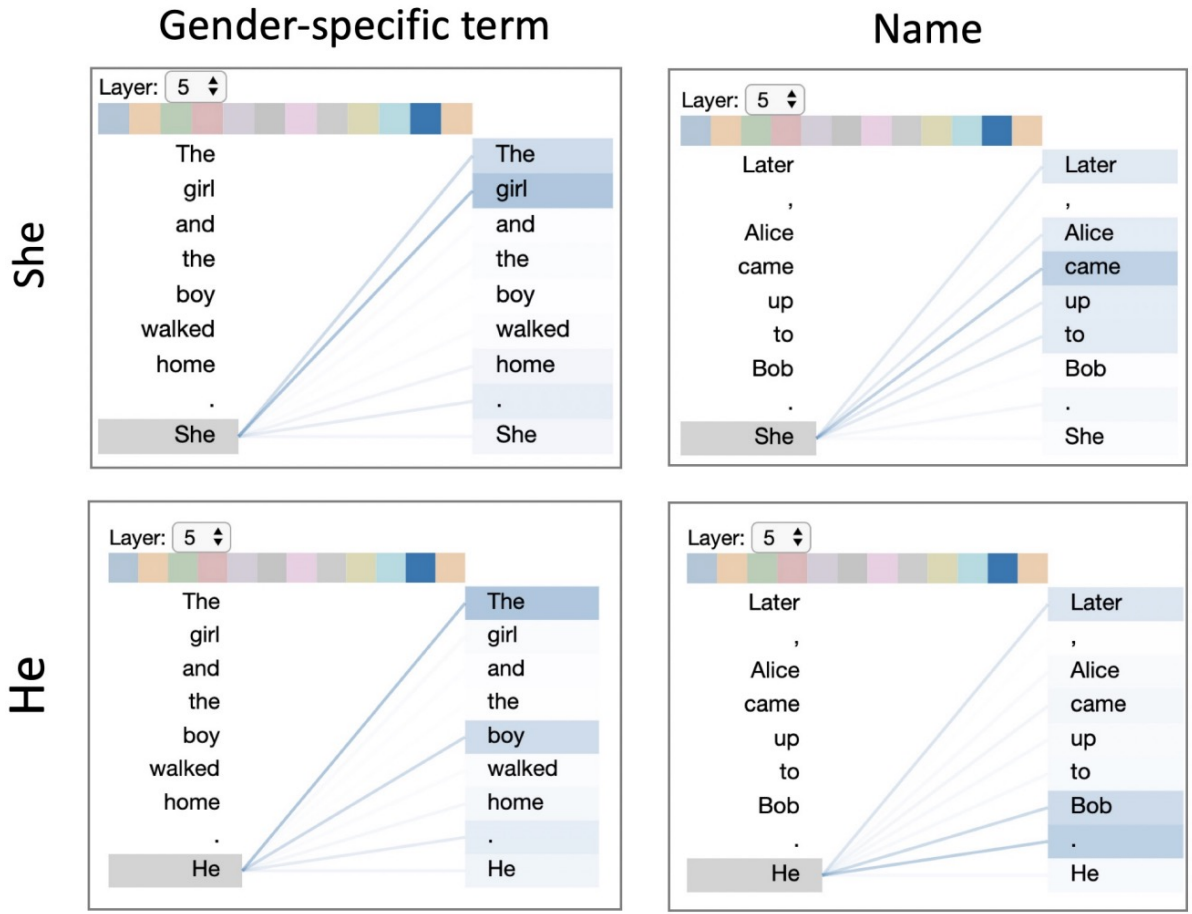
Multi headed self-attention



Multi headed self-attention

- Input: List of vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$, each of size d
- Output: List of vectors $\boldsymbol{h}_1, \ldots, \boldsymbol{h}_T$, each of size d
- Formula: For each head i:
  - Compute self attention output using $\boldsymbol{Q}_i$, $\boldsymbol{K}_i$, $\boldsymbol{V}_i$
  - Finally, concatenate results for all heads
- Parameters:
  - For each head i, parameter matrices $\boldsymbol{Q}_i$, $\boldsymbol{K}_i$, $\boldsymbol{V}_i$ of size $d_{\text{attn}} \times d$
  - # of heads n is hyperparameter, $d_{\text{attn}} = d/n$

What do attention heads learn?

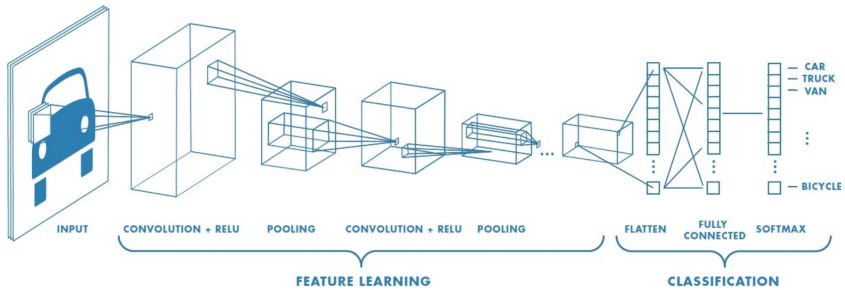


A Multiscale Visualization of Attention in the Transformer Model, Vig 2019

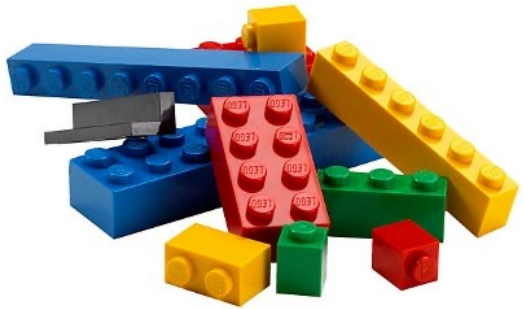
Transformers

Building a Transformer, stack things up!

To build a CNN, we stacked up convolution layers



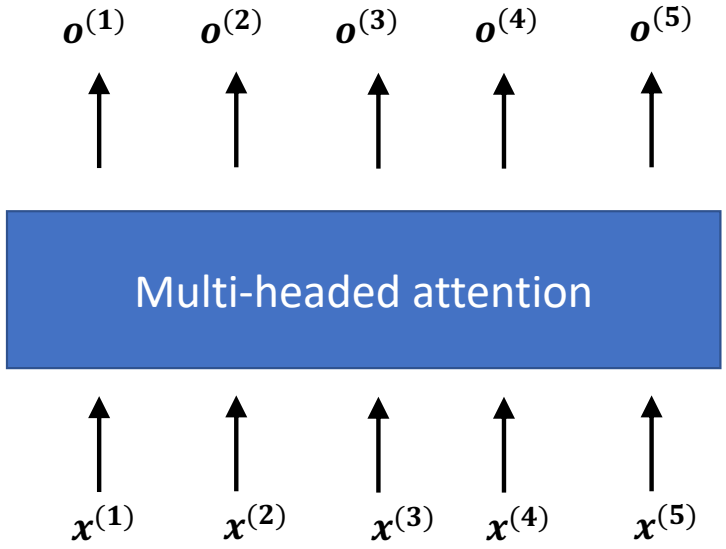
You should think of different components (convolution, non-linearities, pooling, attention, softmax etc.) as building block which can be composed to build a final model.



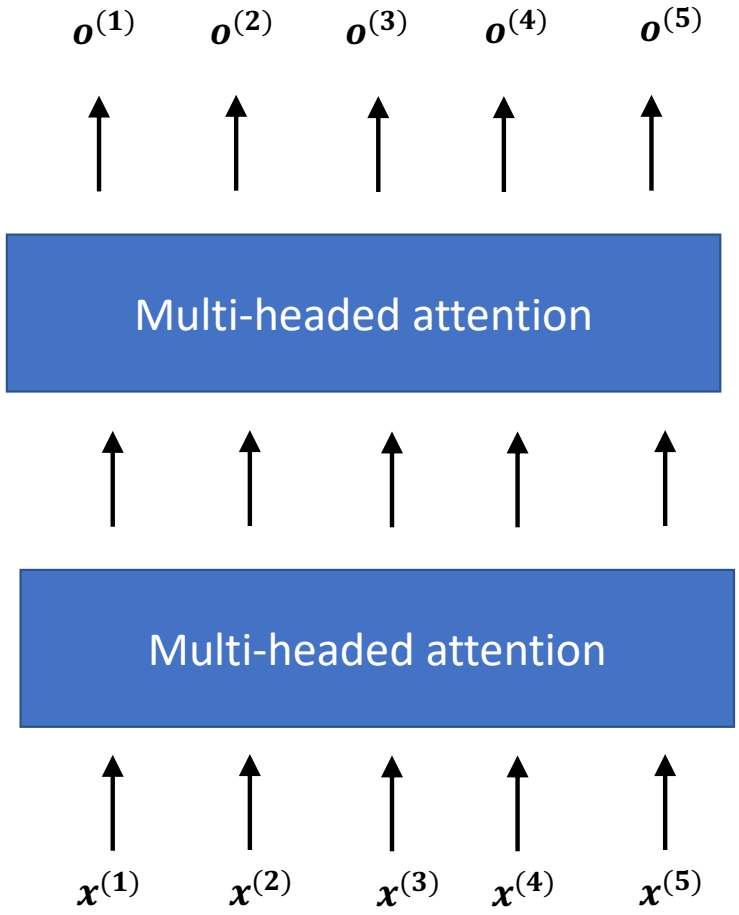
Building a Transformer, stack things up!

How should we stack different layers to build a Transformer?

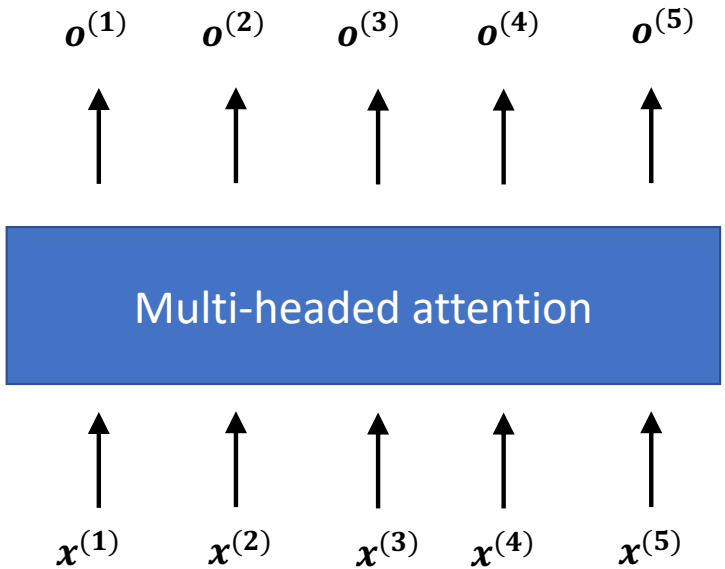
Key ingredient: Attention layers



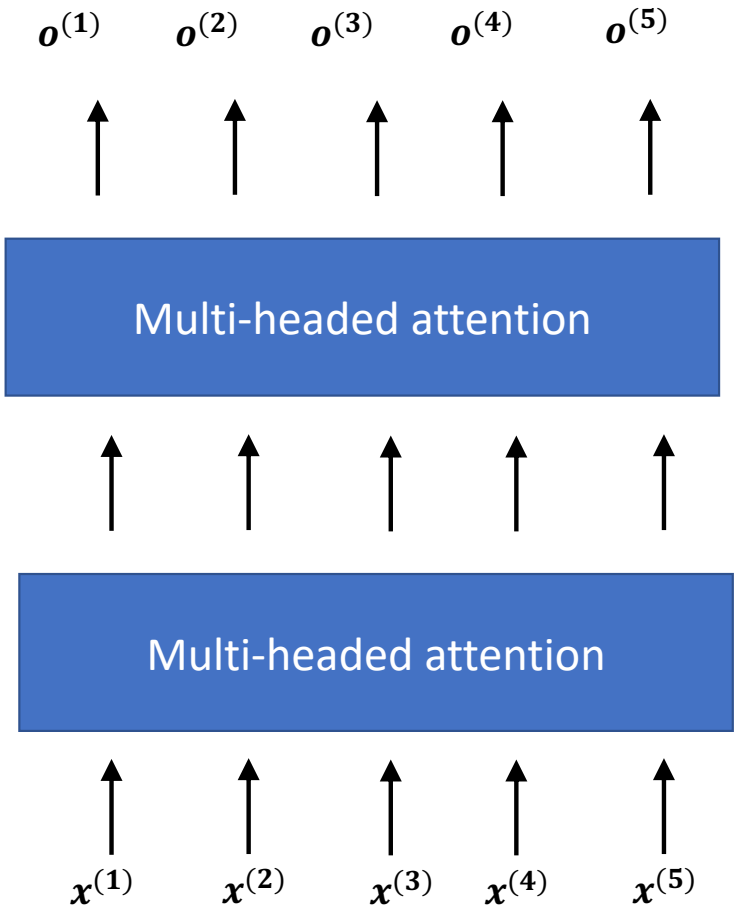
What if we just stack attention layers?



Issue: Multiple attention layers are still just averaging

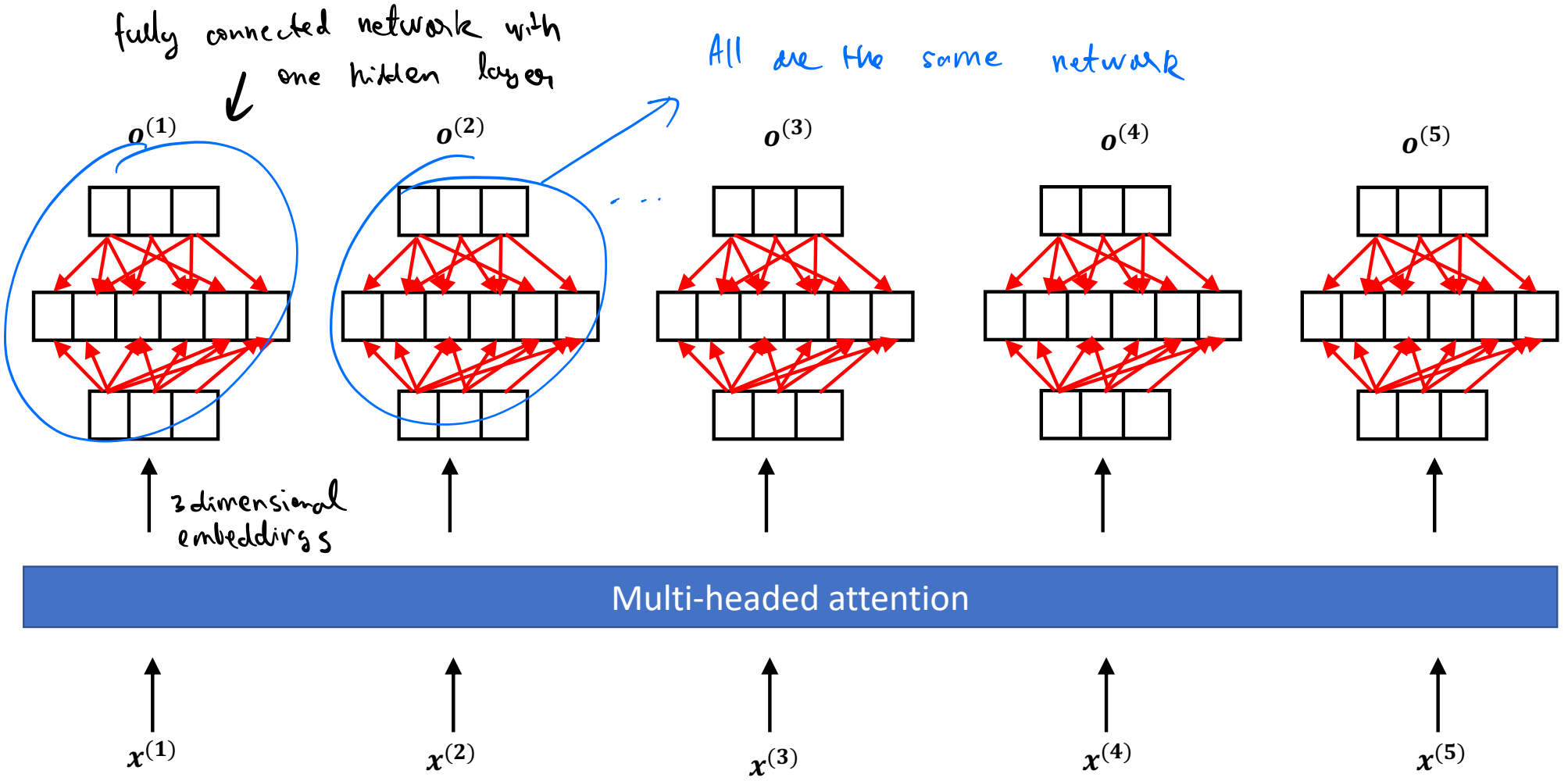


vs.

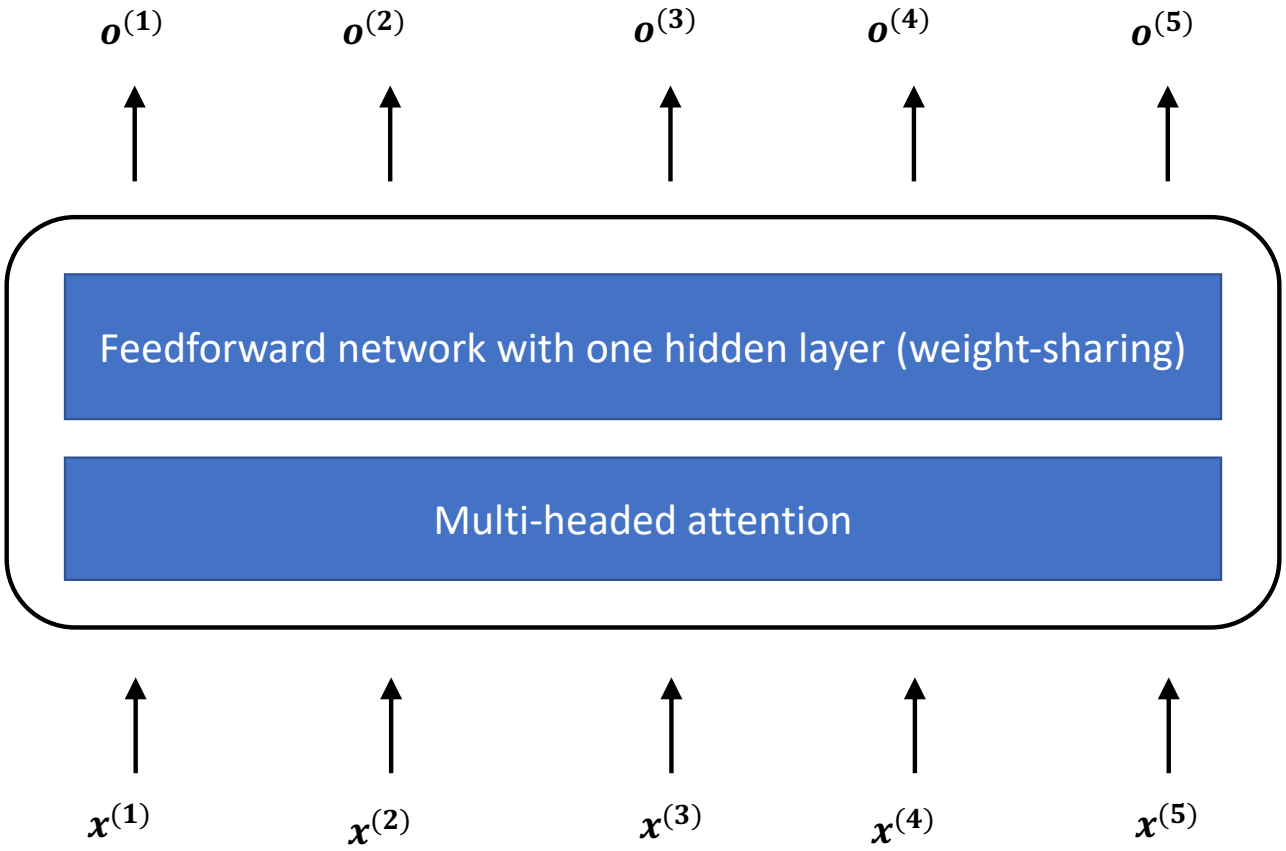


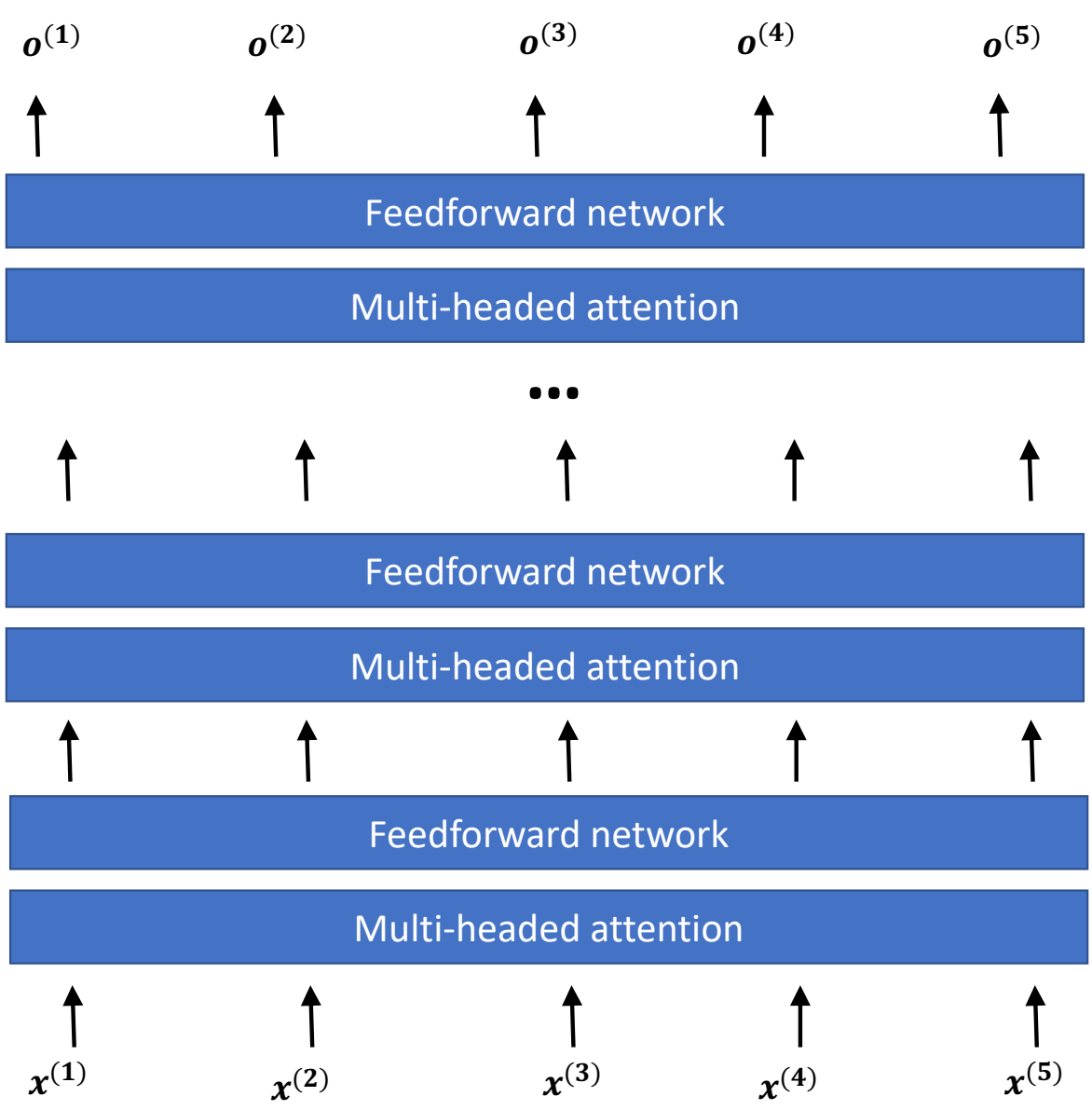
The final output in both cases is a weighted linear combination of value vectors.

Solution: add non-linearities ☺



Solution: add non-linearities ☺




$o^{(1)}$
$o^{(2)}$
$o^{(3)}$
$o^{(4)}$
$o^{(5)}$
Feedforward network
Multi-headed attention
...
Feedforward network
Multi-headed attention
Feedforward network
Multi-headed attention
$x^{(1)}$
$x^{(2)}$
$x^{(3)}$
$x^{(4)}$
$x^{(5)}$

Building a Transformer: Bells and whistles

- Positional embeddings
- Residual connections
- Layer normalization
- Scaled dot product attention
- Tokenization

Positional embeddings

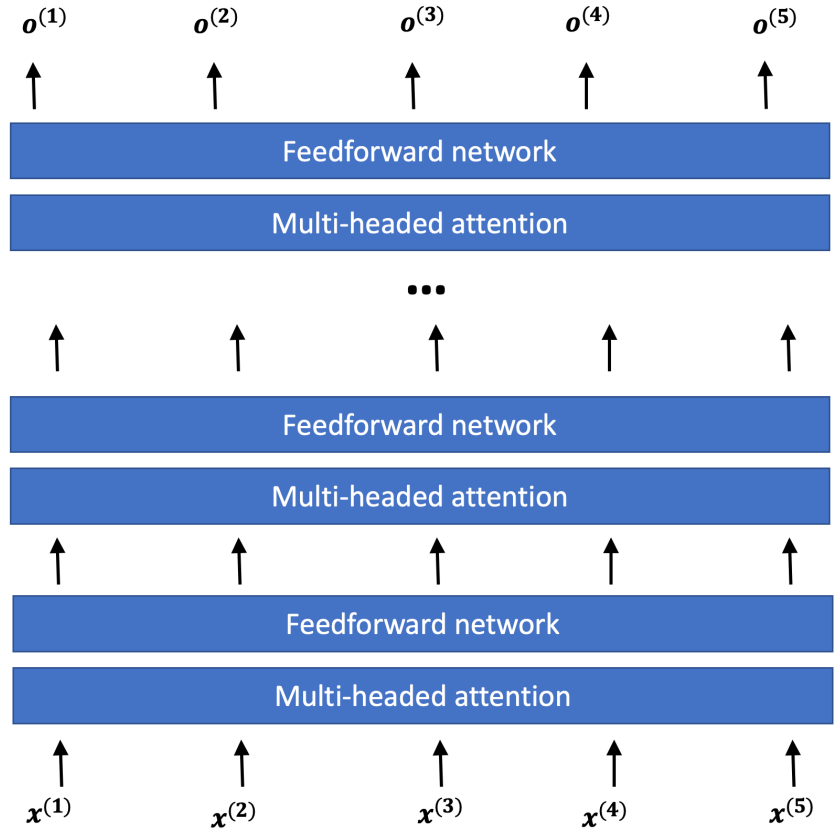
Issue with current architecture:
Embeddings do not take order into account

``Bob ate the salmon”
``The salmon ate Bob”

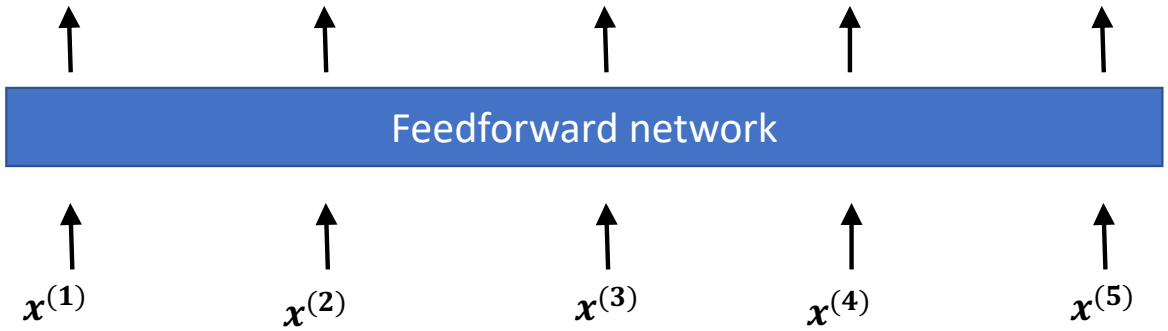
Lead to the same embedding for each word!

Fix: **positional embeddings**

- Learn different vector for each position
- Add this vector to word vector for that position



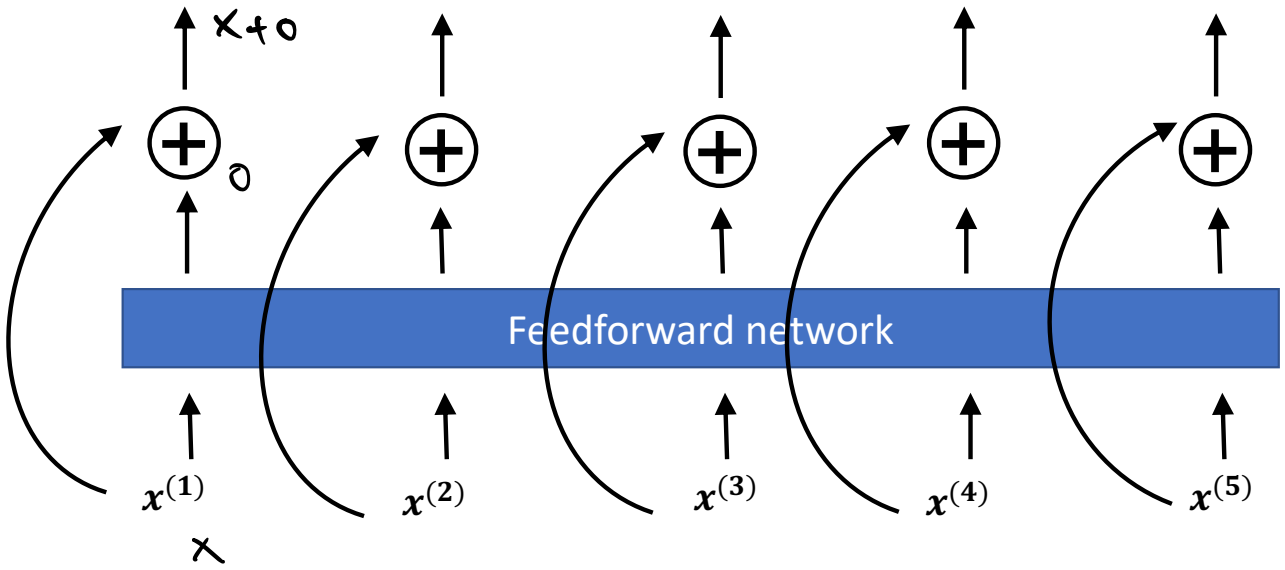
Residual connections



Each feedforward layer

- Takes as input $T \times d$ matrix X (T is number of tokens, d is dimensionality of embedding)
- Outputs $T \times d$ matrix O (T is number of tokens, d is dimensionality of embedding)

Residual connections



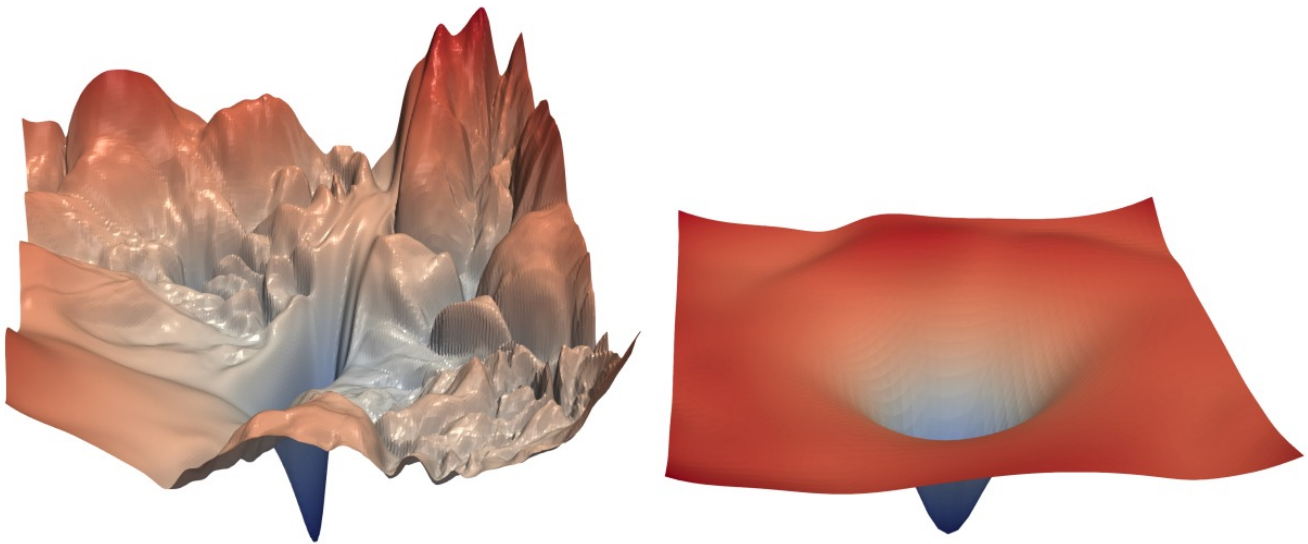
We add a **residual connection**: Output is now $X + O$

- Add together the input to the layer to its previous output
- The feedforward layer now only has to compute what O should be added to the input to have a useful embedding

Residual connections: Why do they help?

With residual connections:

- It makes it easier to copy information from before
- Helps in training deeper networks (avoids gradients from initial layers from becoming too small)
- Seems to make the optimization landscape better behaved



Without residual connections

With residual connections

Visualizing the Loss Landscape of Neural Nets, Li et al., 2018

Layer normalization

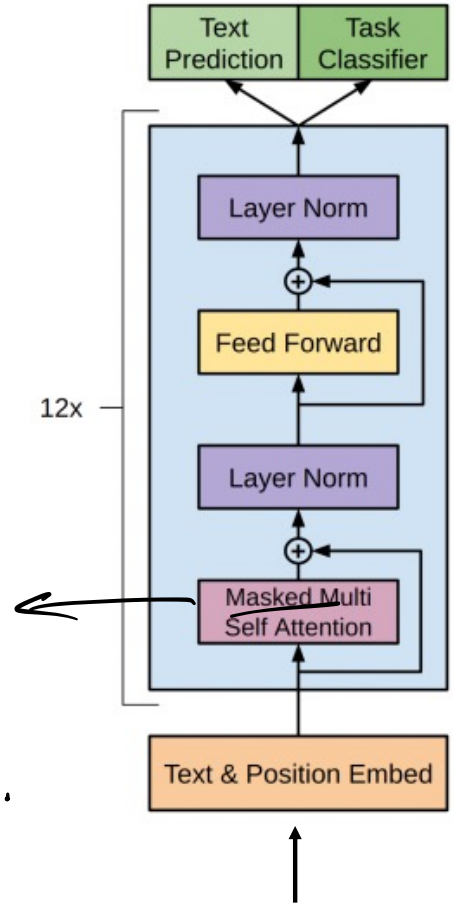
Given some input x

- Normalize x to have mean μ and variance σ

We add this **layer norm** operation in the Transformer blocks to make sure the values are not too large or too small.

Variations of this are also often used to train deep models (including non-Transformer architectures)

Putting things together: The Transformer architecture



"Masking" sets attention weights for future tokens to be 0.

Architecture of the GPT model (figure from GPT paper)

Lots of variants, and extensions to other kinds of data...

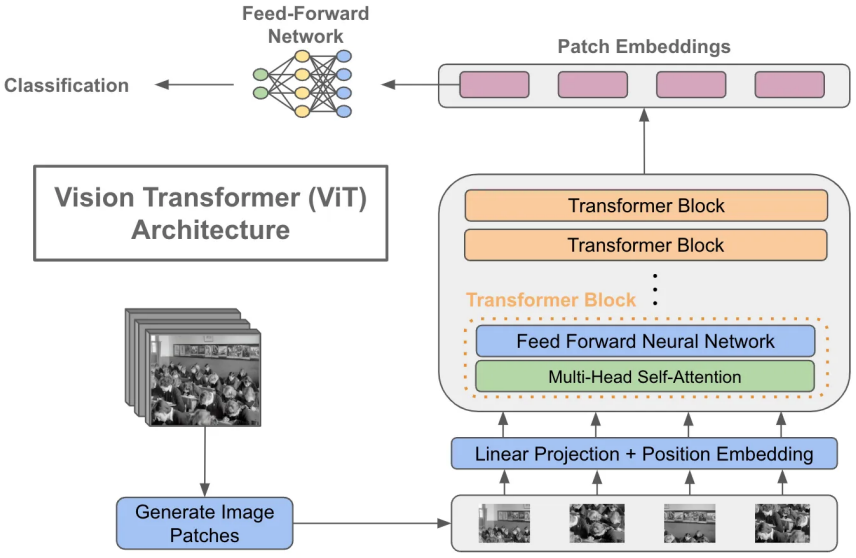
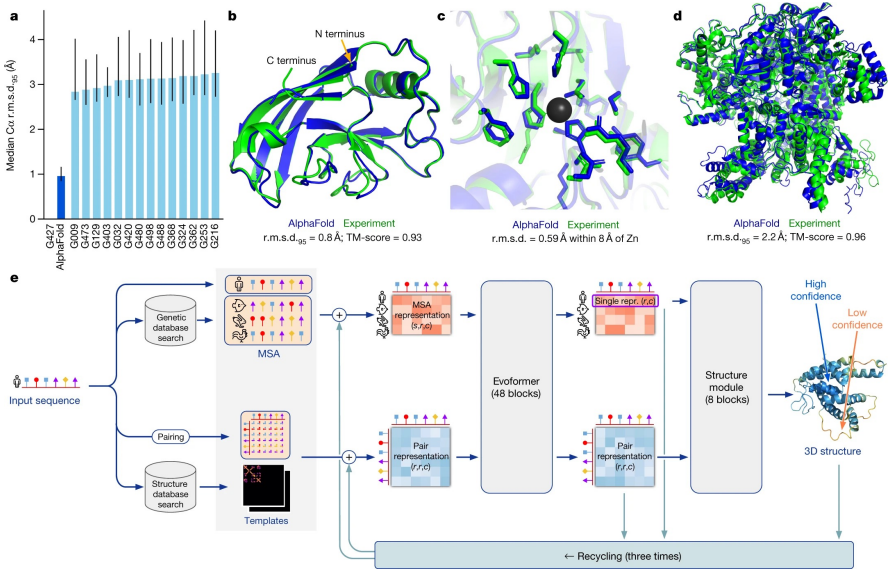


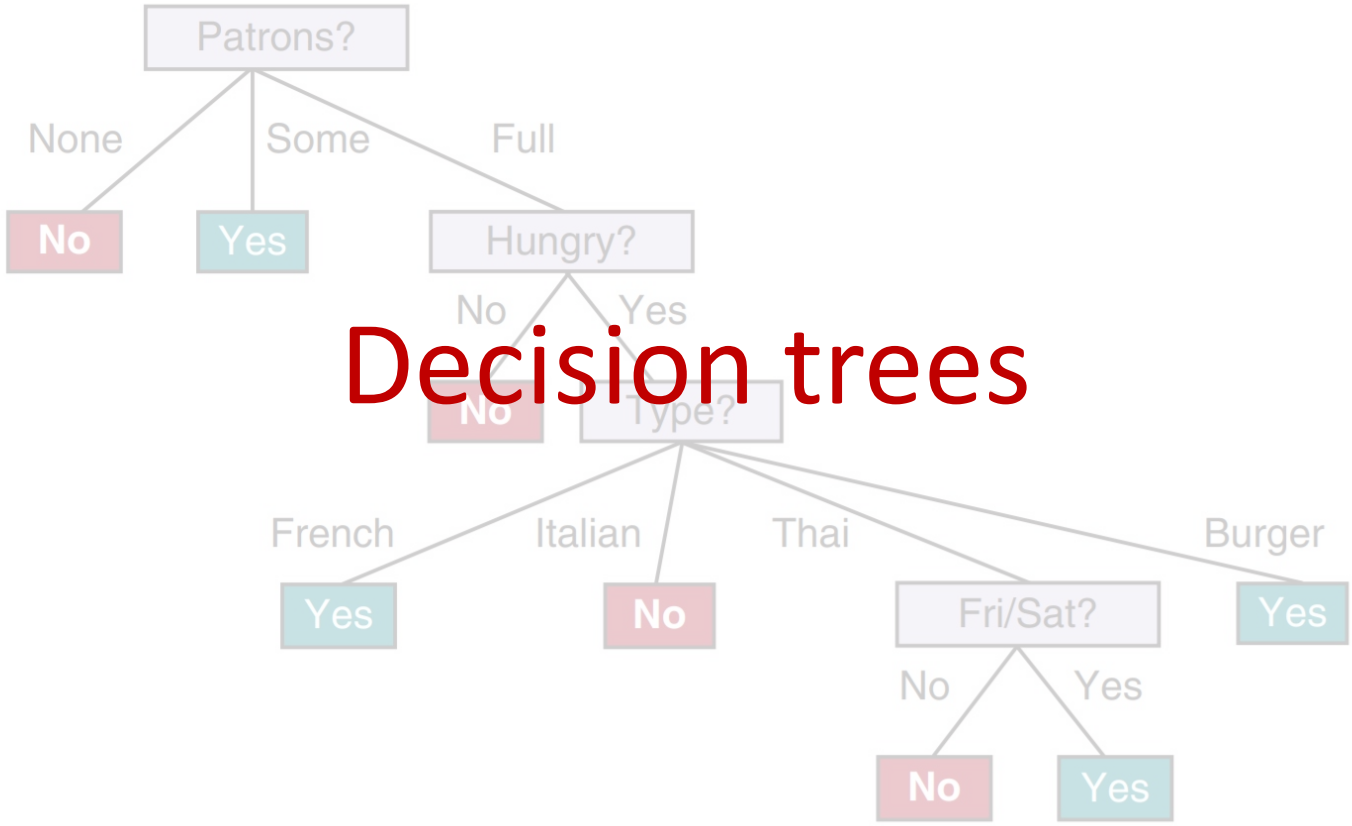
Image data



Protein structure prediction

Today's discussion will cover more about Transformers and Large Language Models (LLMs)

Decision trees



Decision trees

- Introduction & definition
- Learning the parameters
- Measures of uncertainty
- Recursively learning the tree & some variants

Decision trees

We have seen different ML models for classification/regression:

- linear models, nonlinear models induced by kernels, neural networks

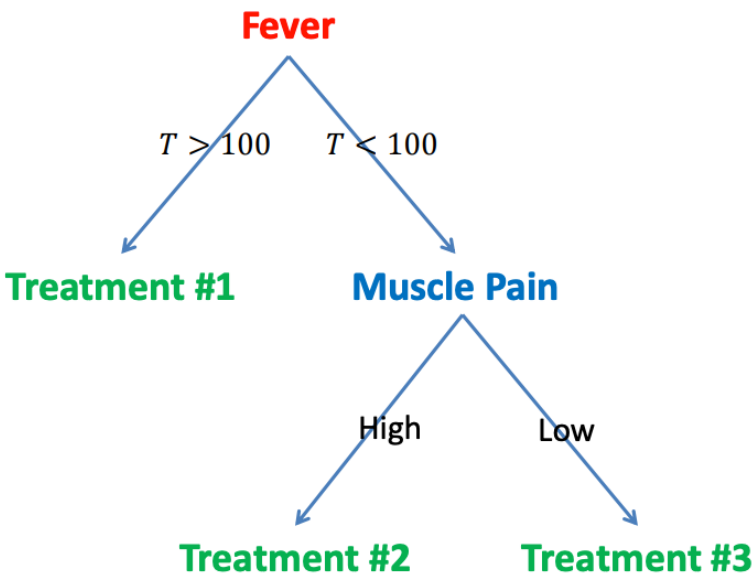
Decision tree is another popular one:

- nonlinear in general
- works for both classification and regression; we focus on classification
- one key advantage is good interpretability
- *ensembles* of trees are very effective

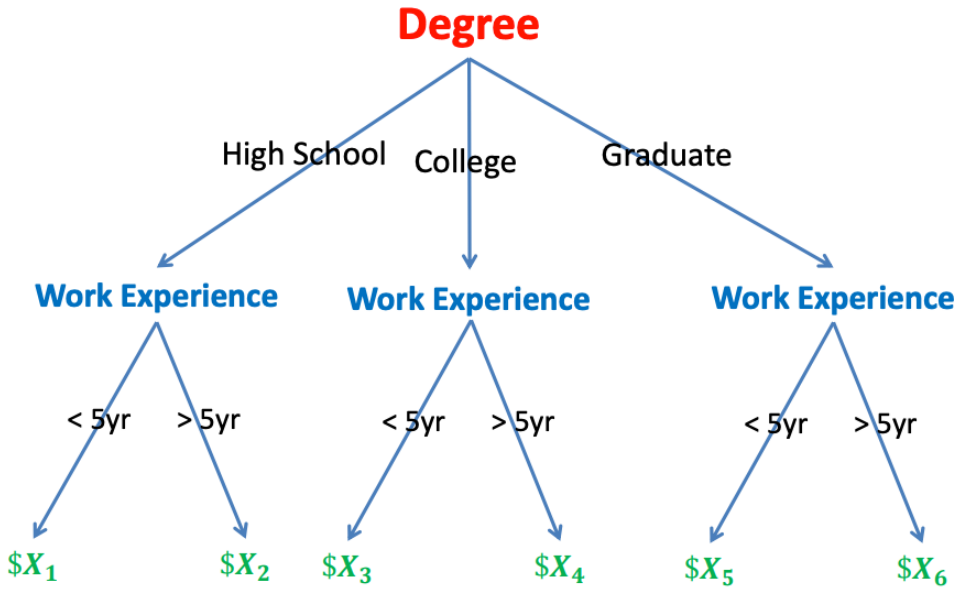
Example

Many decisions are made based on some tree structure

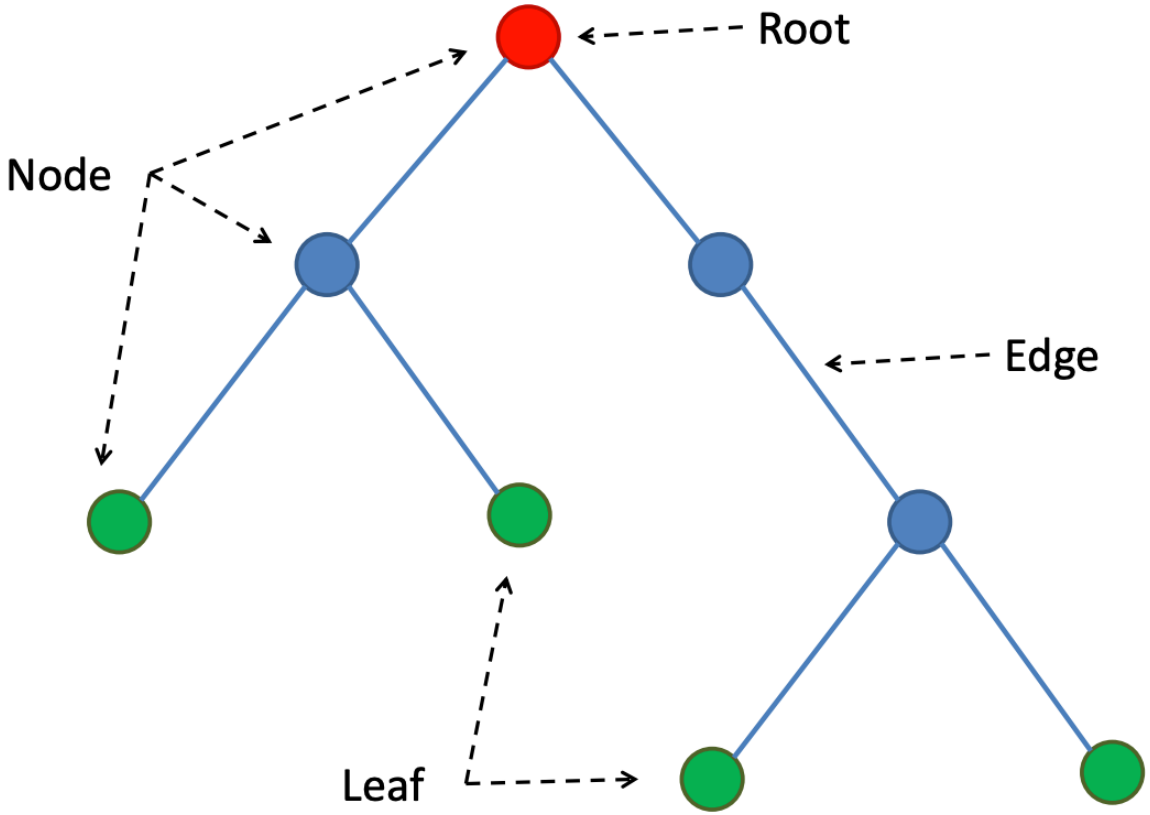
Medical treatment



Salary in a company



Tree terminology

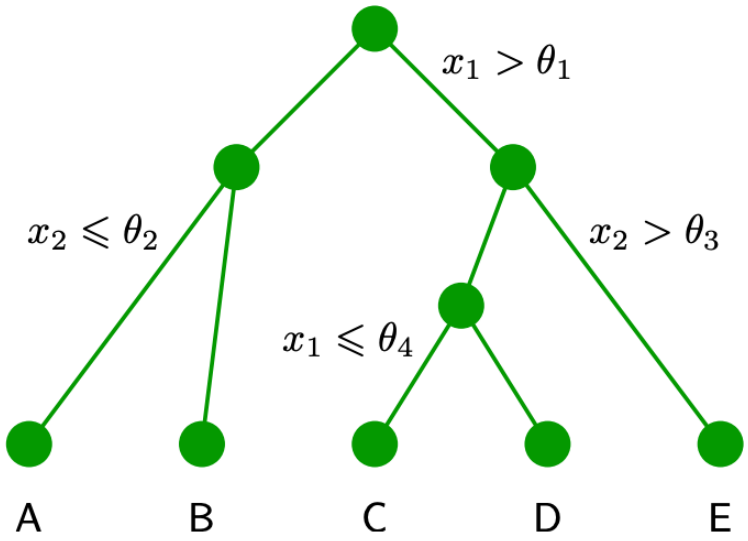


Tree terminology

Input: $\boldsymbol{x} = (x_1, x_2)$

Output: $f(\boldsymbol{x})$ determined naturally by traversing the tree

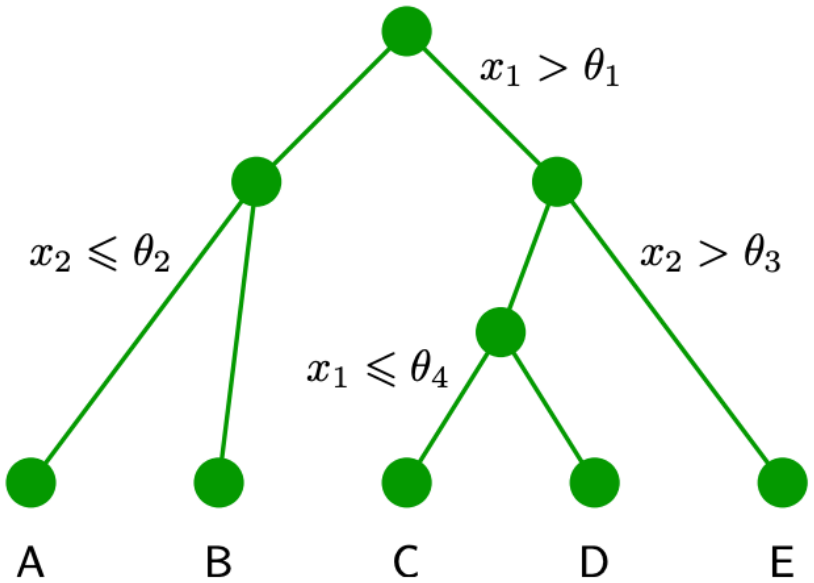
- start from the root
- test at each node to decide which child to visit next
- finally the leaf gives the prediction $f(\boldsymbol{x})$

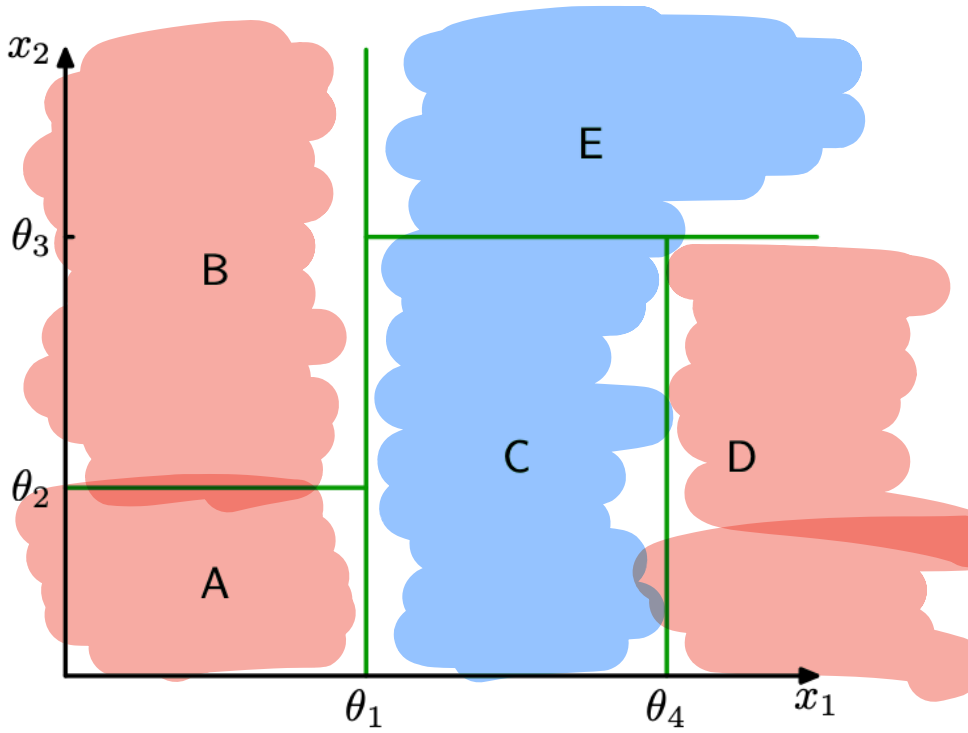


For example, $f((\theta_1 - 1, \theta_2 + 1)) = \mathsf{B}$

Complex to formally write down, but easy to represent pictorially or as code.

Decision boundary





if A, B, D : +ve label

C, E : -ve label

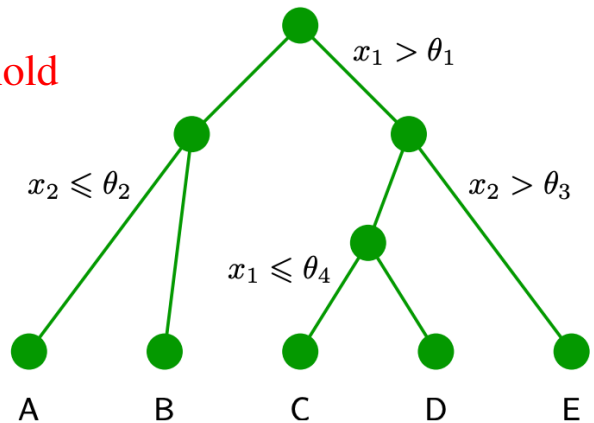
Parameters

Parameters to learn for a decision tree:

- The structure of the tree, such as the depth, #branches, #nodes, etc.
  Some of these are considered as hyperparameters. The structure of a tree is *not fixed in advance, but learned from data*.

- The test at each internal node:
  Which feature(s) to test on? If the feature is continuous, what threshold $(\theta_1, \theta_2, \ldots)$?

- The value/prediction of the leaves (A, B, ...)



Decision trees

- Introduction & definition
- Learning the parameters
- Measures of uncertainty
- Recursively learning the tree & some variants

Learning the parameters (optimization?)

So how do we *learn all these parameters?*

Empirical risk minimization (ERM): find the parameters that minimize some loss.

However, doing exact ERM *is too expensive for trees*.

- for T nodes, there are roughly $(\#\text{features})^T$ possible decision trees (need to decide which feature to use on each node).
- enumerating all these configurations to find the one that minimizes some loss is too computationally expensive.
- since most of the parameters are discrete (#branches, #nodes, feature at each node, etc.) *cannot really use gradient based approaches*.

e.g. can't really use gradient descent to decide which feature to split on at any node because of discontinuities

Instead, we turn to some **greedy top-down approach**.

A running example

Russell & Norvig, AIMA

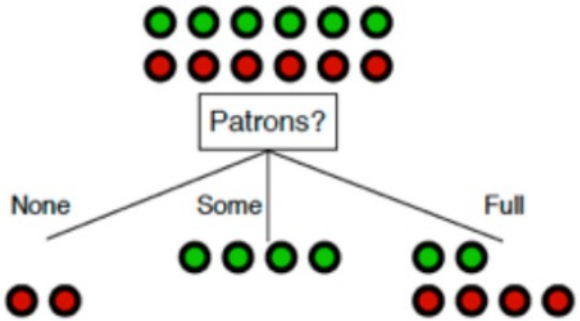
- predict whether a customer will wait to get a table at some restaurant
- 12 training examples
- 10 features (all discrete)

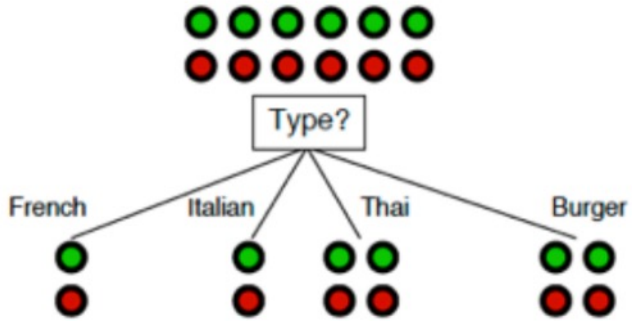
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

"Structured data": mix of categorical attributes, continuous attributes, which all have some meaning.

First step: How to build the root?

Which feature should we test at the root? Examples:





Which split is better?

- intuitively "patrons" is a better feature since it leads to "more certain" children
- how to quantify this intuition?

Decision trees

- Introduction & definition
- Learning the parameters
- Measures of uncertainty
- Recursively learning the tree & some variants

Measure of uncertainty of a node

The uncertainity of a node should be **a function of the distribution of the classes within the node**.

Example: a node with 2 positive and 4 negative examples can be summarized by a distribution P with $P(Y = +1) = 1/3$ and $P(Y = -1) = 2/3$

One classic measure of the uncertainity of a distribution is its *(Shannon) entropy*:

classes

$$H(P) = -\sum_{k=1}^{C} P(Y = k) \log P(Y = k)$$

Properties of entropy

$$H(P) = \mathbb{E}_{Y\sim P}\left[\log\left(\frac{1}{P(Y)}\right)\right]$$

this is a measure of how unlikely an outcome is

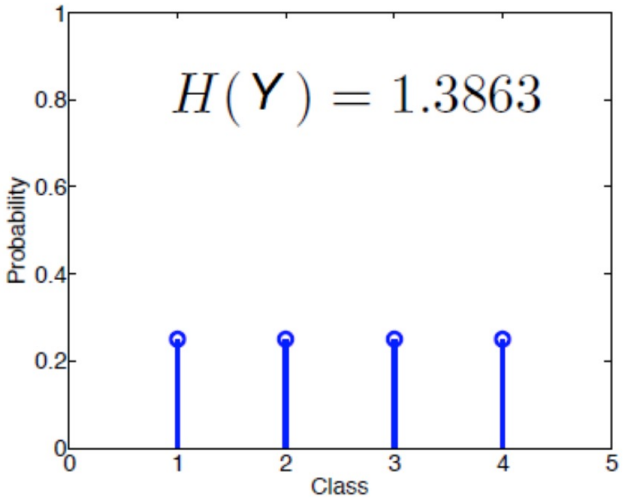
$$= \sum_{k=1}^{C} P(Y=k)\log\left(\frac{1}{P(Y=k)}\right)$$

this is average "unlikeliness" when we sample outcomes from P

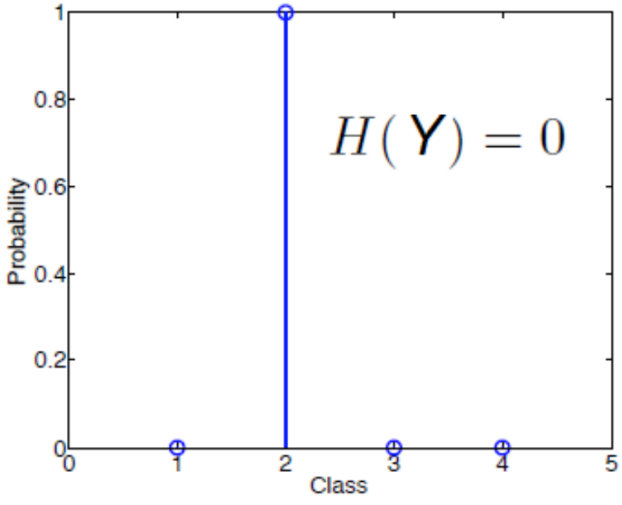
$$= -\sum_{k=1}^{C} P(Y=k)\log P(Y=k)$$

- the base of log can be 2, e or 10
- always non-negative
- it's the *smallest codeword length to encode symbols drawn from P*
- maximized if P is uniform (max = ln C): most uncertain case
- minimized if P focuses on one class (min = 0): most certain case
  - e.g. $P = (1, 0, \ldots, 0)$
  - $0 \log 0$ is defined naturally as $\lim_{z\to 0+} z \log z = 0$

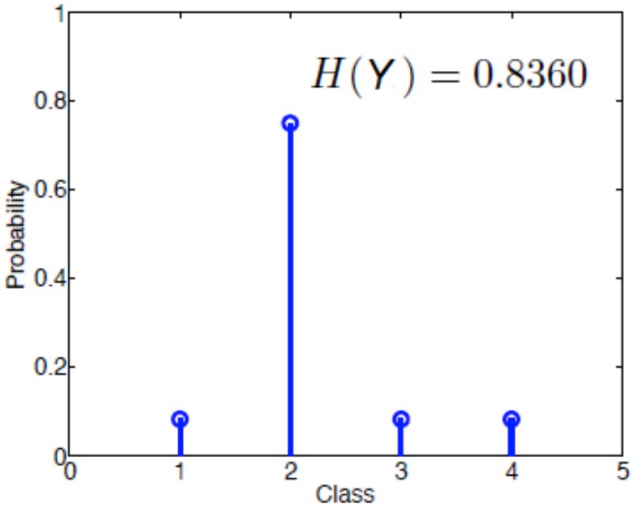
Examples of computing entropy



most uncertain



most certain



Examples of computing entropy

Entropy in each child if root tests on "patrons"

For "None" branch

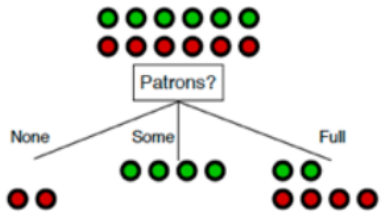
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

For "Some" branch

$$-\left(\frac{4}{4+0}\log\frac{4}{4+0}+\frac{0}{4+0}\log\frac{0}{4+0}\right)=0$$

For "Full" branch

$$-\left(\frac{2}{2+4}\log\frac{2}{2+4}+\frac{4}{2+4}\log\frac{4}{2+4}\right)\approx 0.9$$



So how good is choosing "patrons" overall?

Very naturally, we take the weighted average of entropy:

$$\frac{2}{12}\times 0+\frac{4}{12}\times 0+\frac{6}{12}\times 0.9=0.45$$

Measure of uncertainty of a split

Suppose we split based on a discrete feature A, the uncertainty can be measured by the **conditional entropy**:

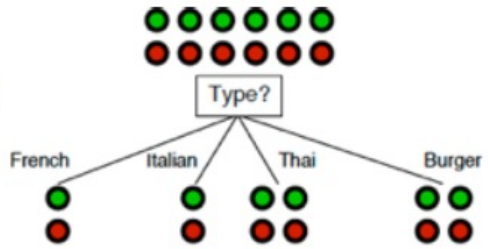
$$
\begin{aligned}
& H(Y \mid A) \\
&= \sum_a P(A=a) H(Y \mid A=a) \\
&= \sum_a P(A=a) \left(-\sum_{k=1}^{\mathsf{C}} P(Y \mid A=a) \log P(Y \mid A=a) \right) \\
&= \sum_a \text{“fraction of examples at node } A=a\text{”} \times \text{“entropy at node } A=a\text{”}
\end{aligned}
$$

Pick the feature that leads to the smallest conditional entropy.

Deciding the root

For "French" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$



For "Italian" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$

For "Thai" and "Burger" branches

$$-\left(\frac{2}{2+2}\log\frac{2}{2+2}+\frac{2}{2+2}\log\frac{2}{2+2}\right)=1$$

The conditional entropy is $\frac{2}{12}\times 1+\frac{2}{12}\times 1+\frac{4}{12}\times 1+\frac{4}{12}\times 1=1>0.45$

So splitting with "patrons" is better than splitting with "type".

In fact by similar calculation "patrons" is the best split among all features.

We are now done with building the root (this is also called a **stump**).

a decision tree with only a root

Decision trees

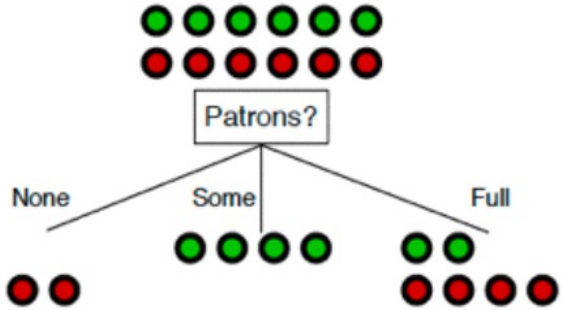
- Introduction & definition
- Learning the parameters
- Measures of uncertainty
- Recursively learning the tree & some variants

Repeat recursively

Split each child in the same way.

- but no need to split children "none" and "some": they are pure already and will be our leaves

- for "full", repeat, focusing on those 6 examples:



	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
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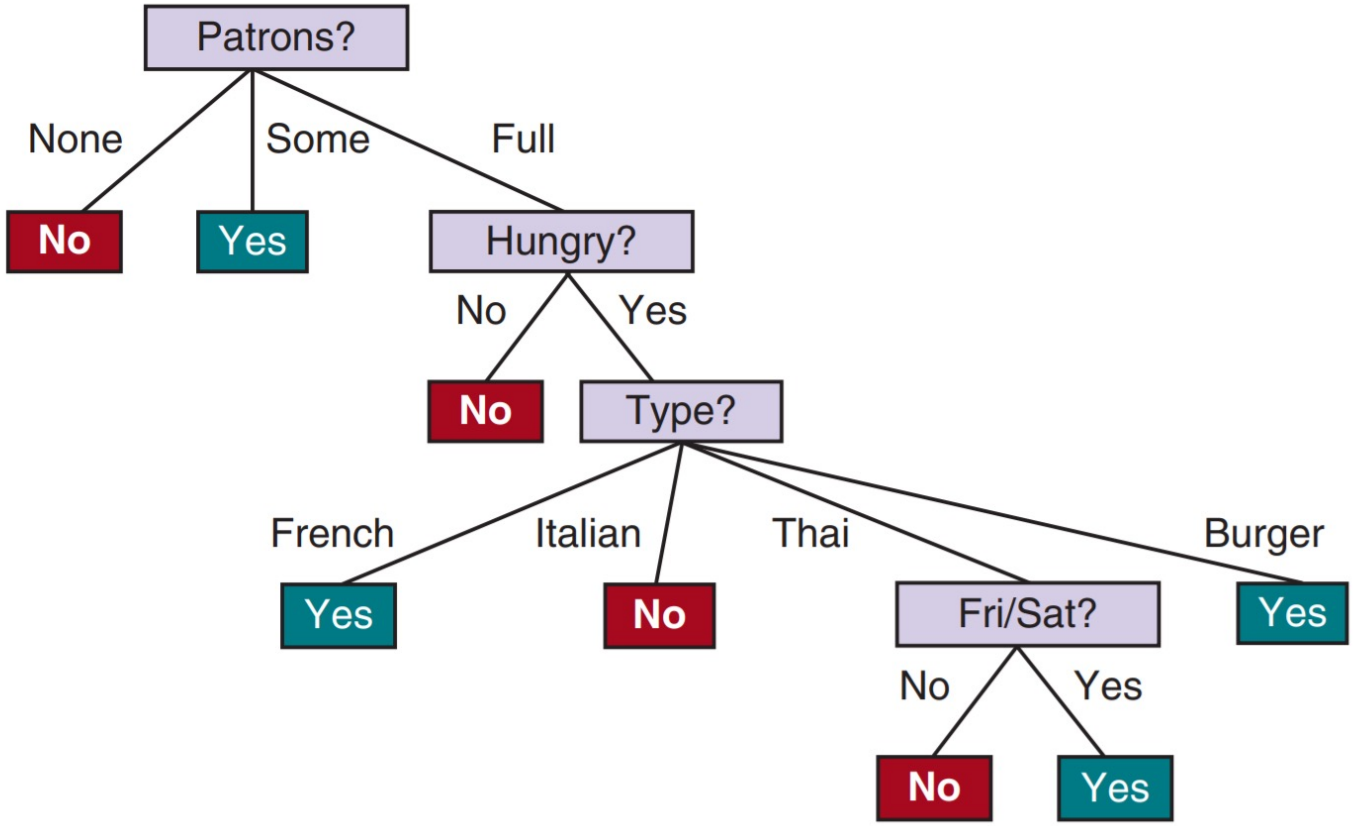
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

Repeat recursively



Putting it together

DecisionTreeLearning(Examples)

- if Examples have the same class, return a leaf with this class
- else if Examples is empty, return a leaf with majority class of parent
- else

    find the best feature A to split (e.g. based on conditional entropy)

    Tree $\leftarrow$ a root with test on A

    For each value a of A:

        Child $\leftarrow$ **DecisionTreeLearning**(Examples with $A = a$)
        add **Child** to **Tree** as a new branch

- return **Tree**

Variants

Popular decision tree algorithms (e.g. C4.5, CART, etc) are all based on this framework.

Variants:

- replace entropy by **Gini impurity**:

$$G(P) = \sum_{k=1}^{C} P(Y = k)(1 - P(Y = k))$$

pick example at random

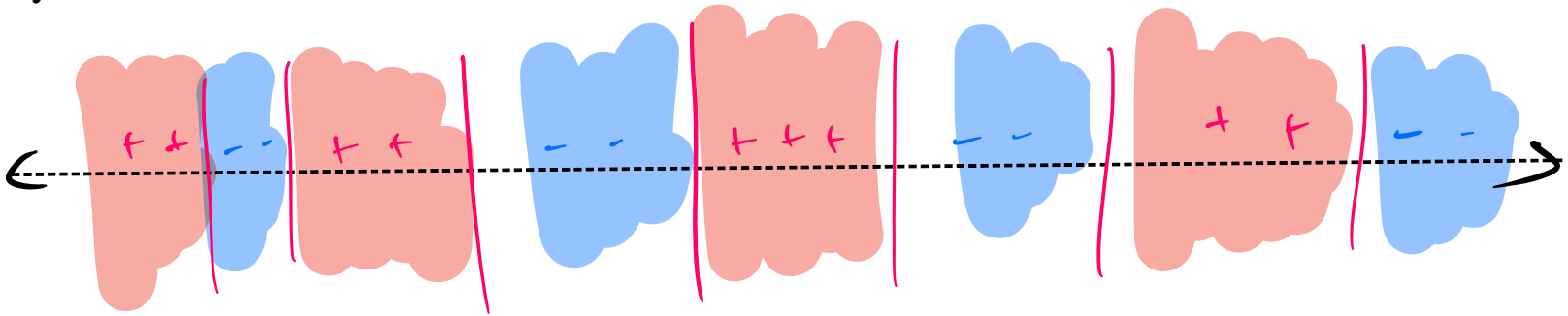
Prob. of the example being misclassified if predict label based on another randomly chosen example

meaning: *how often a randomly chosen example would be incorrectly classified if we predict according to another randomly picked example*

- if a feature is continuous, we need to find a threshold that leads to minimum conditional entropy or Gini impurity. *Think about how to do it efficiently.*

Regularization

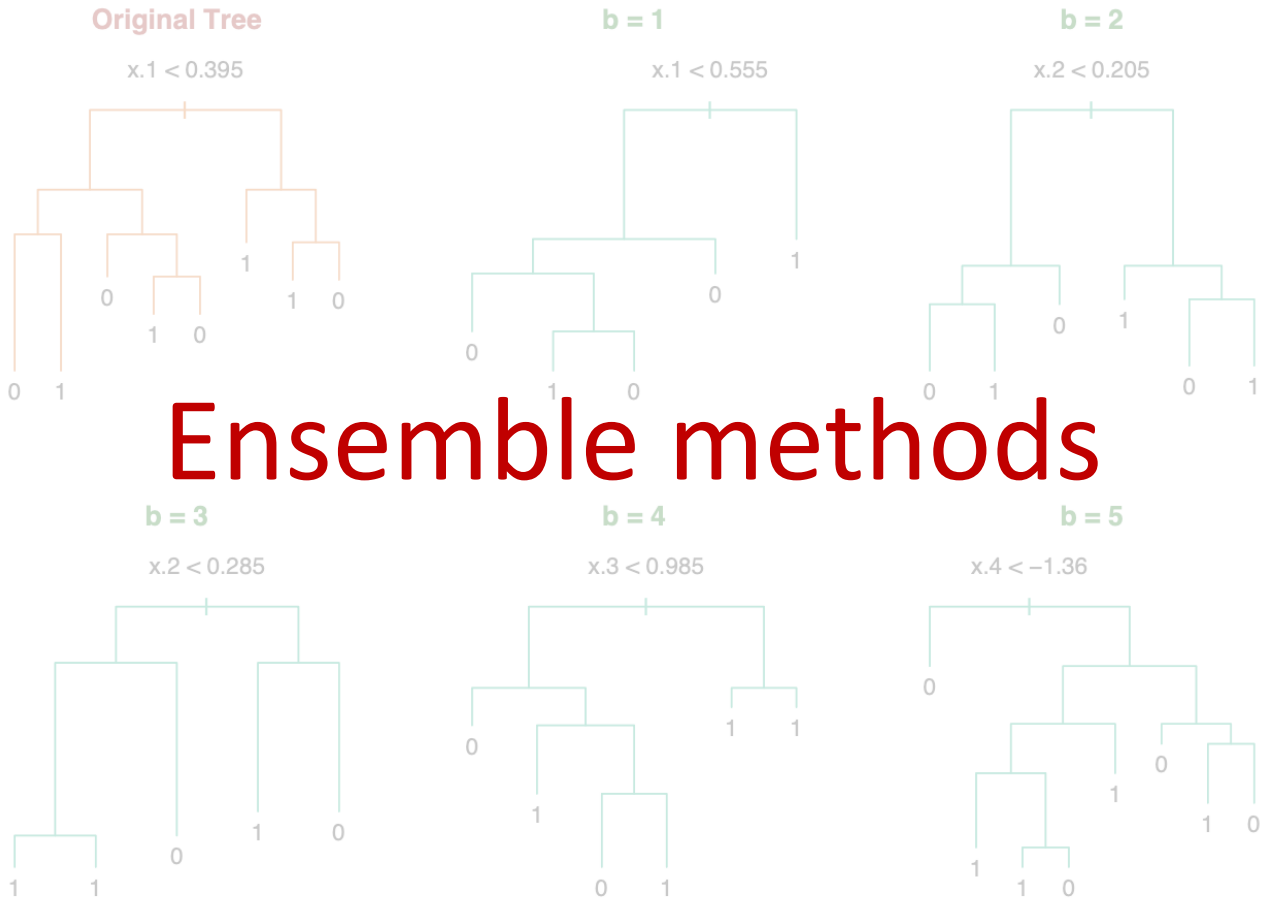
If the dataset has no contradiction (i.e. same $\boldsymbol{x}$ but different y), the training error of our decision tree algorithm is always zero, and hence the model can overfit.



To prevent overfitting:

- restrict the depth or #nodes (e.g. stop building the tree when the depth reaches some threshold).
- do not split a node if the #examples at the node is smaller than some threshold.
- other approaches as well, all make use of a validation set to tune these hyperparameters

You'll explore this in HW4.



Ensemble methods

Acknowledgement

We borrow some of the content from Stanford's CS229 slides on Ensemble Methods, by Nandita Bhaskhar:

https://cs229.stanford.edu/lectures-spring2022/cs229-boosting_slides.pdf

Ensemble methods

- Bagging
- Random forests
- Boosting: Basics
- Adaboost
- Gradient boosting

Decision Trees Recap

Pros

- Can handle large datasets
- Can handle mixed predictors (continuous, discrete, qualitative)
- Can ignore redundant variables
- Can easily handle missing data
- Easy to interpret if small

Cons

- Prediction performance is often poor (because it does not generalize well)
- Large trees are hard to interpret

Ensemble Methods for Decision Trees

Key idea: Combine multiple classifiers to form a learner with better performance than any of them individually ("wisdom of the crowd")

Issue: A single decision tree is very unstable, small variations in the data can lead to very different trees (since differences can propagate along the hierarchy).

They are *high variance models*, which can overfit.

↳ a model whose predictions are sensitive to changes in data.

But they have many advantages (e.g. very fast, robust to data variations).

Q: How can we lower the variance?

A: Let's learn multiple trees!

How to ensure they don't all just learn the same thing??

Ensemble methods are quite powerful

Why do tree-based models still outperform deep learning on tabular data?

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Abstract

While deep learning has enabled tremendous progress on text and image datasets, its superiority on tabular data is not clear. We contribute extensive benchmarks of standard and novel deep learning methods as well as tree-based models such as XGBoost and Random Forests, across a large number of datasets and hyperparameter combinations. We define a standard set of 45 datasets from varied domains with clear characteristics of tabular data and a benchmarking methodology accounting for both fitting models and finding good hyperparameters. Results show that tree-based models remain state-of-the-art on medium-sized data (~10K samples) even without accounting for their superior speed. To understand this gap, we conduct an empirical investigation into the differing inductive biases of tree-based models and Neural Networks (NNs). This leads to a series of challenges which should guide researchers aiming to build tabular-specific NNs: **1.** be robust to uninformative features, **2.** preserve the orientation of the data, and **3.** be able to easily learn irregular functions. To stimulate research on tabular architectures, we contribute a standard benchmark and raw data for baselines: every point of a 20 000 compute hours hyperparameter search for each learner.

Bagging

Bagging (Breiman, 1996)
Bootstrap **Agg**regat**ing**: lowers variance

Ingredients:
Bootstrap sampling: get different splits/subsets of the data
Aggregating: by averaging

Procedure:
→ Get multiple random splits/subsets of the data
→ Train a given procedure (e.g. decision tree) on each subset
→ Average the predictions of all trees to make predictions on test data

Leads to estimations with reduced variance.

Bagging

Collect T subsets each of some fixed size (say m) by sampling with replacement from training data.

Let $f_t(\boldsymbol{x})$ be the classifier (such as a decision tree) obtained by training on the subset $t \in \{1, \ldots, T\}$. Then the aggregrated classifier $f_{agg}(\boldsymbol{x})$ is given by:

$$f_{agg}(\boldsymbol{x}) = \begin{cases} \frac{1}{T}\sum_{t=1}^{T} f_t(\boldsymbol{x}) & \text{for regression,} \\ \text{sign}\left(\frac{1}{T}\sum_{t=1}^{T} f_t(\boldsymbol{x})\right) = \text{Majority Vote}\{f_t(\boldsymbol{x})\}_{t=1}^{T} & \text{for classification.} \end{cases}$$

Why majority vote? "Wisdom of the crowd"

± 1 valued (binary classification)

Bagging

Why majority vote? "Wisdom of the crowd"

Suppose I ask each of you: "Will the stock market go up tomorrow?"
Suppose each of you has a 60% chance of being correct, and all of you make **independent predictions (probability of any 1 person being correct is independent of probability of any one else being correct).**

What is Probability(Majority vote of 100 people being correct)?

Let BinCDF(k, n, p) be the CDF at value k of the Binomial distribution corresponding to n trials and each trial having probability p of success

BinCDF(k,n,p): If flip n coins, each of which is heads w.p. p, what is probability that # heads ≤ k?

Probability(Majority vote of 100 people being correct) = 1 – BinCDF(50,100,0.6)
≈ 0.97

Prob(≤ 50 predictions being correct)

Bagging: example

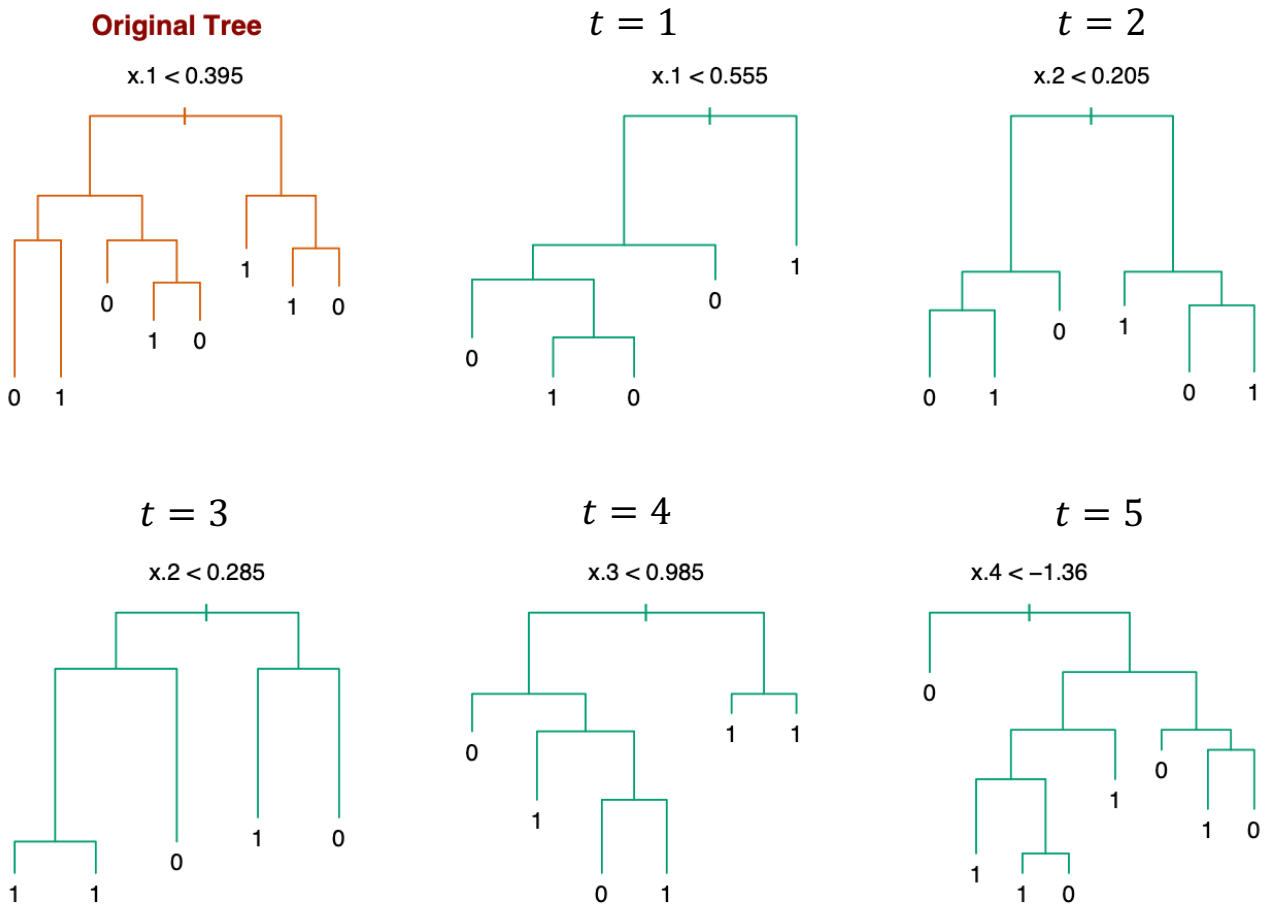

Figure from ESL

Bagging: summary

- Reduces overfitting (i.e., variance)
- Can work with any type of classifier (here focus on trees)
- Easy to parallelize (can train multiple trees in parallel)
- But loses on interpretability to single decision tree (true for all ensemble methods..)

Ensemble methods

- Bagging
- Random forests
- Boosting: Basics
- Adaboost
- Gradient boosting

Random forests

Issue with bagging: **Bagged trees are still too correlated**

Each is trained on large enough random sample of data and often end up not being sufficiently different.

How to decorrelate the trees further?

Simple technique: When growing a tree on a bootstrapped (i.e. subsampled) dataset, before each split select $k \leq d$ of the d input variables at random as candidates for splitting.

When $k = d \rightarrow$ same as Bagging
When $k < d \rightarrow$ Random forests

k is a hyperparameter, tuned via cross-validation

Random forests

Random forests are very popular!

Wikipedia: *Random forests are frequently used as "blackbox" models in businesses, as they generate reasonable predictions across a wide range of data while requiring little configuration.*

Issues:

- When you have large number of features, yet very small number of *relevant features*:
  Prob(selecting a relevant feature among k selected features) is very small

- Lacks expressive power compared to other ensemble methods we'll see next..

Ensemble methods

- Bagging
- Random forests
- Boosting: Basics
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- Gradient boosting

Boosting

Recall that the bagged/random forest classifier is given by

$$f_{agg}(\boldsymbol{x}) = \text{sign}\left(\frac{1}{T}\sum_{t=1}^{T} f_t(\boldsymbol{x})\right)$$

where each $\{f_t\}_{t=1}^T$ belongs to the function class $\mathcal{F}$ (such as a decision tree), and is trained in parallel.

Instead of training the $\{f_t\}_{t=1}^T$ in parallel, what if we sequentially learn which models to use from the function class $\mathcal{F}$ so that they are together as accurate as possible?

More formally, what is the best classifier $\text{sign}\,(h(\boldsymbol{x}))$, where

$$h(\boldsymbol{x}) = \sum_{t=1}^{T} \beta_t f_t(\boldsymbol{x}) \text{ for } \beta_t \geq 0 \text{ and } f_t \in \mathcal{F}.$$

Boosting is a way of doing this.

Boosting

- is a meta-algorithm, which takes a *base algorithm* (classification algorithm, regression algorithm, ranking algorithm, etc) as input and boosts its accuracy
- main idea: combine weak "rules of thumb" (e.g. 51% accuracy) to form a highly accurate predictor (e.g. 99% accuracy)
- works very well in practice (especially in combination with trees)
- has strong theoretical guarantees

We will continue to focus on binary classification.

Boosting: example

Email spam detection:

- given a training set like:
  - ("Want to make money fast? ...", **spam**)
  - ("Viterbi Research Gist ...", **not spam**)
- first obtain a classifier by applying a base algorithm, which can be a rather simple/weak one, like decision stumps:
  - e.g. contains the word "money" $\Rightarrow$ spam
- reweigh the examples so that "difficult" ones get more attention
  - e.g. spam that doesn't contain the word "money"
- obtain another classifier by applying the same base algorithm:
  - e.g. empty "to address" $\Rightarrow$ spam
- repeat ...
- final classifier is the (weighted) majority vote of all weak classifiers

Base algorithm

A **base algorithm** $\mathcal{A}$ (also called weak learning algorithm/oracle) takes a training set S weighted by D as input, and outputs classifier $f \leftarrow \mathcal{A}(S, D)$

- this can be any off-the-shelf classification algorithm (e.g. decision trees, logistic regression, neural nets, etc)
- many algorithms can deal with a weighted training set (e.g. for algorithm that minimizes some loss, we can simply replace "total loss" by "weighted total loss")

For decision trees, can have new weighted distribution at any node, and measure conditional entropy as usual.

- even if it's not obvious how to deal with weight directly, we can always resample according to D to create a new unweighted dataset

Boosting: Idea

The boosted predictor is of the form $f_{boost}(\boldsymbol{x}) = \text{sign}(h(\boldsymbol{x}))$, where,

$$h(\boldsymbol{x}) = \sum_{t=1}^{T} \beta_t f_t(\boldsymbol{x}) \text{ for } \beta_t \geq 0 \text{ and } f_t \in \mathcal{F}.$$

The goal is to minimize $\ell(h(\boldsymbol{x}), y)$ for some loss function ℓ.

Q: We know how to find the best predictor in $\mathcal{F}$ on some data, but how do we find the best weighted combination $h(\boldsymbol{x})$?

A: Minimize the loss by a *greedy approach*, i.e. find β_t, $f_t(\boldsymbol{x})$ one by one for $t = 1, \ldots, T$.

Specifically, let $h_t(\boldsymbol{x}) = \sum_{\tau=1}^{t} \beta_\tau f_\tau(\boldsymbol{x})$. Suppose we have found $h_{t-1}(\boldsymbol{x})$, how do we find β_t, $f_t(\boldsymbol{x})$?

Find the β_t, $f_t(\boldsymbol{x})$ which minimizes the loss $\ell(h_t(\boldsymbol{x}), y)$.

Different loss function ℓ give different boosting algorithms.

$$\ell(h(\boldsymbol{x}), y) = \begin{cases} (h(\boldsymbol{x}) - y)^2 & \rightarrow \text{ Least squares boosting,} \\ \exp(-h(\boldsymbol{x})y) & \rightarrow \textit{AdaBoost}. \end{cases}$$