Large Language Models eXplainable AI

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Outline

- Demystifying large language models (LLMs)
- Introduction to XAI

Demystifying large language models

What is a language model (LM)?

- Probability model that estimates the conditional probability of the next word given the preceding sequence of words
- Applications
  - Speech recognition
  - Translation
  - Language generation
  - Handwriting recognition
  - and many, many more

The best thing about AI is that it ___

Word	P(w|s)
learns	4.5%
predicts	3.5%
understands	3.2%
helps	3.1%
does	2.9%

How can we create LM?

- Gather a large corpus of text documents
- Naive approach
  - Compute the empirical frequency of each word
  - Generate next word by probabilistic selection
  - Can we extend this to multi-word (n-gram) sequence empirical probabilities? Given ~40K common English words this yields:
    - 1.6 billion 2-word combinations
    - 60 trillion 3-word combinations
  - All of text in the world amounts to “only” O(100B) words
- What else can we do?

Self-supervised learning

- Gather a large corpus of text documents
- Train a deep learning model to approximate the language model, p(w|s)
- How can we get around labeling? Use "self" supervised learning where the model is trained to predict the next word given the preceding words

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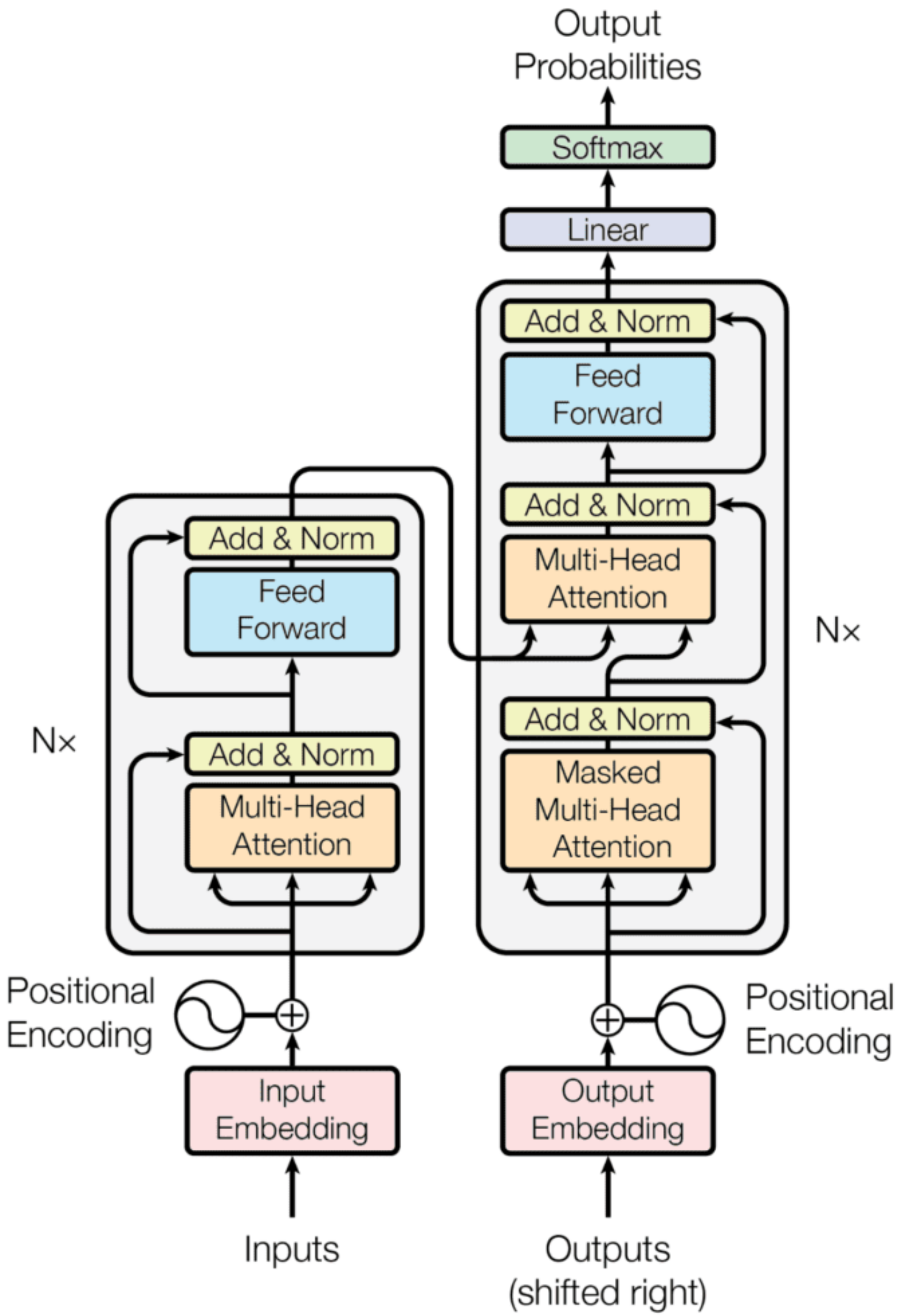


Transformers are transformative

- Transformers have been instrumental in the development of modern large language models
- Overcome many of the challenges associated with RNN language models (notably long sequences and gradient vanishing)
- Generative Pre-Trained Transformers (GPT) are stacked transformers (decoder only) trained on the next word prediction task

*Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).

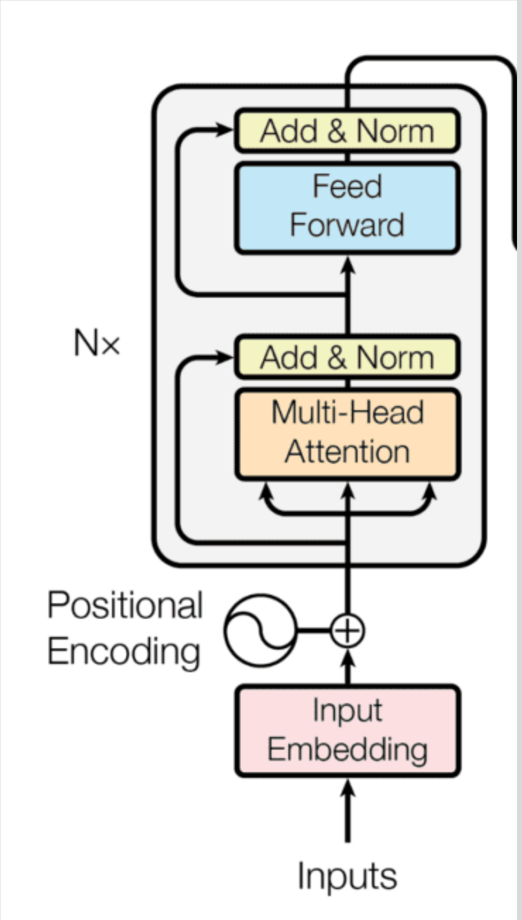
Transformer **Encoder** Pretraining

- Many language tasks require a pretrained encoder only (or just a library of embeddings generated by an encoder)
- Example pretraining approaches
  - **Masked Language Modeling** – predict hidden words

    The dog _____ down the street after the ____.
  - **Consecutive sentence prediction**

  True: *The weather forecast calls for rain. Bring an umbrella.*

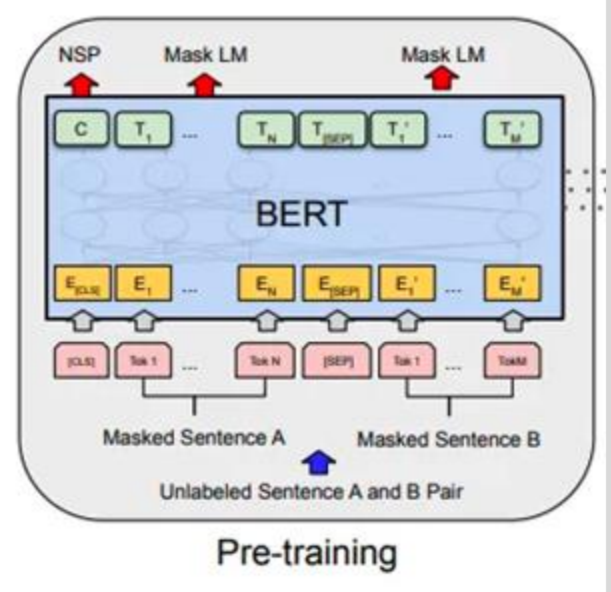
  False: *The weather forecast calls for rain. I work for Clemson.*

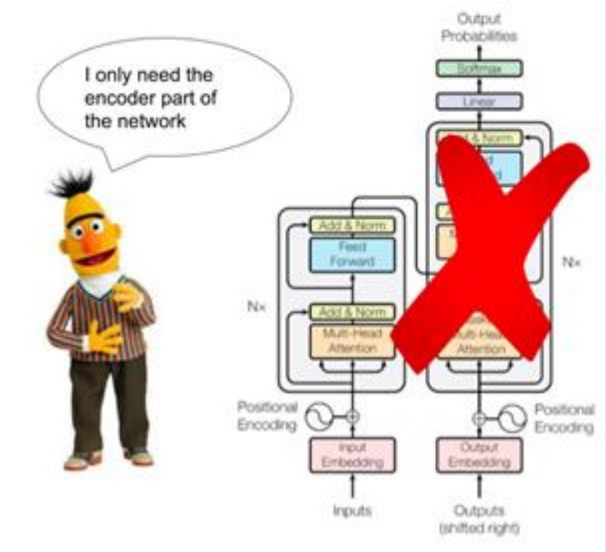


*Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).

Bidirectional Transformers for Language Understanding

- Introduced in 2019 by Devlin et al.
- Applies masked language model task with sentence pairs for encoder pre-training
- Approach originally used in chatGPT to form word embedding library (more on this later)
- Pretrained encoder can be paired with downstream network for ”encoder” only tasks:
  - Document classification
  - Sentiment analysis
  - Named entity recognition



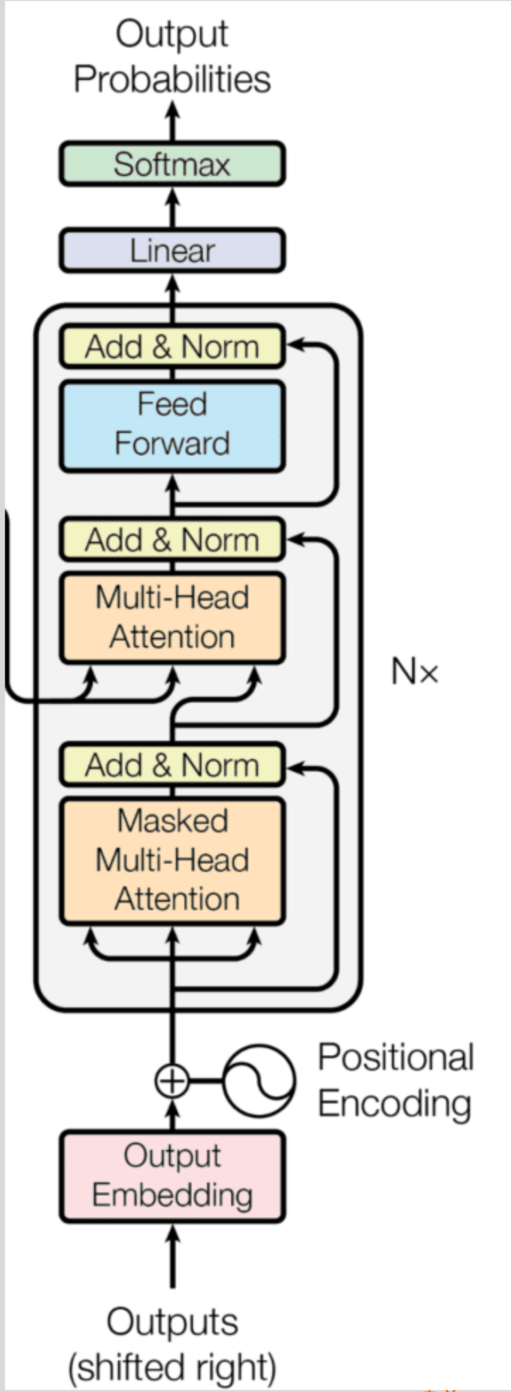


Transformer Decoder Pretraining

- Some language tasks require a pretrained decoder only
- Next word (or token) prediction

  The dog ran down the street after the ____

- This is the foundation of *Generative Pre-Trained* (GPT) models
  - Tokens of current output are represented using an embedding library (previously generated, e.g. with BERT)
  - The decoder generates the probabilities for the next output token using only the previous outputs (no encoder)



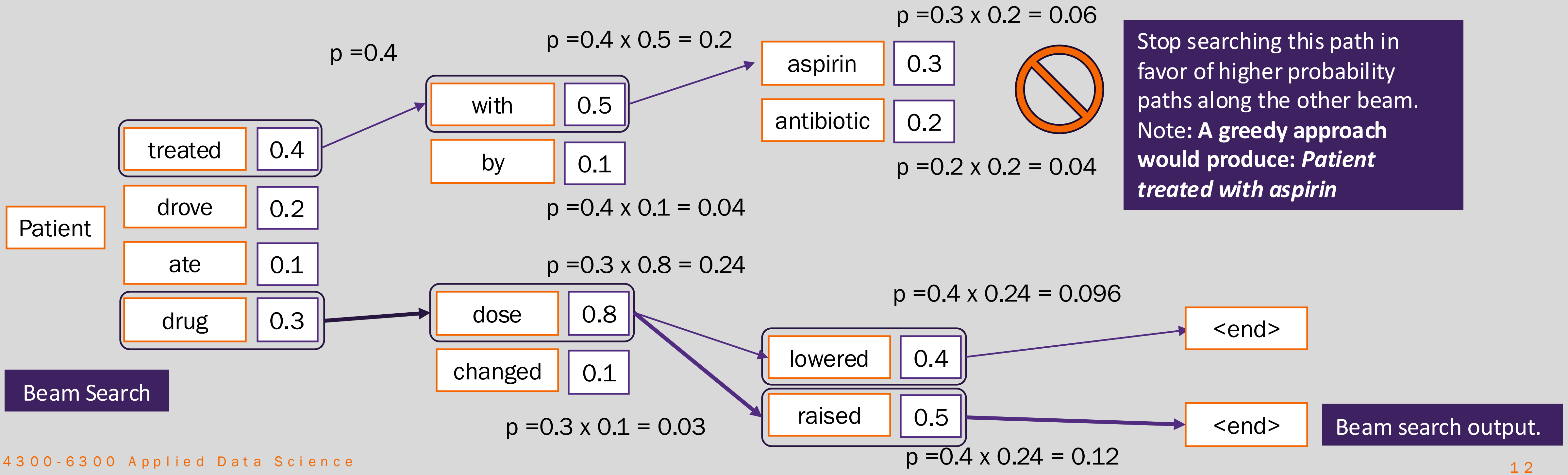
*Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems 30 (2017).

What about ChatGPT (and similar)?

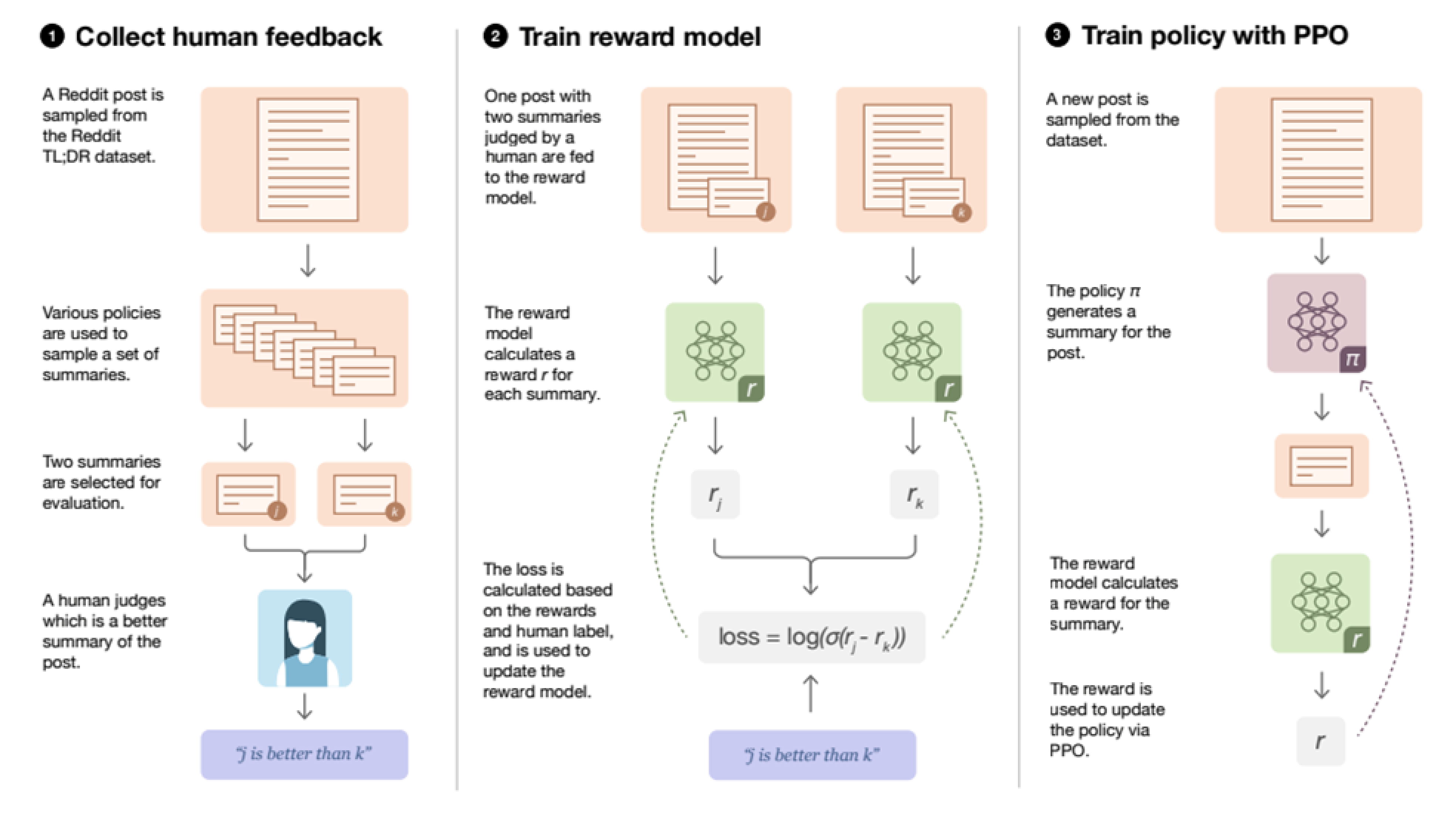
- Built on a generative pretrained (GPT) model
  - Composed of GPT layers
  - Trained to predict next word in a sequence
  - Huge amounts of data (GPT-3 was pretrained on >45 TB of data)
- Is that all?
  - No, add in some reinforcement learning (which is critical):
    - Humans rate “chat” results
    - Another NNet is trained to predict the rating
    - This NNet is then used as a loss function to further train the language generation model
  - Prompting strategies: Retrieval Augmented Generation, Chain of Thought, Ensemble Refinement, …

Language generation process, or “this is what ChatGPT does”

- Assume we have a trained LM (e.g., GPT)
- Given the current input, how do we select the next word?
  - Greedy – select the word with highest probability
  - Beam search – iteratively select the top K words and select the most probable path
- Both can be modified to select the next word / path probabilistically



OpenAI - Reinforcement Learning with Human Feedback



https://github.com/CarperAI/trlx

Text Generation Parameters

Temperature: This controls the randomness of the model's output. A higher value (closer to 1) makes the output more random, while a lower value (closer to 0) makes it more deterministic and focused on the most likely completion.

Maximum length: This specifies the maximum number of tokens (words or parts of words) that the model can generate for a single response

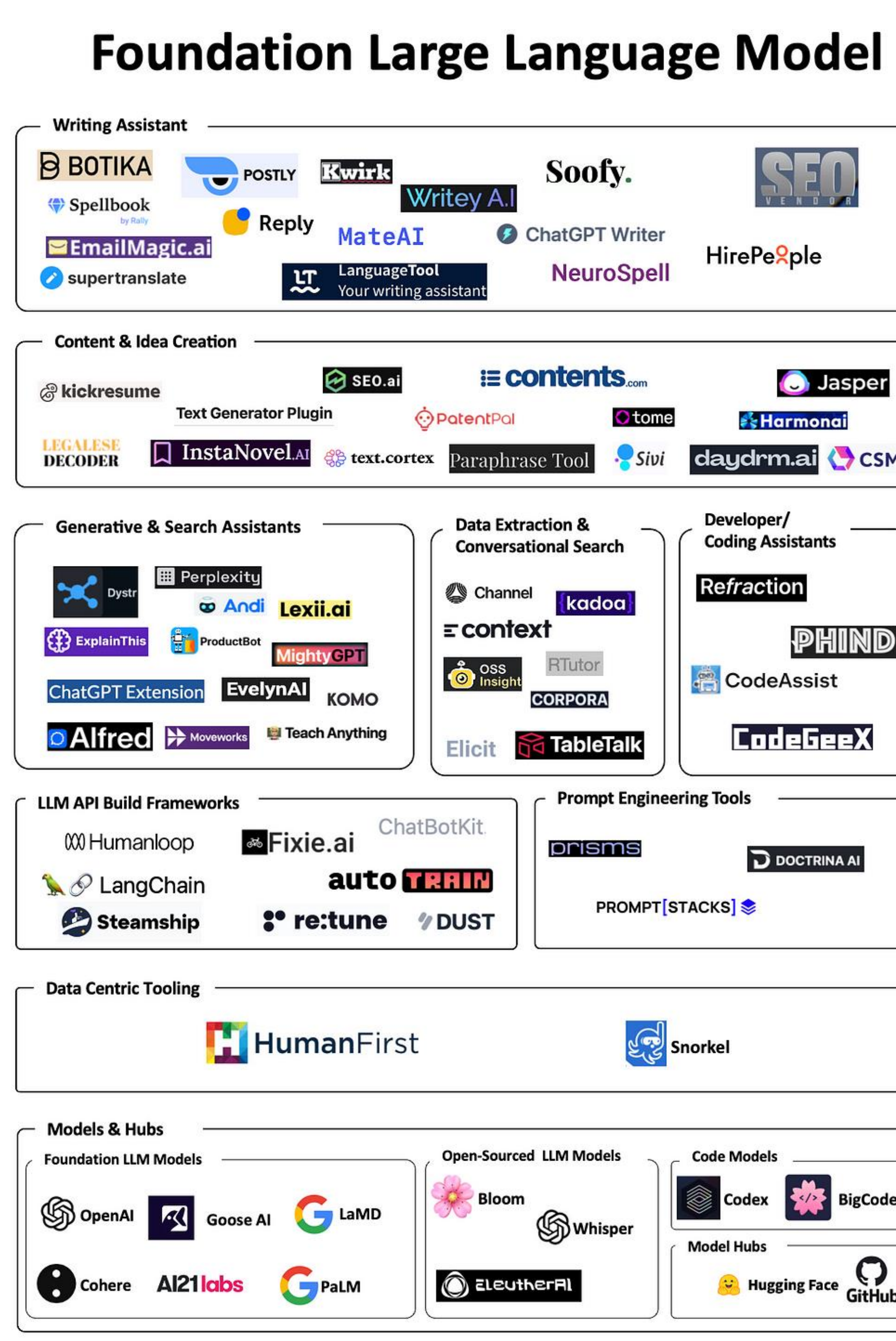
Stop sequences: These are specific strings of text that, if generated by the model, will cause it to stop generating further text.

Top P: This is a parameter for nucleus sampling, a method of generating text that involves choosing the next word from a subset of the vocabulary (the "nucleus") that has a cumulative probability larger than some value p. A higher value of p (up to 1) includes more of the vocabulary in the nucleus, making the output more random.

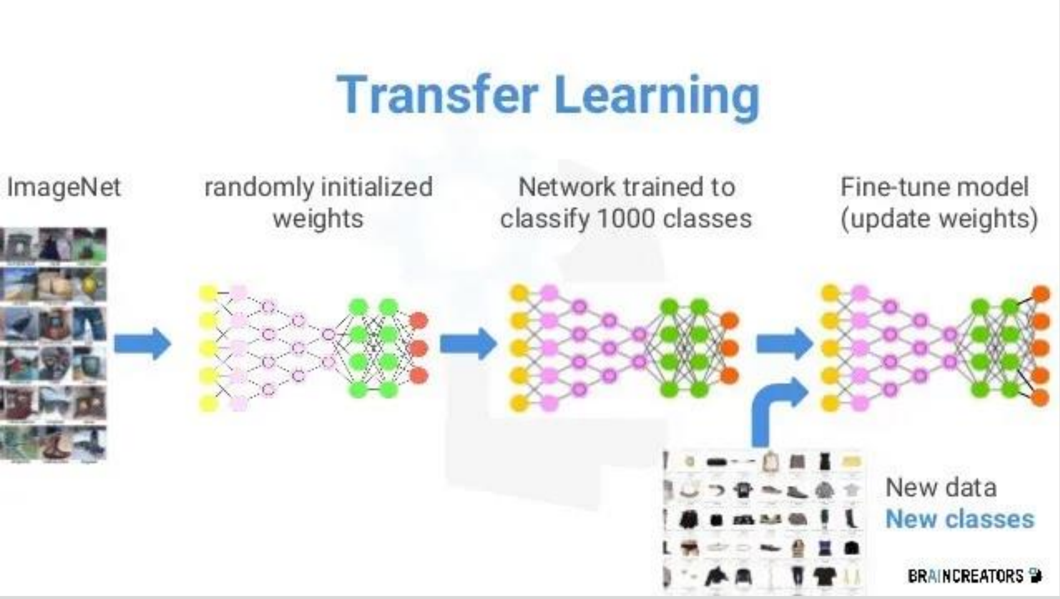
Frequency penalty: This value determines how the model handles frequently used words. A higher frequency penalty makes the model less likely to use common words and phrases.

Free and Open LLMs - Foundational

- Open Foundational
  - LLaMA (1 & 2) (Meta)
  - BLOOM (BigScience)
  - GLM (General Language Model)
  - GPT-J
  - GPT-NeoX
  - Pythia
  - StabilityLM
  - Cerebras-GPT (Cerebras)
  - Polyglot
  - RWKV
  - Falcon
  - OpenLLaMa
  - more …



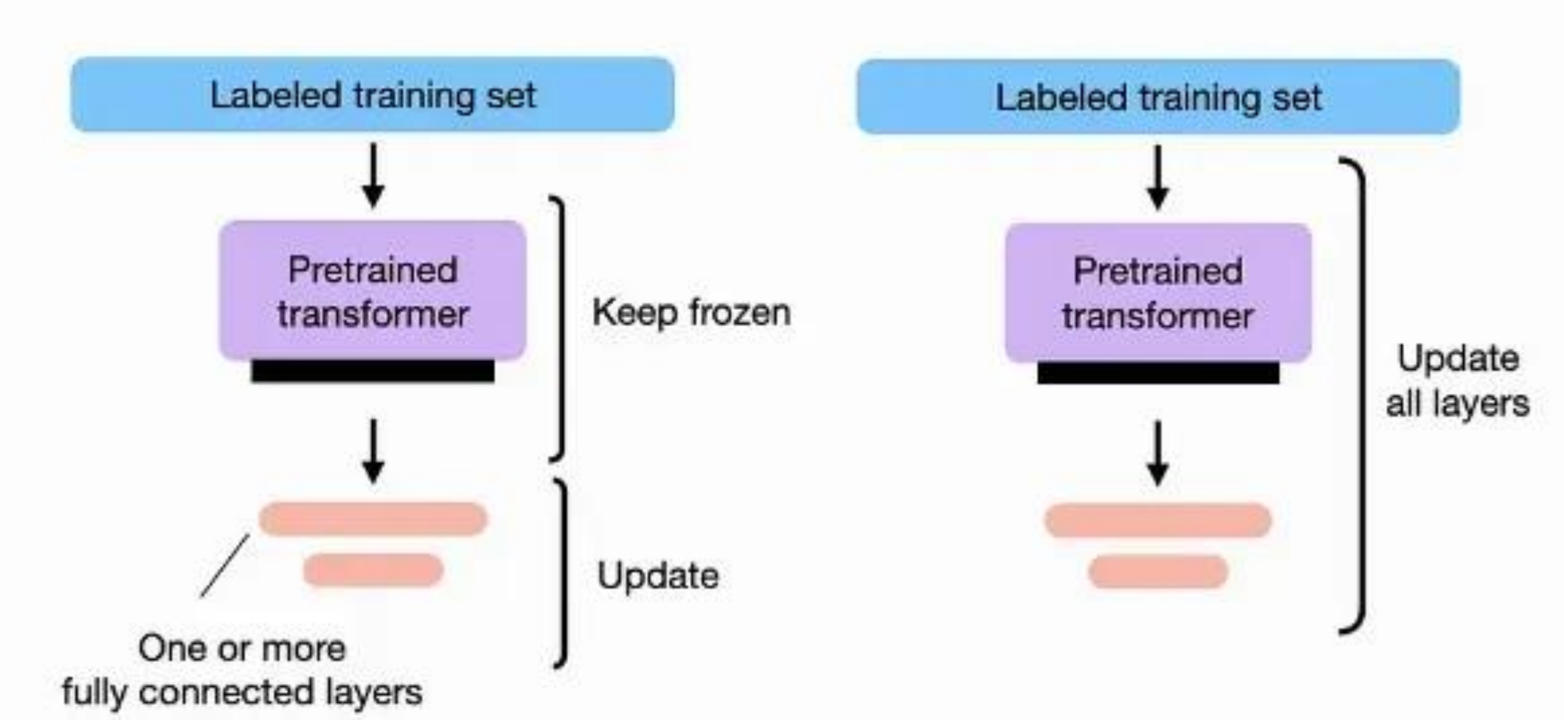
Transfer learning



1. Model is trained on a *generic* task for which a large dataset is available
2. The trained model is used as a starting point for a new, more specific task
3. **Fine tuning** – the original model is further trained on data for the new task
4. **Frozen encoder** – often, the pretrained model acts as the encoder and is not updated. Only the new decoder weights are updated for the new task

LLM Parameter Efficient Finetuning (PEFT)

- Full finetuning is time-consuming and expensive due to the computation and memory requirements.
- In the PEFT, only train a small subset of parameters while keeping most of the LLM model's weights frozen.



https://medium.com/intro-to-artificial-intelligence/parameter-efficient-finetuning-peft-of-llm-710831c0ffb3

eXplainable AI (XAI)

What is explainability?

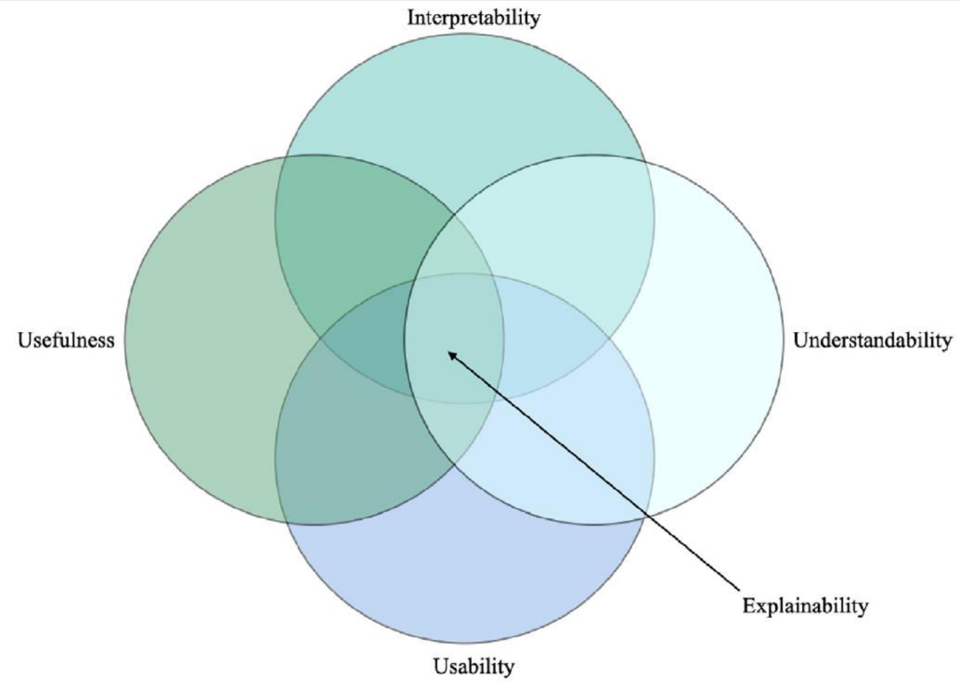
- *“… the ability to explain or to present in understandable terms to a human”* (Doshi-Velez & Kim 2017)
- *“descriptions are diverse … refers to more than one concept”* (Lipton 2016)
- There is no single definition
- Attempts to quantify explainability require subjective decisions on desiderata and measurement

What is eXplainable Artificial Intelligence (XAI)

- An emerging research area in AI
- Goal is to develop knowledge and methods that can be used to "explain":
  - How AI systems arrive at specific solutions
  - Which features most influenced a given output
  - Which and how features interact
  - Operating characteristics
  - Model biases
  - Accuracy relative to input regions
  - How the model learned

School of COMPUTING Clemson University

What makes an AI explainable?



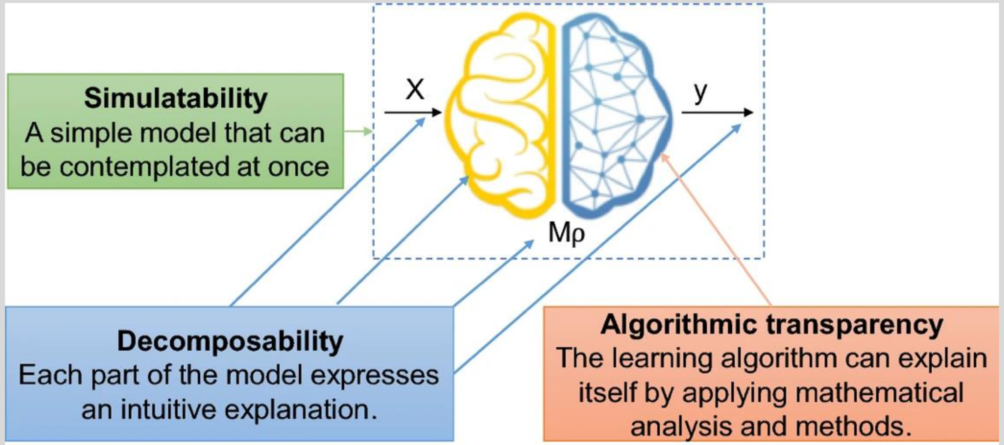
No consensus definition but most researchers agree explainability is a construct encompassing several concepts including:

- *Interpretability* – degree to which a human can infer the cause of and predict a model output
- *Understandability* – degree to which a user can determine how the system works
- *Usability* – the ease with which a user can operate the AI
- *Utility* – the practical usefulness of the AI

Figure credit: Combi, Carlo, et al. "A manifesto on explainability for artificial intelligence in medicine." Artificial Intelligence in Medicine 133 (2022): 102423.

What makes an AI understandable?

- No consensus definition
- Intrinsically linked to human cognition
- *Lipton proposed a framework for assessing model understandability composed of:



  - Simulatability – the degree to which a human can take the input and model parameters and step through every calculation required to produce a prediction
  - Decomposability – the degree to which each part of the model (inputs, parameters, calculations) allow for an explanation
  - Algorithmic transparency – the degree to which theoretical guarantees for learning algorithm properties (e.g., convergence) can be provided

*Lipton, Zachary C. "The mythos of model interpretability: In machine learning, the concept of interpretability is both important and slippery." Queue 16.3 (2018): 31-57.
Figure credit: Minh, Dang, et al. "Explainable artificial intelligence: a comprehensive review." Artificial Intelligence Review (2022): 1-66.

Why do we need explainability?

Need for explainability arises when formal learning objectives fail to capture other real-world desiderata

Prediction Loss

$$L(y, \hat{y}) + G(\lambda, \widehat{\boldsymbol{\Theta}}) + ?$$

Regularization

Objective Function Limitations

- Difficult to formalize many real-world desiderata in mathematical form
- For example, how would one form an objective to encode ”trust” or “fairness”

AI desiderata beyond prediction accuracy

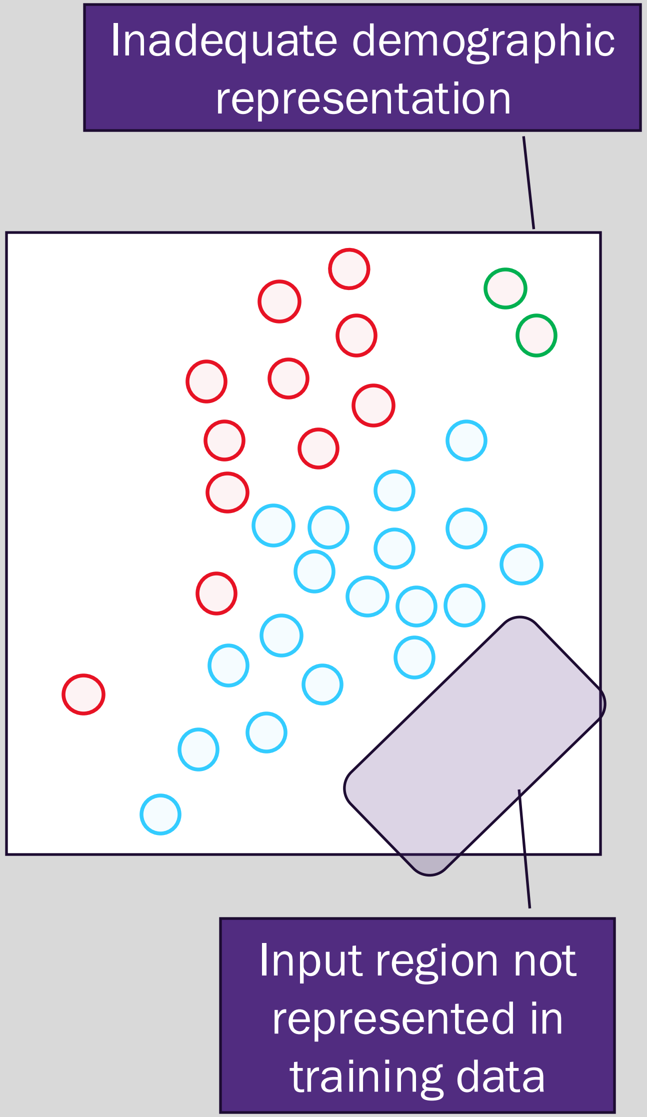
- Trust – relates to subjective human emotion that the model “is fair” or “can be left in control”
- Scientific knowledge
- Decision support information
- Fair, ethical, legal decisions
- Safety
- Privacy

Explainability through data characterization

- Examine standard statistical measures (mean, stdev, range) of input features and target (supervised learning problems) data
    - Are there outliers? Are outliers due to measurement error or are they real?
- Examine missing data rates for input features
    - Imputation may be used in some cases should be restricted to cases where missing data rate is below some threshold
    - Rule of thumb: Require missing data rate <30% for imputation
- Feature reduction:
    - Are there redundant features that can be removed (e.g., highly correlated features)?

Data quality and explainability

- Training data coverage
  - Range/counts of continuous/categorical valued input features
  - Sample input and output density (i.e., assess sparsity)
- Demographic representation
  - Which and to what extent are population groups represented in the data?
  - Medical data: should report comorbidities, procedures, medications
- Data collection methodology
  - How was the data collected?
  - What inclusion/exclusion criteria were used?



"Inherently" explainable models

- Some models are often cited as *inherently explainable* including:
  - Linear / logistic regression
  - Decision trees
  - Rule sets
- Why?
  - Relation between variables is usually clear
  - Direction of relation between input and output is usually discernable
  - Computation of output is usually straightforward

$$y = \sigma[\beta_1 x_1 - \beta_2 x_2]$$

Human simulatable!

In a linear model with a small number of predictors, it's easy to "simulate" the result (here two multiplications and a sum >0 results in positive class) and to "infer" relations (e.g., as x_2 increases the likelihood of the positive class decreases)

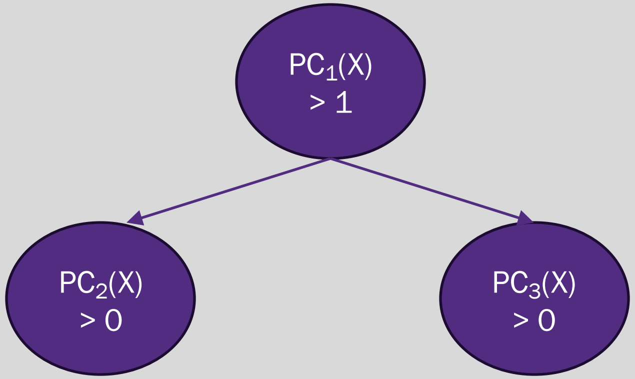
Are “Inherently” explainable models always understandable?

- What if there are many variables?

$$y = \sum_{i=1}^{10,000} \beta_i x_i$$

Not human simulatable!

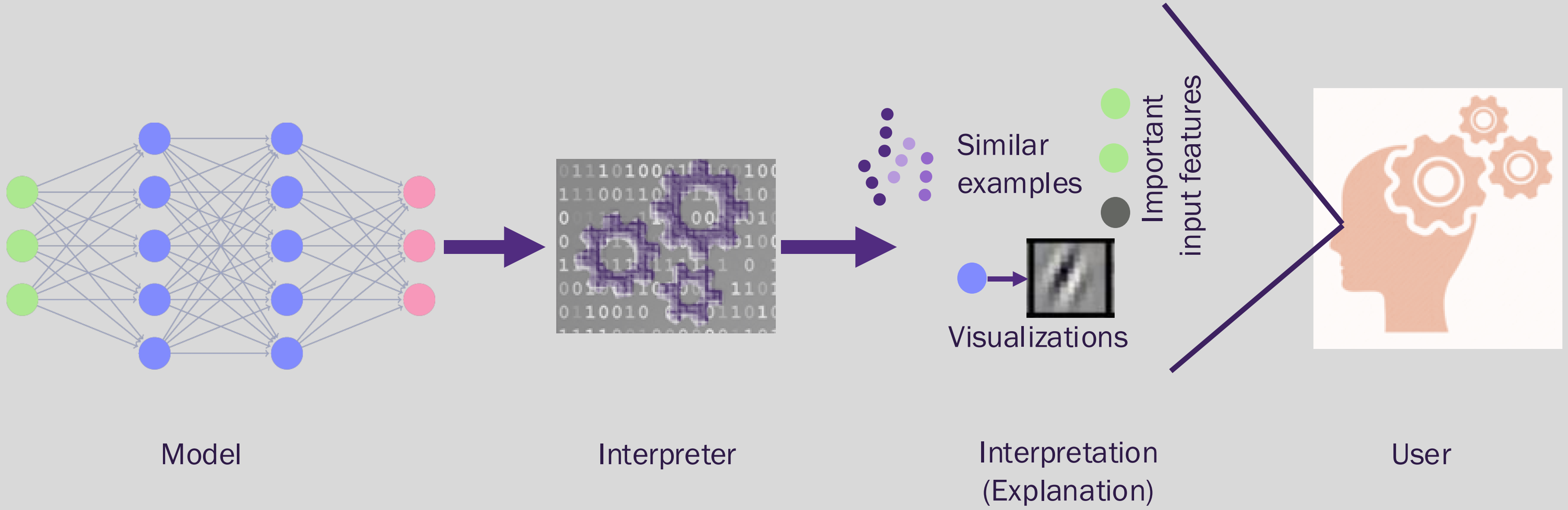
- What if the input variables are highly engineered? For example, the principal components as input to a shallow decision tree?



Not human simulatable!

Post-hoc explanation method

Methods applied to models and their outputs to create explanatory information

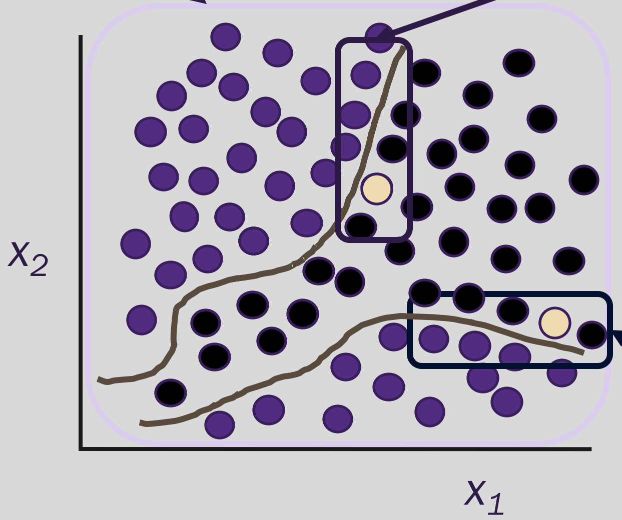


Global vs. local feature importance

Global explanation: x_1 and x_2 equally important

Local explanation: x_1 is more important here …

Global explanation: **independent** of input sample
Local explanation: **depends** on input sample



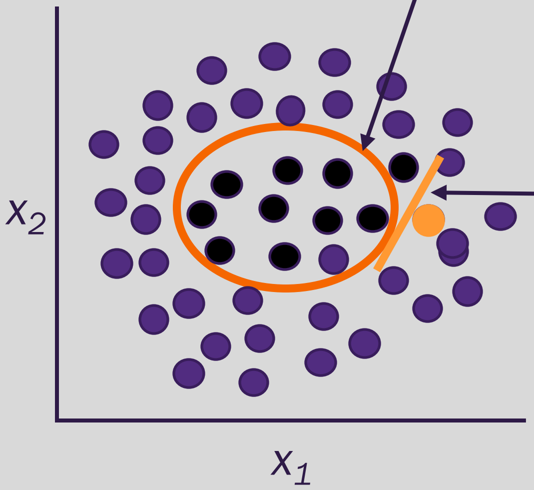
Local explanation: x_2 is more important here

Global feature importance assessment

- Permutation analysis
  - Only applicable to structured data
  - Method
    1. Train model as usual
    2. Shuffle the observed values among samples for one feature
    3. Measure performance
    4. Repeat steps 2-3 for each column
    5. Rank features by model performance (shuffled features that lead to higher reductions in model performance or more important)
- Ablation analysis
  1. Remove one feature
  2. Train model and measure performance performance
  3. Repeat steps 1-2 for each feature
  4. Rank features with same approach as permutation analysis

Local feature importance via additive feature attribution

Global model: $f(x_1, x_2) = class$



Local explanation model

$$g(x_1, x_2) = \phi_0 + \boxed{\phi_1} x_1 + \boxed{\phi_2} x_2$$

x_1 , x_2
importance

SHapley Additive exPlanation (SHAP)

For a model $f(x) = y$, form a linear approximation:

$$g(z) = \underbrace{\boxed{\phi_0}}_{\text{Baseline risk}} + \sum_{i=1}^{M} \underbrace{\boxed{\phi_i}}_{\text{Feature importance}} z_i \qquad \underbrace{\boxed{z = h_x^{-1}(x)}}_{\text{Binary feature mapping}}$$

$$\phi_i(f, x) = \sum_{z' \subseteq x'} \underbrace{\boxed{\frac{|z'|!\,(M - |z'| - 1)!}{M!}}}_{\text{Weighting term}} \underbrace{\boxed{\left[f[h_x(z')] - f[h_x(z' \backslash i)]\right]}}_{\text{Output difference when removing feature } i}$$

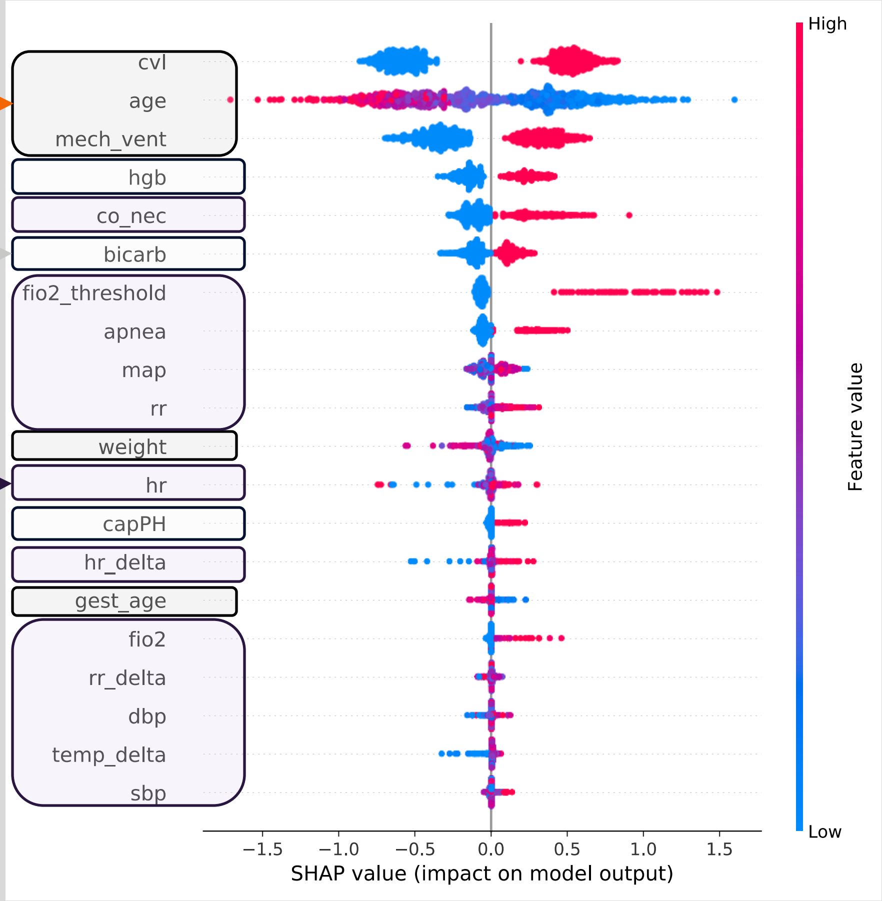
A Unified Approach to Interpreting Model Predictions. Lundberg & Lee. 2017.

SHAP Visualization

Known risk factors

Lab indicators

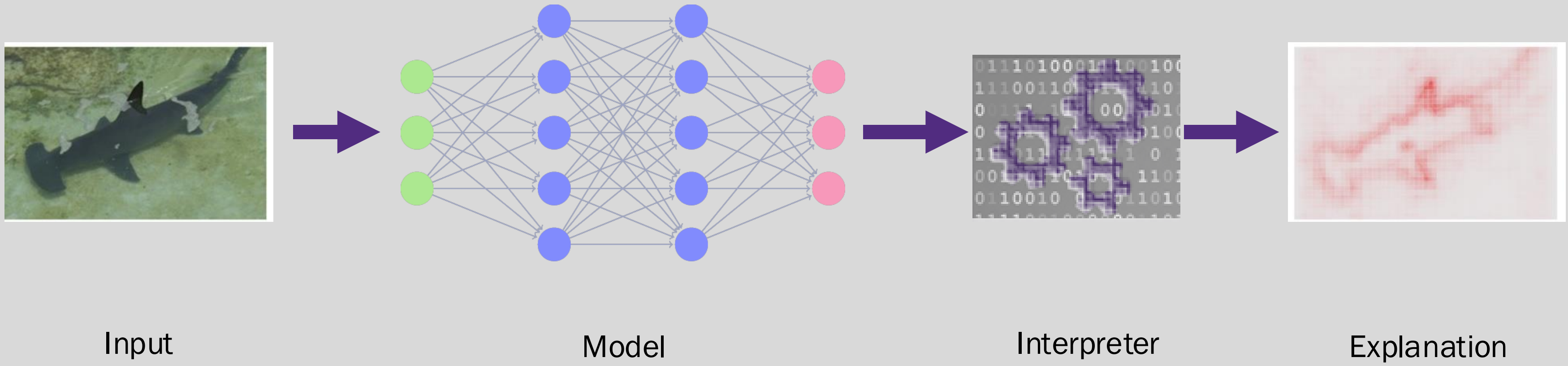
Clinical status change?



Visualization local feature importance methods

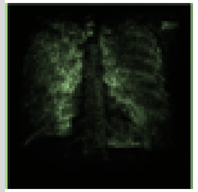
For a model $f: R^d \rightarrow R^+$, associate with each input element a relevance score, $R_p(x)$, that indicates importance

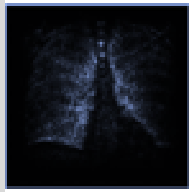
- Gradient methods: $\sum_p \left({}^{\partial f}/_{\delta x_p} \right)^2 = \|\nabla_x f(x)\|^2$
- Perturbation: Mask image areas
- Decomposition methods: $f(x) = \sum_p R_p(x)$



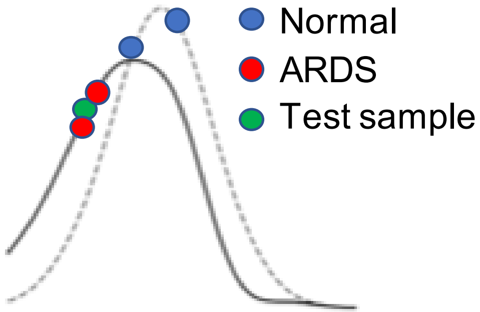
Instance based explanations with influence functions

- Robust statistical methods that identify the training example(s) that most influence the current prediction
  - Deletion diagnostics (linear models)
  - Influence functions (twice differentiable loss function)
- Useful in model development as a means of identifying outliers with undue influence on predictions
- For deployed models can be used to indicate how important features of test sample compare to influential samples





SpO2/Fi02 Data Distribution



Report Findings Comparison

Test Sample

Opacification (Right)

Pleural Apical Thickening

Influential ARDS Training Samples

Opacification

Influential Normal Training Samples

Opacification (negated)

Python XAI resources

- SHAP - https://shap.readthedocs.io/en/latest/
- ELI5 - https://eli5.readthedocs.io/en/latest/
- Captum - https://captum.ai/ (deep learning XAI library)
- Interpretable Machine Learning by Molnar (free online text) https://christophm.github.io/interpretable-ml-book/