

10-423/10-623 Generative Al

Machine Learning Department School of Computer Science Carnegie Mellon University

Course Overview + RNN-LMs + Automatic Differentiation

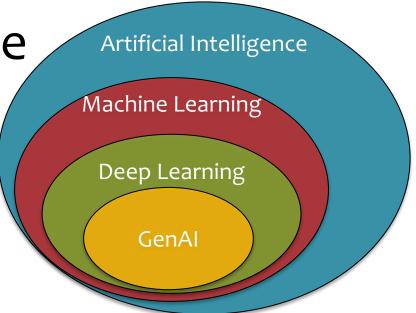
Matt Gormley & Pat Virtue Lecture 1 Jan. 11, 2024

WHAT IS GENERATIVE AI?

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning



Artificial Intelligence

Machine Learning

Deep Learning

GenAl

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

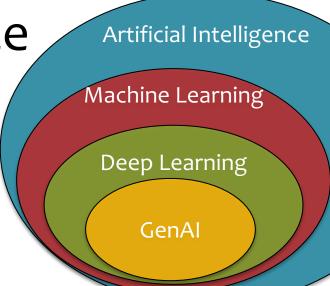
Deep Learning



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning



☐ Q: What does Generative Al have to do with **any of these goals**?

☐ A: It's making in-roads into all of them.

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning

- ☐ Communication comprises the comprehension and generation of human language.
- ☐ Large language models (LLMs) excel at both
- ☐ (Even though they are most often trained autoregressively, i.e. to **generate** a next word, given the previous ones)

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Machine Learning

Deep Learning

GenAl

- ☐ The traditional way of learning in ML is via parameter estimation
- ☐ But in-context learning (i.e. providing training examples as context at test time) shows that learning can also be done via inference

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial IntelligenceMachine LearningDeep Learning

GenAl

- ☐ LLMs are also (unexpectedly) good at certain reasoning tasks
- ☐ cf. Chain-of-Though Prompting (an ex. of in-context learning)

Chain-of-Thought Prompting

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. 5 + 6 = 11. The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Outpu

A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had 23 - 20 = 3. They bought 6 more apples, so they have 3 + 6 = 9. The answer is 9.

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning

GenAl

☐ LLMs are already being used for grounded planning for embodied agents, c.f. LLM-Planner

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning

- ☐ Text-to-image models
 [Midjourney's Discord server has
 18 million members (1.7 million
 were online this morning)]
- ☐ Text-to-music models
 [MusicGen capable of
 conditioning on text and audio
 sample]

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Machine Learning

Deep Learning

- ☐ Multimodal foundation models learn to answer questions about images (and text in images)
- ☐ Diffusion models can be used as zero-shot classifiers

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

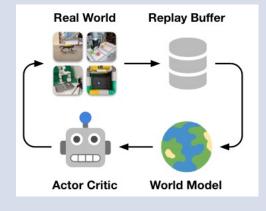
- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning

Artificial Intelligence

Deep Learning

Machine Learning

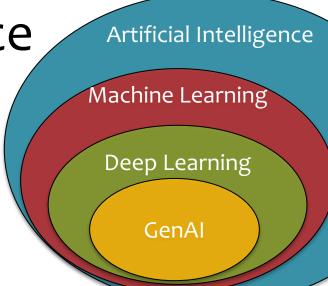
- ☐ DayDreamer learns a generative model of experiences for RL, i.e. a World Model, without
 - simulation
- ☐ Quadruped robot learns to walk in under 1 hour



The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning



☐ Q: What does Generative Al have to do with **any of these goals**?

☐ A: It's making in-roads into all of them.

WHAT IS GENERATIVE AI CAPABLE OF?

Text Generation

Prompt: Write a proof of the fact that there are infinitely many primes; do it in the style of a Shakespeare play through a dialogue between two parties arguing over the proof.

GPT-4: Enter FIRST PARTY and SECOND PARTY.

FIRST PARTY: Thou dost not understand, my friend, There simply is no upper end To primes, those numbers indivisible, No matter if it seems impossible.

SECOND PARTY: But how dost thou so surely know? To prove this truth, what canst thou show?

FIRST PARTY: Consider this, my doubtful peer, A clever proof that will make clear: Assume that there's a final prime, The largest one we'll see in time. Let's call this number "P" for short, And then, my friend, we will purport To build a number "Q" that's new, One larger than "P" and prime too.

SECOND PARTY: But how, my friend, will this be done? The proof is not yet fairly won.

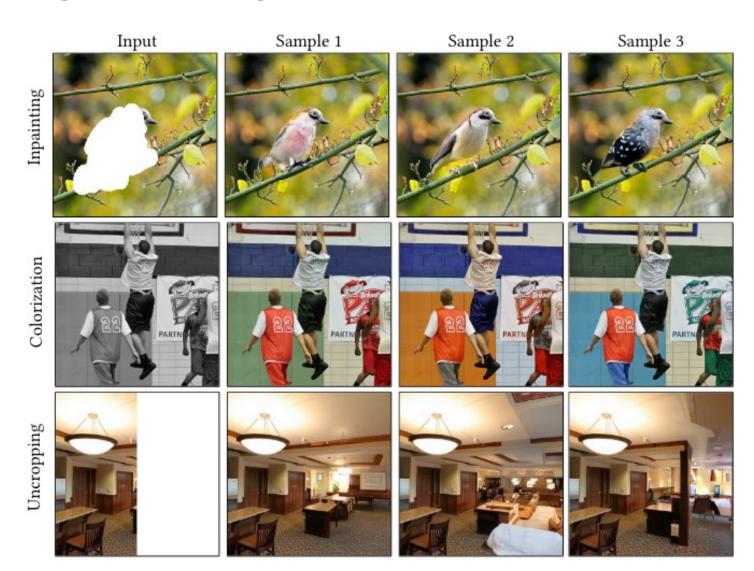
FIRST PARTY: It's simple, friend, just wait and see, We'll multiply the primes, that's key. All primes from two to "P" combined, Will make this new "Q" we will find. But one thing more we must include, To make the proof more watertight, We'll add a one onto the end, And now the proof is in our sight.

SECOND PARTY: I see it now, it's crystal clear, For "Q" must be a prime, my dear. It can't divide by any prime, All smaller than itself in time. And since we chose "P" as the last, This proves that our assumption's past. There is no final prime, we see, The numbers go on endlessly.

Image Editing

A variety of tasks involve automatic editing of an image:

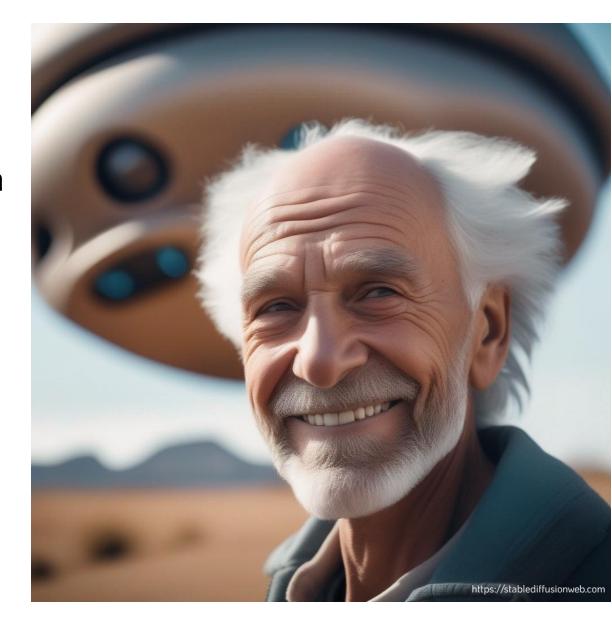
- Inpainting fills in the (prespecified) missing pixels
- Colorization restores color to a greyscale image
- Uncropping creates a photo-realistic reconstruction of a missing side of an image



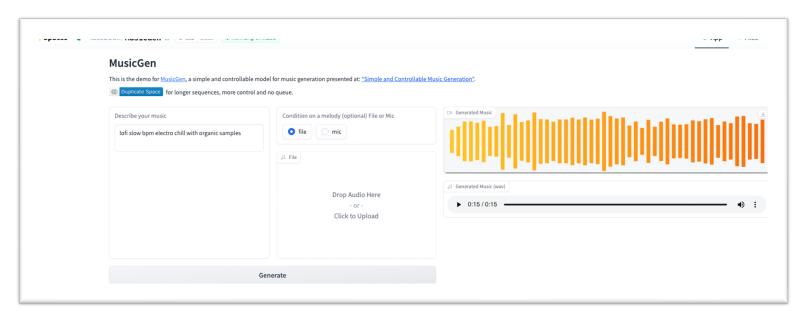
Text-to-Image Generation

- Given a text description, sample an image that depicts the prompt
- The following images are samples from SDXL with refinement

Prompt: close up headshot, futuristic **old man**, wild hair sly smile in front of gigantic UFO, dslr, sharp focus, dynamic composition, **rule of thirds**

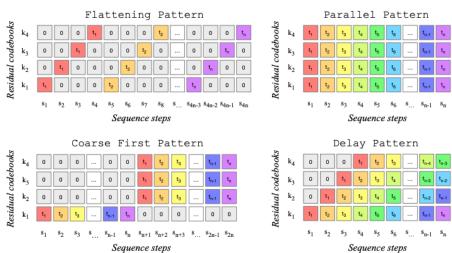


Music Generation



MusicGen

- A transformer decoder model over quantized units (discrete elements of a codebook of audio frames)
- Interleaves sounds by adjusting how codebooks attend to each other
- Permits conditioning on text and/or audio samples





Code Generation



Figure 1.3: We queried GPT-4 three times, at roughly equal time intervals over the span of a month while the system was being refined, with the prompt "Draw a unicorn in TikZ". We can see a clear evolution in the sophistication of GPT-4's drawings.

GPT-4 vs ChatGPT

Prompt:

A function f is called {increasing}_{emphasize!} if f(s) \P f(t) holds for every s \P t. Consider the formula: limit_{x goes to 0} {limit when n approaches infinite} underscore{ waterix [sum of i from 1 to n (f(nx) - integral from 0 to x sin(nx) dx), ((x + 2/8)^2 - 5)/((4x-1/x^2) /(n xor 3)), \\ , ..., partial f(x/n) over partial x * (e^f-i*emega n x} + 3(x#7)), f inverse of (x mod n)]] multiply whatrix{i}, 1, ..., 1\\ 1, \\ 1, 1, ..., 1} } {grey_color{this gives us a good impression about the function}}

Convert the above paragraph to LaTeX.

GPT-4:

A function f is called *increasing* if $f(s) \leq f(t)$ holds for every $s \leq t$. Consider the formula:

$$\lim_{x \to 0} \lim_{n \to \infty} \left[\begin{array}{c} \sum_{i=1}^{n} \left(f(nx) - \int_{0}^{x} \sin(nx) \, dx \right), & \frac{\left(x + \frac{2}{8}\right)^{2} - 5}{\frac{4x - 1/x^{2}}{n \oplus 3}}, \\ \vdots & \vdots & \vdots \\ \frac{\partial f(x/n)}{\partial x} \cdot \left(e^{-i\omega nx} + 3(x\#7) \right), & f^{-1}(x \bmod n) \end{array} \right] \times \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$
this gives us a good impression about the function

GPT-4 vs ChatGPT Prompt: I want to write a customized optimizer in pytorch, the optimizer should do: 1. the parameters for the optimizer is learning rate, momentum ,weigth decay, d_dim, k and factor alpha 2. the optimizer goes through each parameter in the network, and then -- Get the gradient of this parameter, reshape it to 2D by looping through the dimensions, and keeping the dimension whose actual dimension (shape) is equal to d_dim, do an SVD decomposition of the parameter so W = U\Sigma V. -- Keep the top k singular vectors of W, so we get a new matrix W_k = U \Sigma_k V. -- Keep the top 2k singular vectors of W, so we get a new matrix W_{2k} = U \Sigma_{2k} V. -- Normalize W_k according to the momentum of the F-norm of W_{2k}. -- Truncate each coordinate of W_k to the top alpha percentile of all the coordinates, in absolute value. -- Apply momentum on W_k, and then update the network parameters using this momentum. -- Apply weight decay. GPT-4: ChatGPT: def step(self): def step(self): for group in self.param_groups: for group in self.param_groups: for p in group['params']: for p in group['params']: if p.grad is None: if p.grad is None: grad = p.grad.data grad = p.grad.data grad = grad.reshape(-1, grad.shape[-1]) # reshape to 2D # reshape grad to 2D grad_2d = grad.reshape(-1, group['d_dim']) # SVD decomposition U, S, V = torch.svd(grad_2d) u, s, v = torch.svd(grad) # keep top k singular vectors G_k = U[:, :group['k']] @ torch.diag(S[:group['k']]) @ # Keep top k and 2k singular vectors k = group['k'] V[:, :group['k']].T u_k = u[:,:k] # keep top 2k singular vectors s_k = s[:k] G_2k = U[:, :2*group['k']] torch.diag(S[:2*group['k']]) v_k = v[:,:k] 0 V[:, :2*group['k']].T $u_2k = u[:,:2*k]$ # normalize G_k s_2k = s[:2*k] G_k /= torch.norm(G_2k, p=2) $v_2k = v[:,:2*k]$ # truncate G_k threshold = torch.quantile(torch.abs(G_k), # Normalize according to momentum of F-norm of G_2k group['alpha']) grad_k = u_k 0 torch.diag(s_k) 0 v_k.t() $G_k[torch.abs(G_k) < threshold] = 0$ norm_2k = s_2k.norm() # apply momentum grad_k = grad_k * group['momentum'] / norm_2k if 'momentum_buffer' not in group: group['momentum_buffer'] = torch.zeros_like(G_k) # Truncate to top alpha percentile group['momentum_buffer'] = group['momentum'] * alpha = group['alpha'] group['momentum_buffer'] + G_k percentile = grad_k.abs().flatten().kthvalue(int(alpha * # update parameters grad_k.numel())) p.data.add_(-group['lr'] * group['momentum_buffer']) grad_k[grad_k.abs() < percentile] = 0 # apply weight decay if group['weight_decay'] != 0: # Apply weight decay p.data.add_(-group['weight_decay'] * group['lr'], p.data.add_(-group['lr'], grad_k + group['weight_decay']

Figure 3.4: GPT-4 vs ChatGPT at implementing a customized Pytorch optimizer module. We highlight the astuteness of GPT-4 vs the mistake by ChatGPT at 'applying momentum'.

Video Generation

- Latent diffusion models use a lowdimensional latent space for efficiency
- Key question: how to generate multiple correlated frames?
- 'Align your latents' inserts temporal convolution / attention between each spatial convolution / attention
- 'Preserve Your Own Correlation' includes temporally correlated noise

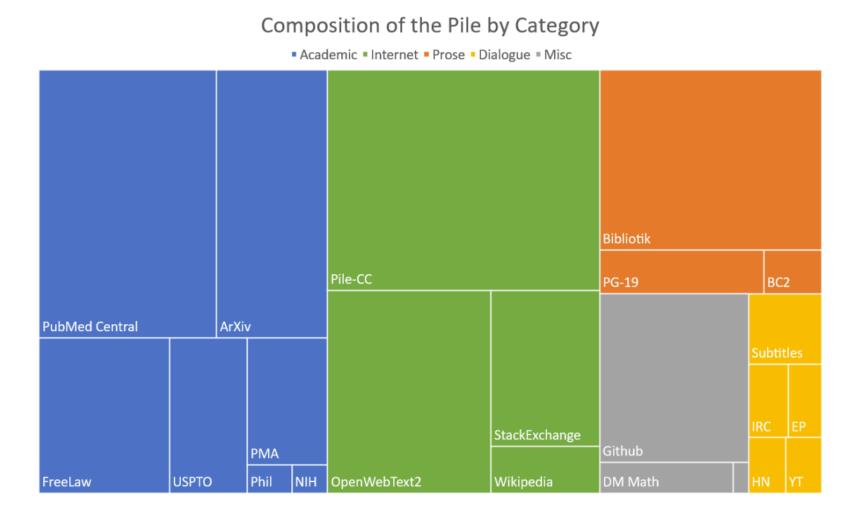


SCALING UP

Training Data for LLMs

The Pile:

- An open source dataset for training language models
- Comprised of 22 smaller datasets
- Favors high quality text
- 825 Gb ≈ 1.2 trillion tokens



RLHF

- InstructGPT uses
 Reinforcement
 Learning with Human
 Feedback (RLHF) to
 fine-tune a pre trained GPT model
- From the paper:
 "In human
 evaluations on our
 prompt distribution,
 outputs from the 1.3B
 parameter
 InstructGPT model are
 preferred to outputs
 from the 175B GPT-3,
 despite having 100x
 fewer parameters."

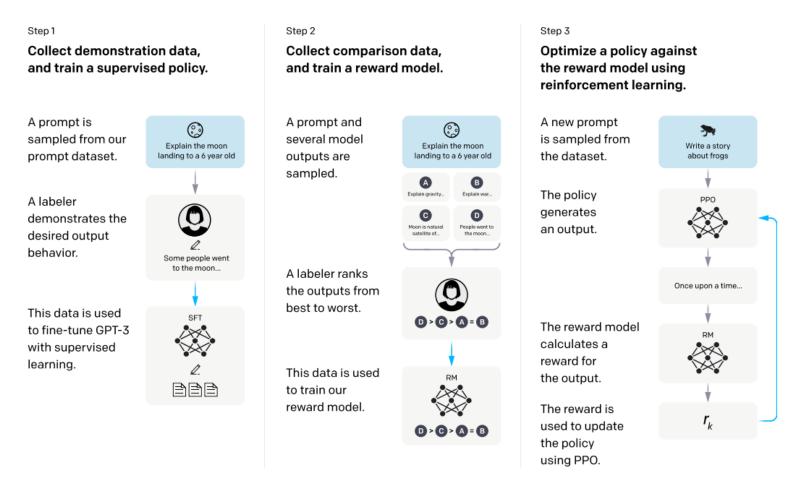


Figure 2: A diagram illustrating the three steps of our method: (1) supervised fine-tuning (SFT), (2) reward model (RM) training, and (3) reinforcement learning via proximal policy optimization (PPO) on this reward model. Blue arrows indicate that this data is used to train one of our models. In Step 2, boxes A-D are samples from our models that get ranked by labelers. See Section 3 for more details on our method.

Memory Usage of LLMs

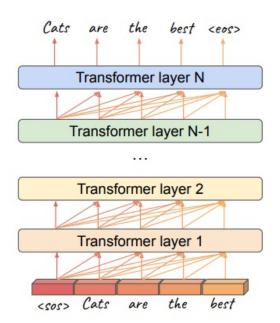
How to store a large language model in memory?

- full precision: 32-bit floats
- half precision: 16-bit floats
- Using half precision not only reduces memory, it also speeds up GPU computation
- "Peak float16 matrix multiplication and convolution performance is 16x faster than peak float32 performance on A100 GPUs."
 from Pytorch docs

Model	Megatron-LM	GPT-3
# parameters	8.3 billion	175 billion
full precision	30 Gb	651 Gb
half precision	15 Gb	325 Gb

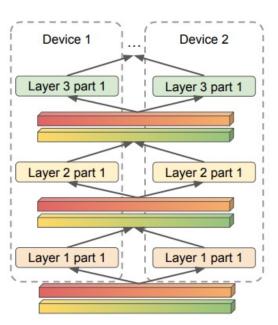
GPU / TPU	Max Memory
TPU v2	16 Gb
TPU v3/v4	32 Gb
Tesla V100 GPU	32 Gb
NVIDIA RTX A6000	48 Gb
Tesla A100 GPU	80 Gb

Distributed Training: Model Parallel



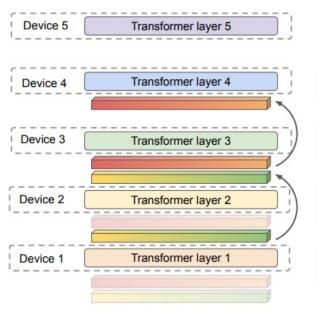
(a) Transformer-based LM

There are a variety of different options for how to distribute the model computation / parameters across multiple devices.



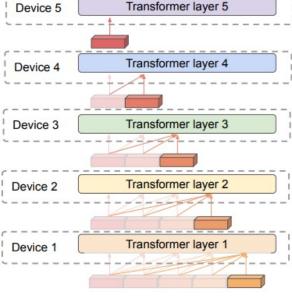
(b) Operation partitioning (Megatron-LM)

Matrix multiplication comprises most Transformer LM computation and can be divided along rows/columns of the respective matrices.



(c) Microbatch-based pipeline parallelism (GPipe)

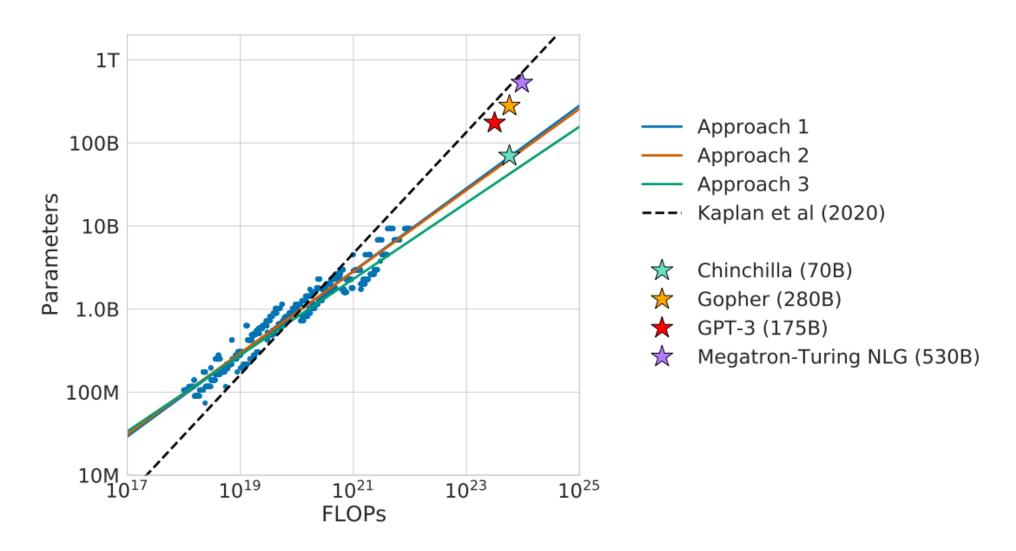
The most natural division is by layer: each device computes a subset of the layers, only that device stores the parameters and computation graph for those layers.



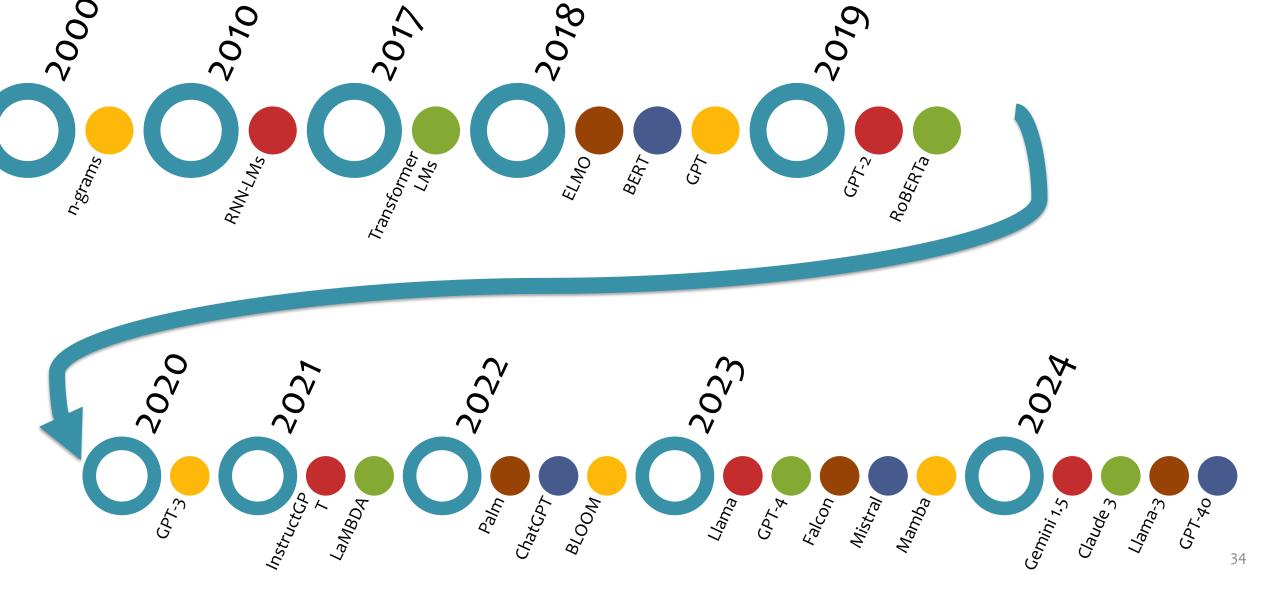
(d) Token-based pipeline parallelism (TeraPipe)

A more efficient solution is to divide computation by token and layer. This requires careful division of work and is specific to the Transformer LM.

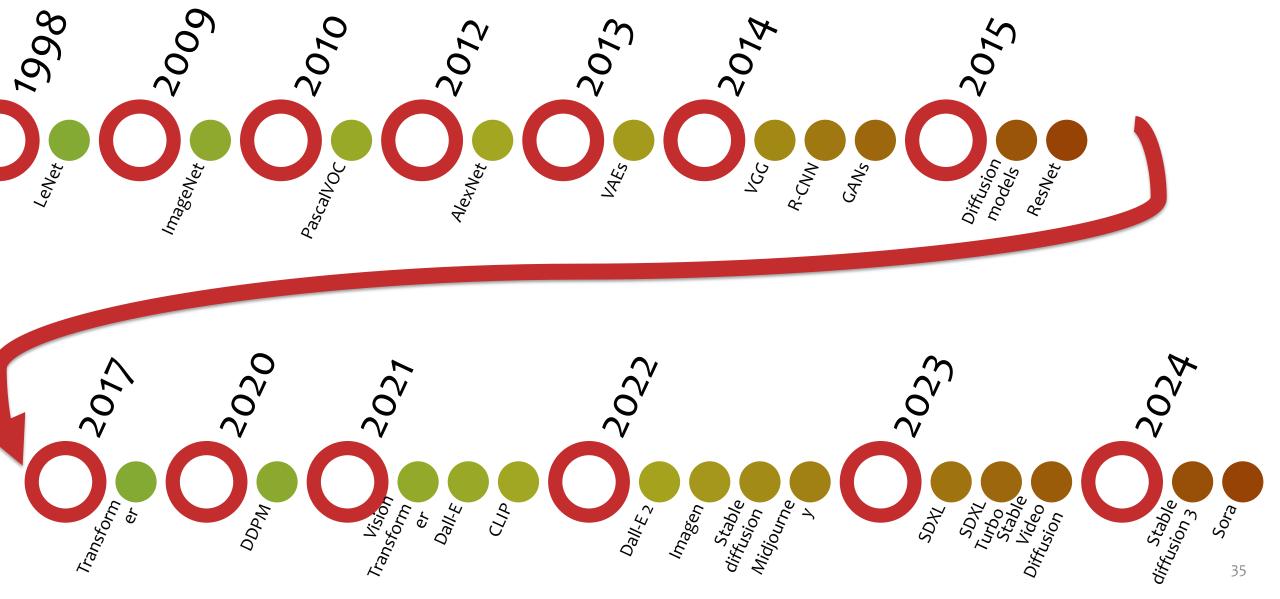
Cost to train



Timeline: Language Modeling



Timeline: Image Generation

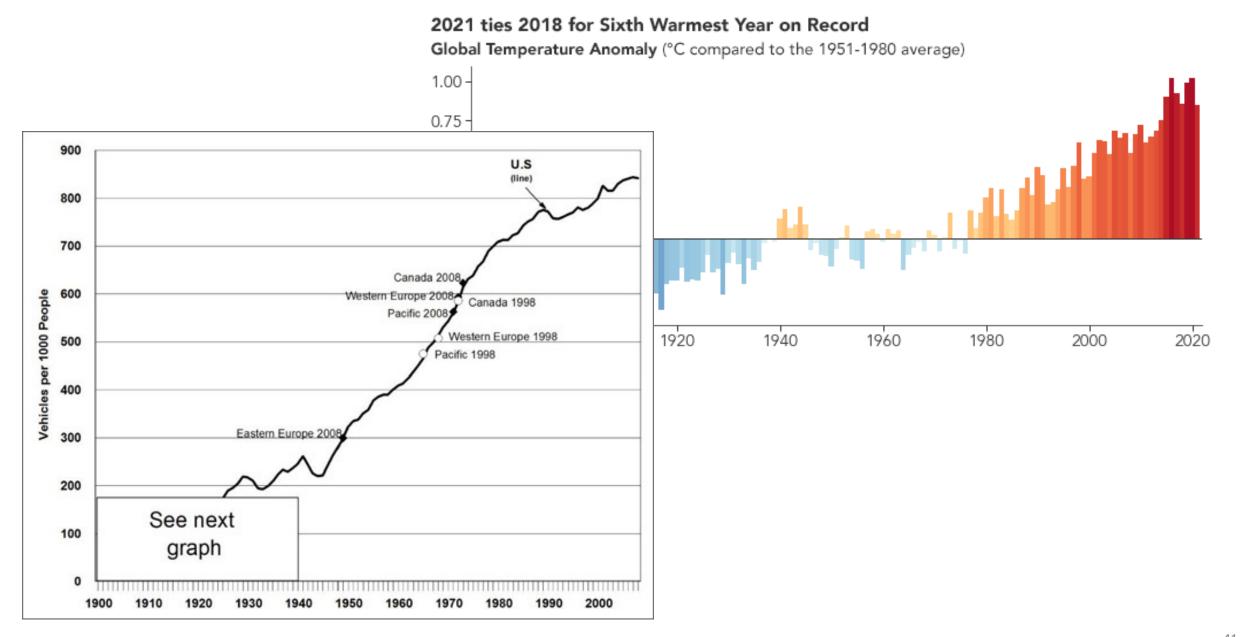


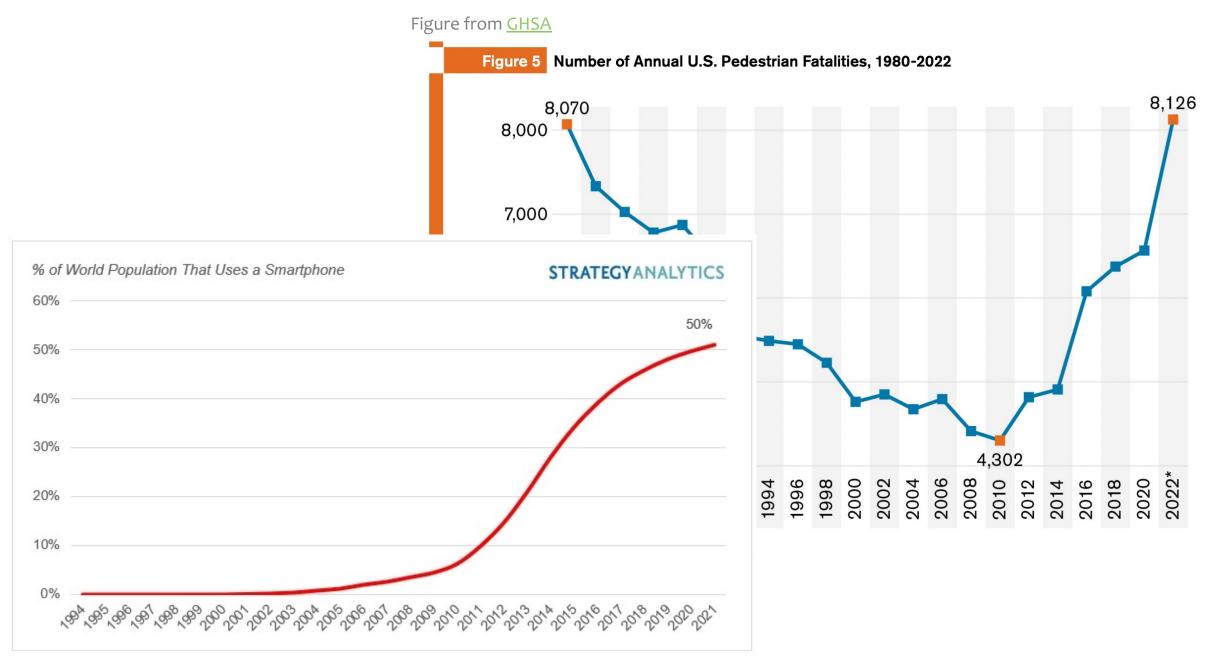
Why learn the innerworkings of GenAl?

(a metaphor)











GENERATIVE AI IS PROBABILISTIC MODELING

GenAl is Probabilistic Modeling

$$p(x_{t+1} \mid x_1, \ldots, x_t)$$

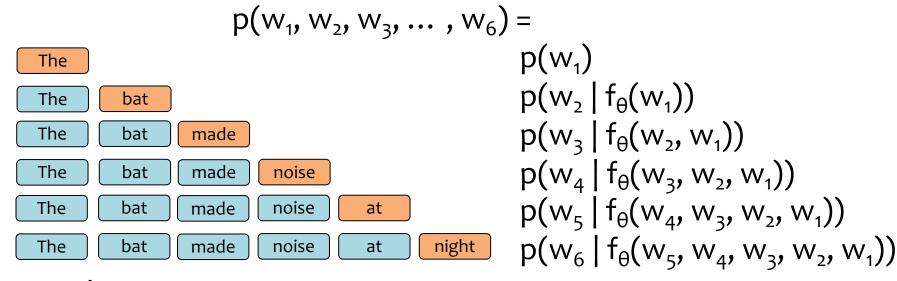
What if I want to model EVERY possible interaction?

... or at least the interactions of the current variable with all those that came before it...

(RNN-LMs)

RNN Language Model

RNN Language Model:
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid f_{\boldsymbol{\theta}}(w_{t-1}, \dots, w_1))$$



Key Idea:

- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector

Topics

- Generative models of text
 - RNN LMs / Autodiff
 - Transformer LMs
 - Pre-training, fine-tuning, evaluation, decoding
- Generative models of images
 - CNNs / Transformers for vision
 - GANs, Conditional GANs
 - VAEs and Diffusion models
- Applying and adapting foundation models
 - Reinforcement learning with human feedback (RLHF)
 - Parameter-efficient fine tuning
 - In-context learning for text
 - In-context learning for vision
- Multimodal foundation models
 - Text-to-image generation
 - Aligning multimodal representations
 - Visual-language foundation models

- Scaling models
 - Efficient decoding strategies
 - Distributed training
 - Scaling laws and data
 - Mixture of experts / FlashAttention
- What can go wrong?
 - Safety/bias/fairness, Hallucinations, Adversarial (e.g., prompt injection) attacks
 - Cheating how to watermark, Legal issues, e.g., copyright,...
 - Drift in performance, Data contamination, Lack of ground truth
- Advanced Topics
 - State space models
 - Code generation
 - Audio understanding and synthesis
 - Video synthesis

SYLLABUS HIGHLIGHTS

Syllabus Highlights

The syllabus is located on the course webpage:

http://423.mlcourse.org http://623.mlcourse.org



https://www.cs.cmu.edu/~mgormley/courses/10423/

The course policies are required reading.

Syllabus Highlights

- Grading: 40% homework, 10% quizzes, 20%
 exam, 25% project, 5% participation
- Exam: in-class exam, Mon, Mar. 31
- Homework: 5 assignments
 - 8 grace days for homework assignments
 - Late submissions: 80% day 1, 60% day 2, 40% day 3, 20% day 4
 - No submissions accepted after 4 days w/o extension
 - Extension requests: only for emergency situations, see syllabus
- Recitations: Fridays, same time/place as lecture (optional, interactive sessions)
- Readings: required, online PDFs, recommended for after lecture

Technologies:

- Piazza (discussion),
- Gradescope (homework),
- Google Forms (polls),
- Zoom (livestream),
- Panopto (video recordings)

Academic Integrity:

- Collaboration encouraged, but must be documented
- Solutions must always be written independently
- No re-use of found code / past assignments
- Severe penalties (i.e., failure)
- (Policies differ from 10-301/10-601)
- Office Hours: posted on Google Calendar on "Office Hours" page

Lectures

- You should ask lots of questions
 - Interrupting (by raising a hand) to ask your question is strongly encouraged
 - Asking questions later (or in real time) on Piazza is also great
- When I ask a question...
 - I want you to answer
 - Even if you don't answer, think it through as though I'm about to call on you
- Interaction improves learning (both in-class and at my office hours)

Prerequisites

What they are:

Introductory machine learning. (i.e. 10-301, 10-315, 10-601, 10-701)

If you instead took an introduction to deep learning course, that is also fine (i.e. 11-485/11-685/11-785)

What is not required:

- Deep learning
- PyTorch

Depending on which prerequisite course you took and in which semester you took it, you may or may not have been exposed to deep learning and/or PyTorch.

Either way is fine.

Homework

There will be 5 homework assignments during the semester. The assignments will consist of both conceptual and programming problems.

	Main Topic	Implementation	Application Area	Туре
HWo	PyTorch Primer	image classifier + Text classifier	vision + language	written + programming
HW1	Large Language Models	TransformerLM with GQA and RoPE	text gen	written + programming
HW2	Image Generation	Diffusion model	image gen	written + programming
HW3	Adapters for LLMs	GPT-2 + LoRA	instruction fine- tuning	written + programming
HW4	Multimodal Foundation Models	text-to-image editing model	vision + language	written + programming
HW623	(10-623 only)	read / analyze a recent research paper	genAl	video presentation

Project

Goals:

- Explore a generative modeling technique of your choosing
- Deeper understanding of methods in real-world application
- Report back to the class during a poster session to be held sometime over finals period
- Work in teams of 3 students



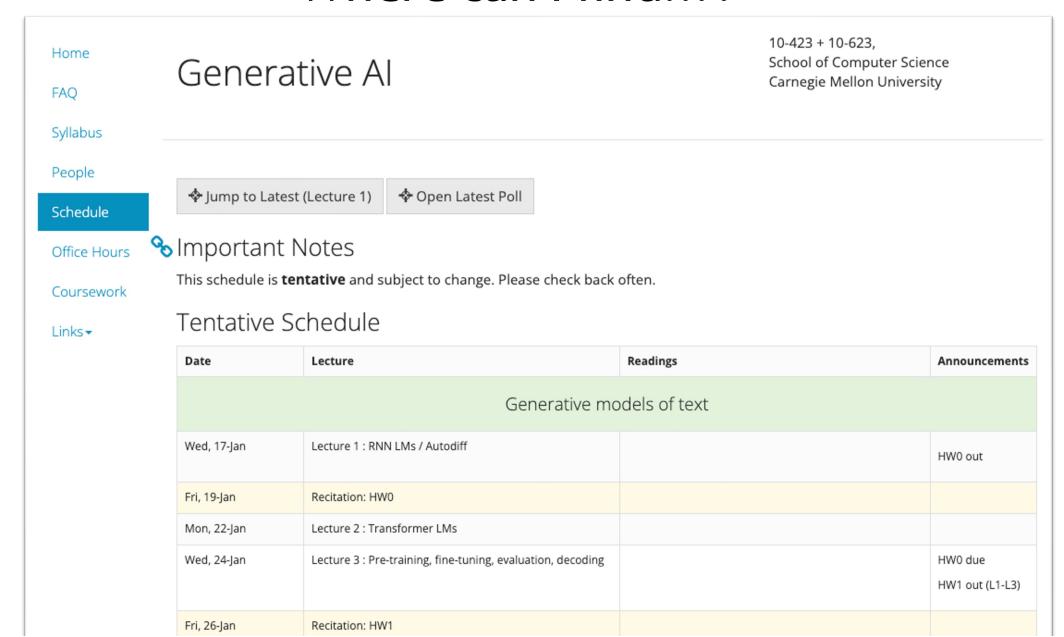
Prompt to ChatGPT-4o: Create an image of three Scottish terriers in traditional Scottish outfits working collaboratively on a project for a generative AI course

Textbooks

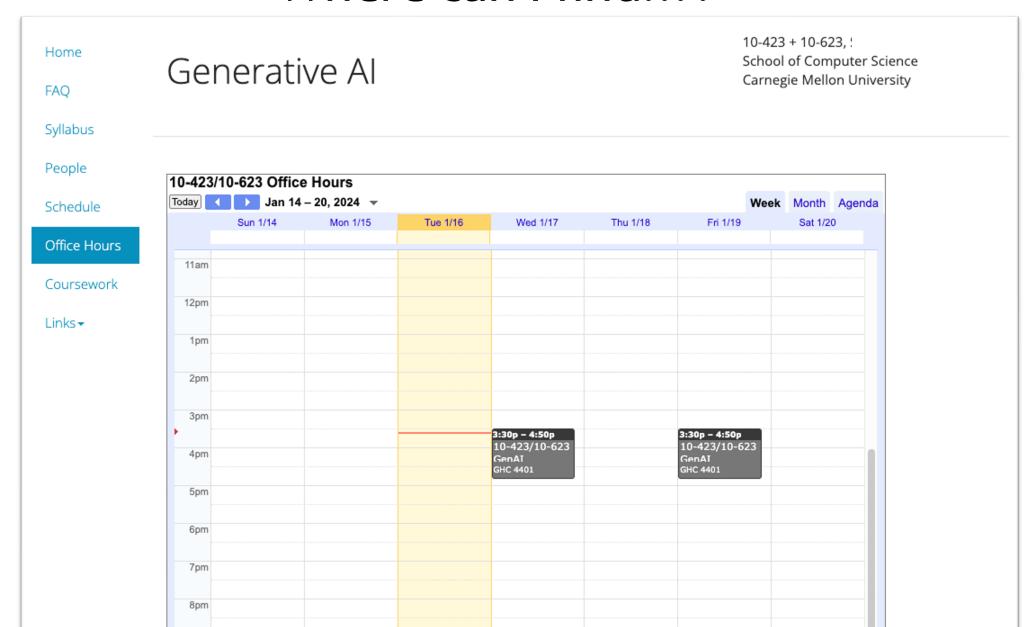
... do not exist for this course.

Instead, we will be directing your reading time to current research papers.

Where can I find...?



Where can I find...?



Where can I find...?

Home

FAQ

Generative Al

10-423 + 10-623, ! School of Computer Science

Carnegie Mellon University

Syllabus

People

Schedule

Office Hours

Coursework

Links **▼**

Assignments

There will be 5 homework assignments (and a special extra assignment for 10-623 only). The assignments will consist of both theoretical and programming problems. Homework assignments will be released via a Piazza announcement explaining where to find the handout, LaTeX template, etc.

- Homework 0: PyTorch Primer
- · Homework 1: Large Language Models
- · Homework 2: Image Generation
- · Homework 3: Adapters for LLMs
- · Homework 4: Multimodal Foundation Models
- Homework 623: (10-623 only)

Tentative release dates and due dates are listed on the Schedule page.



There will be 5 quizzes.

- Quiz 1 (Lectures 1 3)
- Quiz 2 (Lectures 4 7)
- Quiz 3 (Lectures 8 11)
- Quiz 4 (Lectures 12 15)
- Quiz 5 (Lectures 16 20)

Reminders

- Homework 0: PyTorch + Weights & Biases
 - Out: Wed, Jan 17
 - Due: Mon, Jan 27 at 11:59pm
 - Two parts:
 - 1. written part to Gradescope
 - 2. programming part to Gradescope
 - unique policy for this assignment: we will grant (essentially) any and all extension requests

Learning Objectives

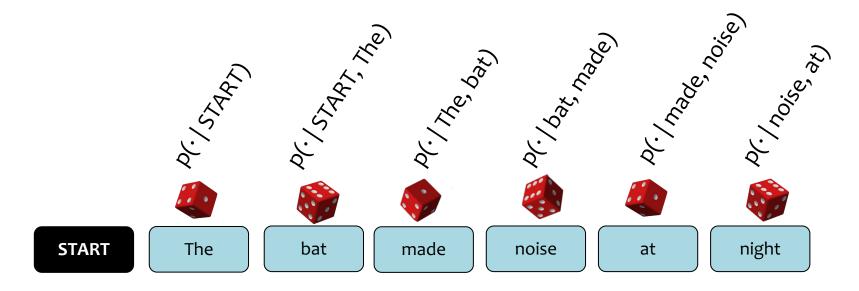
You should be able to...

- Differentiate between different mechanisms of learning such as parameter tuning and in-context learning.
- 2. Implement the foundational models underlying modern approaches to generative modeling, such as transformers and diffusion models.
- 3. Apply existing models to real-world generation problems for text, code, images, audio, and video.
- 4. Employ techniques for adapting foundation models to tasks such as fine-tuning, adapters, and in-context learning.
- 5. Enable methods for generative modeling to scale-up to large datasets of text, code, or images.
- Use existing generative models to solve real-world discriminative problems and for other everyday use cases.
- 7. Analyze the theoretical properties of foundation models at scale.
- 8. Identify potential pitfalls of generative modeling for different modalities.
- 9. Describe societal impacts of large-scale generative AI systems.

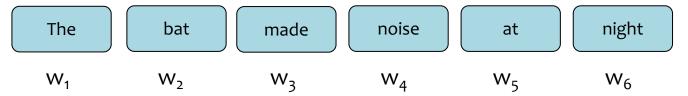
Q&A

BACKGROUND: N-GRAM LANGUAGE MODELS

- <u>Goal</u>: Generate realistic looking sentences in a human language
- <u>Key Idea</u>: condition on the last n-1 words to sample the nth word



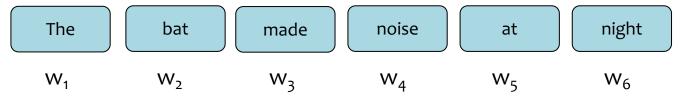
The Chain Rule of Probability



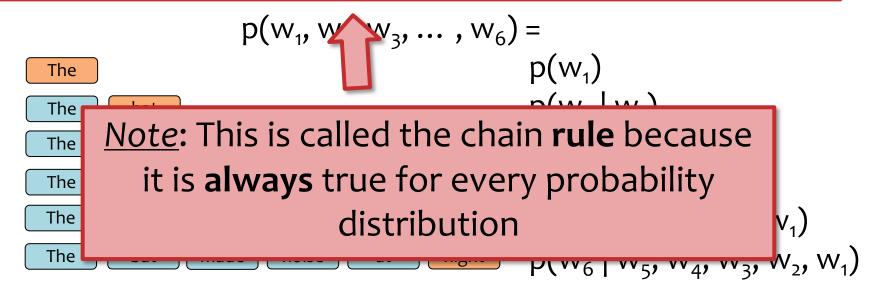
$$p(w_{1},w_{2},w_{3},\ldots,w_{6}) = \\ p(w_{1}) \\ The & bat & p(w_{2} \mid w_{1}) \\ The & bat & made & p(w_{3} \mid w_{2},w_{1}) \\ The & bat & made & noise & p(w_{4} \mid w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & p(w_{5} \mid w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & p(w_{6} \mid w_{5},w_{4},w_{3},w_{2},w_{1}) \\ The & bat & made & noise & at & night & noise &$$

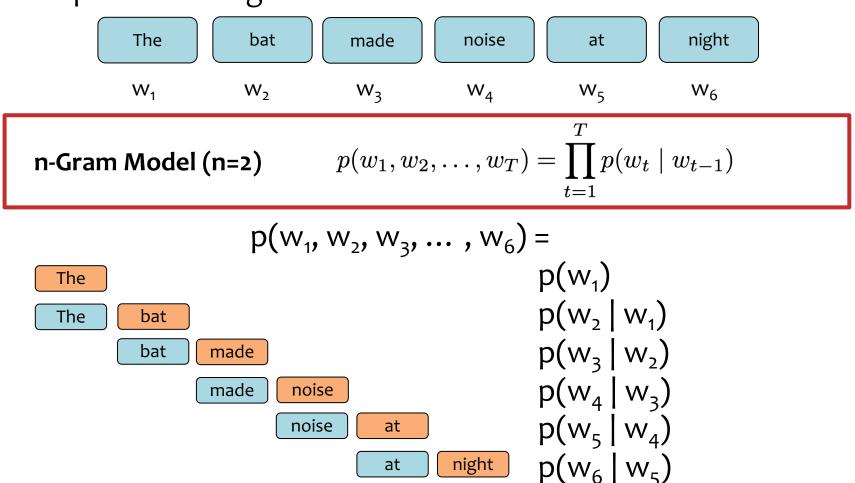
The Chain Rule of Probability

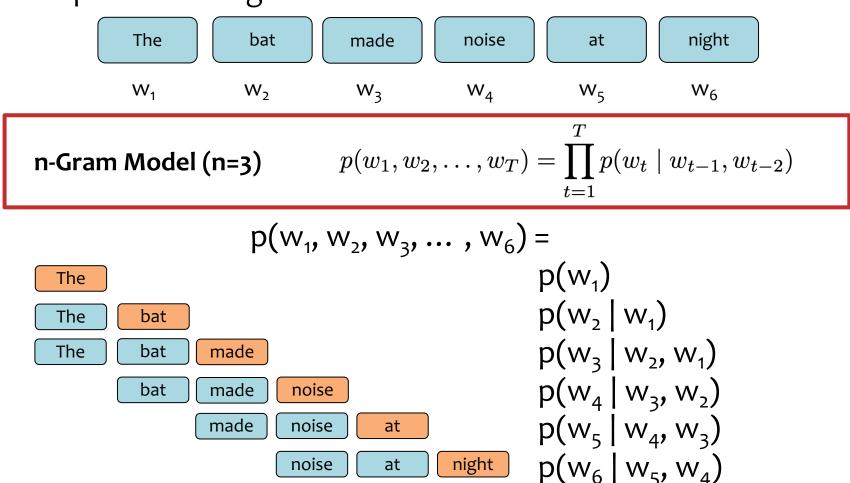
<u>Question</u>: How can we **define** a probability distribution over a sequence of length T?

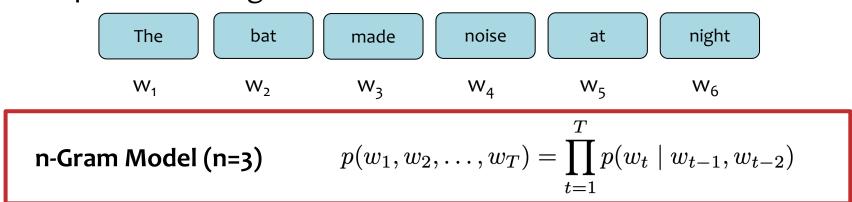


Chain rule of probability: $p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid w_{t-1}, \dots, w_1)$







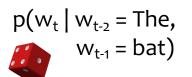


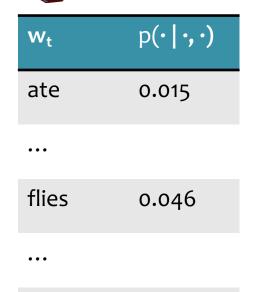
$$p(w_1, w_2, ..., w_6) = p(w_1)$$

The Note: This is called a **model** because we made some **assumptions** about how many previous words to condition on (i.e. only n-1 words)

Learning an n-Gram Model

<u>Question</u>: How do we **learn** the probabilities for the n-Gram Model?



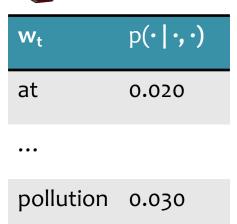


0.000

zebra

$$p(w_t | w_{t-2} = made,$$

 $w_{t-1} = noise)$



0.000

...

zebra

	v _{t-1} = eat)
W _t	p(· ·,·)
corn	0.420
•••	
grass	0.510
•••	

0.000

zebra

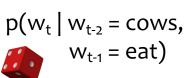
 $p(w_t | w_{t-2} = cows,$

Learning an n-Gram Model

<u>Question</u>: How do we **learn** the probabilities for the n-Gram Model?

Answer: From data! Just count n-gram frequencies

```
... the cows eat grass...
... our cows eat hay daily...
... factory-farm cows eat corn...
... on an organic farm, cows eat hay and...
... do your cows eat grass or corn?...
... what do cows eat if they have...
... cows eat corn when there is no...
... which cows eat which foods depends...
... if cows eat grass...
... when cows eat corn their stomachs...
... should we let cows eat corn?...
```

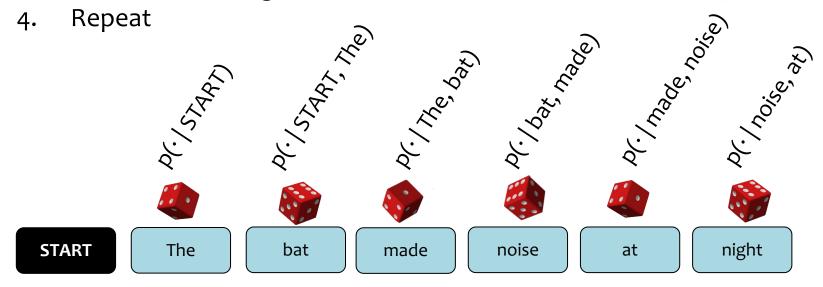


W _t	p(· ·,·)
corn	4/11
grass	3/11
hay	2/11
if	1/11
which	1/11

Sampling from a Language Model

<u>Question</u>: How do we sample from a Language Model? <u>Answer</u>:

- 1. Treat each probability distribution like a (50k-sided) weighted die
- 2. Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w_t lands face up



Sampling from a Language Model

<u>Question</u>: How do we sample from a Language Model? Answer:

- 1. Treat each probability distribution like a (50k-sided) weighted die
- 2. Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w_t lands face up
- 4. Repeat

Training Data (Shakespeaere)

I tell you, friends, most charitable care ave the patricians of you. For your wants, Your suffering in this dearth, you may as well Strike at the heaven with your staves as lift them Against the Roman state, whose course will on The way it takes, cracking ten thousand curbs Of more strong link asunder than can ever Appear in your impediment. For the dearth, The gods, not the patricians, make it, and Your knees to them, not arms, must help.

5-Gram Model

Approacheth, denay. dungy
Thither! Julius think: grant,—O
Yead linens, sheep's Ancient,
Agreed: Petrarch plaguy Resolved
pear! observingly honourest
adulteries wherever scabbard
guess; affirmation—his monsieur;
died. jealousy, chequins me.
Daphne building. weakness: sun—
rise, cannot stays carry't,
unpurposed. prophet—like drink;
back—return 'gainst surmise
Bridget ships? wane; interim?
She's striving wet;

RECURRENT NEURAL NETWORK (RNN) LANGUAGE MODELS

Recurrent Neural Networks (RNNs)

inputs:
$$\mathbf{x} = (x_1, x_2, \dots, x_T), x_i \in \mathcal{R}^I$$

hidden units: $\mathbf{h} = (h_1, h_2, \dots, h_T), h_i \in \mathcal{R}^J$

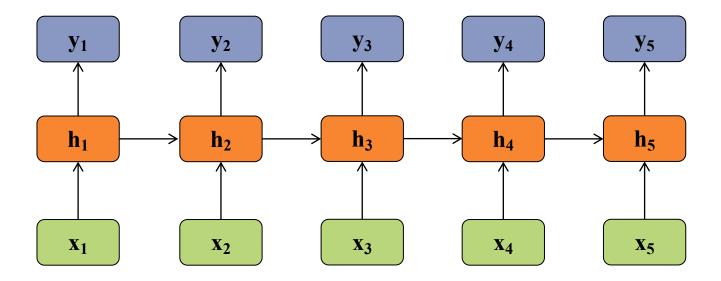
outputs:
$$\mathbf{y} = (y_1, y_2, \dots, y_T), y_i \in \mathcal{R}^K$$
 $y_t = W_{hy}h_t + b_y$

nonlinearity: \mathcal{H}

Definition of the RNN:

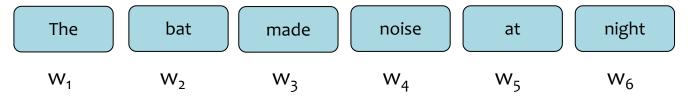
$$h_t = \mathcal{H}\left(W_{xh}x_t + W_{hh}h_{t-1} + b_h\right)$$

$$y_t = W_{hy}h_t + b_y$$

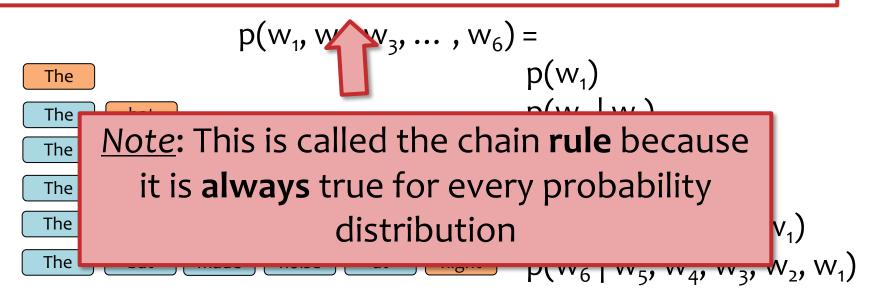


The Chain Rule of Probability

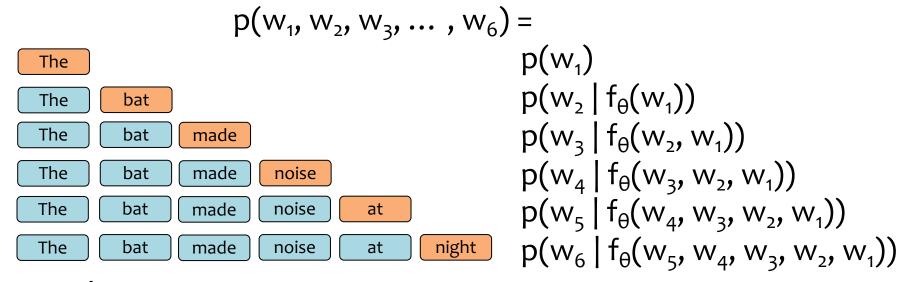
<u>Question</u>: How can we **define** a probability distribution over a sequence of length T?



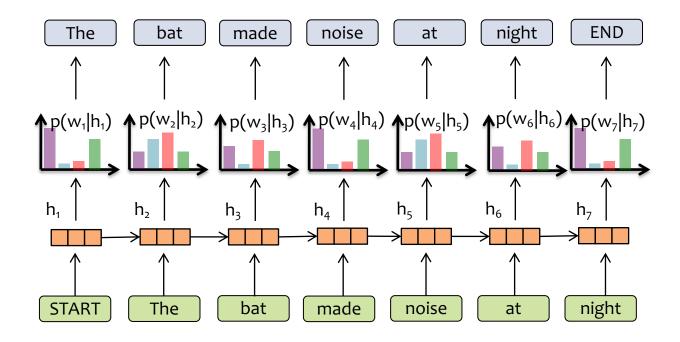
Chain rule of probability: $p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid w_{t-1}, \dots, w_1)$



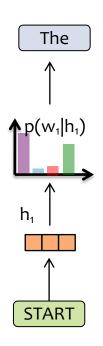
RNN Language Model:
$$p(w_1, w_2, \dots, w_T) = \prod_{t=1}^T p(w_t \mid f_{\boldsymbol{\theta}}(w_{t-1}, \dots, w_1))$$



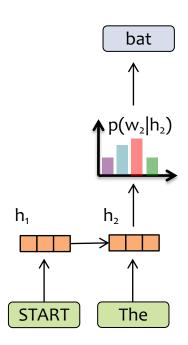
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector



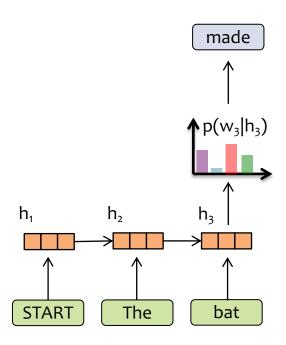
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



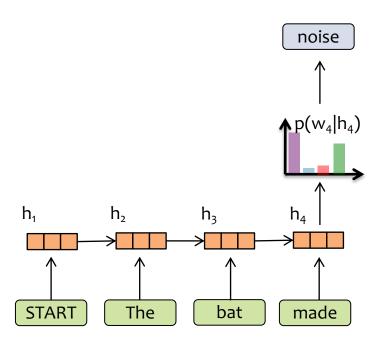
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



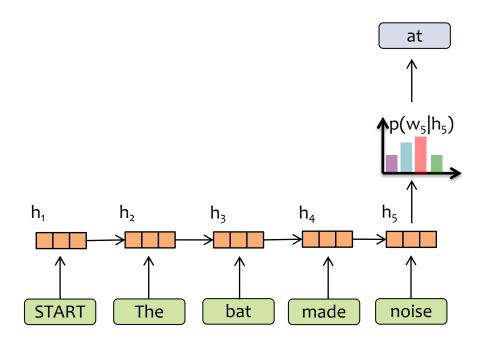
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



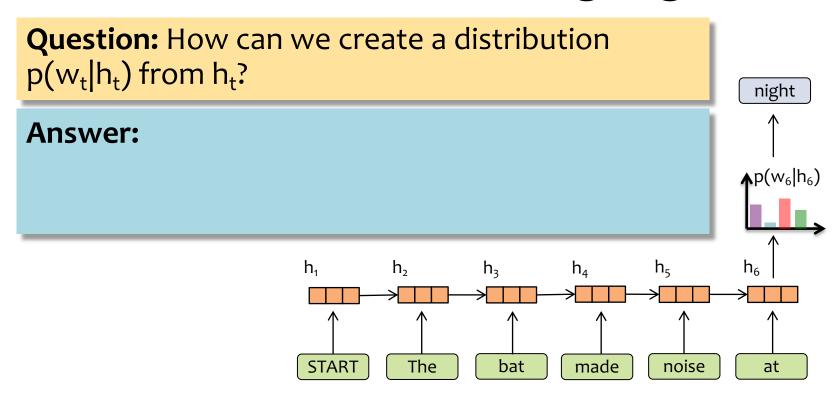
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



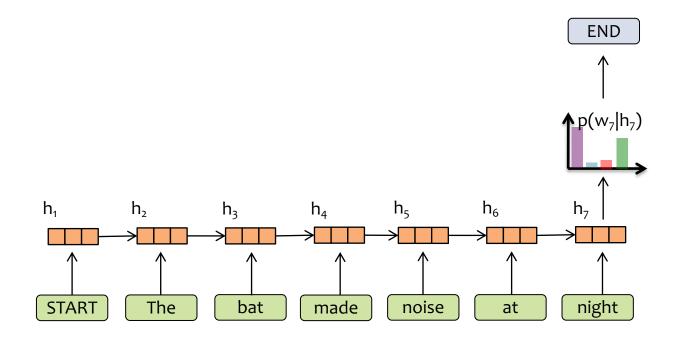
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



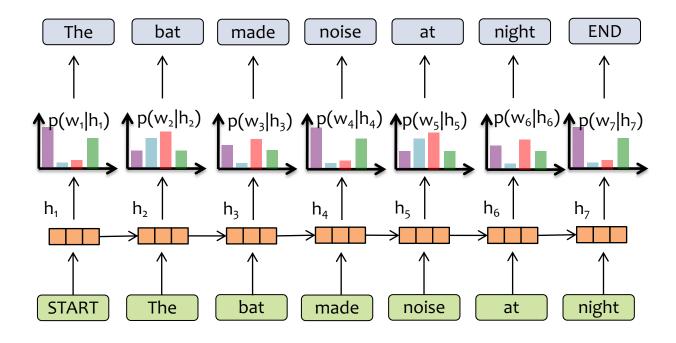
- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$



- (1) convert all previous words to a fixed length vector
- (2) define distribution $p(w_t | f_{\theta}(w_{t-1}, ..., w_1))$ that conditions on the vector $\mathbf{h}_t = f_{\theta}(w_{t-1}, ..., w_1)$

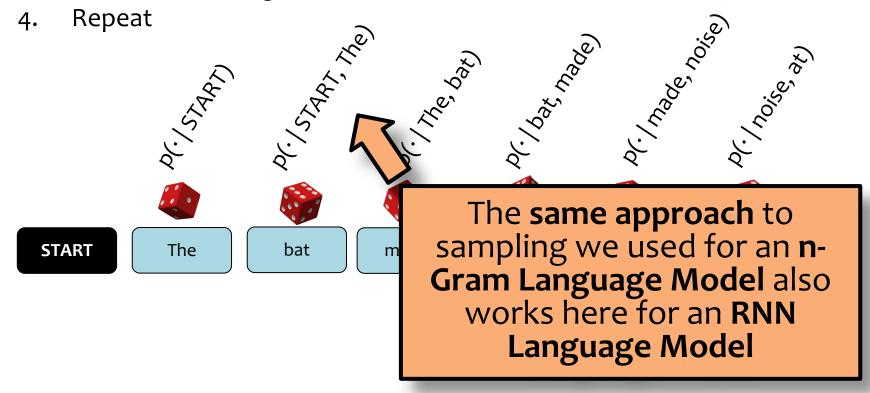


$$p(w_1, w_2, w_3, ..., w_T) = p(w_1 | h_1) p(w_2 | h_2) ... p(w_2 | h_T)$$

Sampling from a Language Model

<u>Question</u>: How do we sample from a Language Model? <u>Answer</u>:

- 1. Treat each probability distribution like a (50k-sided) weighted die
- 2. Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$
- 3. Roll that die and generate whichever word w_t lands face up



??

her wine.

VIOLA: Why, Salisbury must find his flesh and thought
That which I am not aps, not a man and in fire, To show
the reining of the raven and the wars To grace my hand
reproach within, and not a fair are hand, That Caesar and
my goodly father's world; When I was heaven of
presence and our fleets, We spare with hours, but cut thy
council I am great, Murdered and by thy m
there My power to give thee but so much
service in the noble bondman here, Would

KING LEAR: O, if you were a feeble state, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

??

CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without some broken limb shall acquit him well. Your brother is ender; and, for your love, I would be as I must, for my own honour, if he re, out of my love to you, I came hither withal, that either you might stay him from his intends or brook such disgrace well as he shall run into, in the list at him gof his own search and

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

altogether against my will.

Shakespeare's As You Like It

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of presence and our fleets, We spare with hours, but cut thy council I am great, Murdered and by thy master's ready there My power to give thee but so much as hell: Some service in the noble bondman here, Would show him to her wine.

KING LEAR: O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

RNN-LM Sample

CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without some broken limb shall acquit him well. Your brother is but young and tender; and, for your love, I would be loath to foil him, as I must, for my own honour, if he come in: therefore, out of my love to you, I came hither to acquaint you withal, that either you might stay him from his intendment or brook such disgrace well as he shall run into, in that it is a thing of his own search and altogether against my will.

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

RNN-LM Sample

VIOLA: Why, Salisbury must find his flesh and thought That which I am not aps, not a man and in fire, To show the reining of the raven and the wars To grace my hand reproach within, and not a fair are hand, That Caesar and my goodly father's world; When I was heaven of presence and our fleets, We spare with hours, but cut thy council I am great, Murdered and by thy master's ready there My power to give thee but so much as hell: Some service in the noble bondman here, Would show him to her wine.

KING LEAR: O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

Shakespeare's As You Like It

CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without some broken limb shall acquit him well. Your brother is but young and tender; and, for your love, I would be loath to foil him, as I must, for my own honour, if he come in: therefore, out of my love to you, I came hither to acquaint you withal, that either you might stay him from his intendment or brook such disgrace well as he shall run into, in that it is a thing of his own search and altogether against my will.

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

??

VIOLA: Why, Salisbury must find his flesh and thought
That which I am not aps, not a man and in fire, To show
the reining of the raven and the wars To grace my hand
reproach within, and not a fair are hand, That Caesar and
my goodly father's world; When I was heaven of
presence and our fleets, We spare with hours, but cut thy
council I am great, Murdered and by thy m
there My power to give thee but so much
service in the noble bondman here, Would
her wine.

KING LEAR: O, if you were a feeble state, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

??

CHARLES: Marry, do I, sir; and I came to acquaint you with a matter. I am given, sir, secretly to understand that your younger brother Orlando hath a disposition to come in disguised against me to try a fall. To-morrow, sir, I wrestle for my credit; and he that escapes me without some broken limb shall acquit him well. Your brother is ender; and, for your love, I would be as I must, for my own honour, if he re, out of my love to you, I came hither withal, that either you might stay him from his intends or brook such disgrace well as he shall run into, in the list at him gof his own search and

TOUCHSTONE: For my part, I had rather bear with you than bear you; yet I should bear no cross if I did bear you, for I think you have no money in your purse.

altogether against my will.

MODULE-BASED AUTOMATIC DIFFERENTIATION

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

- Write an **algorithm** for evaluating the function y = f(x). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation**" graph")
- 2. Visit each node in **topological order**.

For variable u_i with inputs $v_1, ..., v_N$ a. Compute $u_i = g_i(v_1, ..., v_N)$ b. Store the result at the node

Backward Computation (Version A)

- **Initialize** dy/dy = 1.

Visit each node v_j in **reverse topological order**. Let $u_1, ..., u_M$ denote all the nodes with v_j as an input

- Assuming that $y = h(\mathbf{u}) = h(\mathbf{u}_1, ..., \mathbf{u}_M)$ and $\mathbf{u} = g(\mathbf{v})$ or equivalently $\mathbf{u}_i = g_i(v_1, ..., v_j, ..., v_N)$ for all ia. We already know dy/du_i for all ib. Compute dy/dv_i as below (Choice of algorithm ensures computing

 $\frac{(du_i/dv_j) \text{ is easy}}{dv_j} = \sum_{i=1}^{M} \frac{dy}{du_i} \frac{du_i}{dv_j}$

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

Forward Computation

- Write an **algorithm** for evaluating the function y = f(x). The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation**" graph")
- 2. Visit each node in **topological order**.

For variable u_i with inputs $v_1, ..., v_N$ a. Compute $u_i = g_i(v_1, ..., v_N)$ b. Store the result at the node

Backward Computation (Version B)

- **Initialize** all partial derivatives dy/du_i to 0 and dy/dy = 1.
- Visit each node in reverse topological order.

For variable $u_i = g_i(v_1, ..., v_N)$

- a. We already know dy/du_i
- b. Increment dy/dv_j by (dy/du_i)(du_i/dv_j)
 (Choice of algorithm ensures computing (du_i/dv_i) is easy)

Backpropagation: Procedural Method

Algorithm 1 Forward Computation

```
1: procedure NNFORWARD(Training example (\mathbf{x}, \mathbf{y}), Params \alpha, \beta)
2: \mathbf{a} = \alpha \mathbf{x}
3: \mathbf{z} = \sigma(\mathbf{a})
4: \mathbf{b} = \beta \mathbf{z}
5: \hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{b})
6: J = -\mathbf{y}^T \log \hat{\mathbf{y}}
7: \mathbf{o} = \operatorname{object}(\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J)
8: return intermediate quantities \mathbf{o}
```

Algorithm 2 Backpropagation

```
1: procedure NNBACKWARD(Training example (\mathbf{x}, \mathbf{y}), Params \alpha, \beta, Intermediates \mathbf{o})

2: Place intermediate quantities \mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J in \mathbf{o} in scope

3: \mathbf{g}_{\hat{\mathbf{y}}} = -\mathbf{y} \div \hat{\mathbf{y}}

4: \mathbf{g}_{\mathbf{b}} = \mathbf{g}_{\hat{\mathbf{y}}}^T \left( \operatorname{diag}(\hat{\mathbf{y}}) - \hat{\mathbf{y}}\hat{\mathbf{y}}^T \right)

5: \mathbf{g}_{\beta} = \mathbf{g}_{\mathbf{b}}^T \mathbf{z}^T

6: \mathbf{g}_{\mathbf{z}} = \beta^T \mathbf{g}_{\mathbf{b}}^T

7: \mathbf{g}_{\mathbf{a}} = \mathbf{g}_{\mathbf{z}} \odot \mathbf{z} \odot (1 - \mathbf{z})

8: \mathbf{g}_{\alpha} = \mathbf{g}_{\mathbf{a}} \mathbf{x}^T

9: return parameter gradients \mathbf{g}_{\alpha}, \mathbf{g}_{\beta}
```

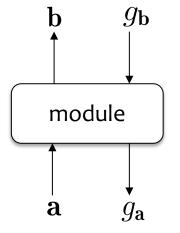
Drawbacks of Procedural Method

- Hard to reuse / adapt for other models
- 2. (Possibly) harder to make individual steps more efficient
- of error if finitedifference check reports an error (since it tells you only that there is an error somewhere in those 17 lines of code)

Module-based AutoDiff

Key Idea:

- componentize the computation of the neural-network into layers
- each layer consolidates multiple real-valued nodes in the computation graph (a subset of them) into one vector-valued node (aka. a module)
- Each module is capable of two actions:
 - 1. Forward computation of output $\mathbf{b} = [b_1, \dots, b_B]$ given input $\mathbf{a} = [a_1, \dots, a_A]$ via some differentiable function f. That is $\mathbf{b} = f(\mathbf{a})$.



2. Backward computation of the gradient of the input $\mathbf{g_a} = \nabla_{\mathbf{a}} J = \left[\frac{\partial J}{\partial a_1}, \ldots, \frac{\partial J}{\partial a_A}\right]$ given the gradient of output $\mathbf{g_b} = \nabla_{\mathbf{b}} J = \left[\frac{\partial J}{\partial b_1}, \ldots, \frac{\partial J}{\partial b_B}\right]$, where J is the final real-valued output of the entire computation graph. This is done via the chain rule $\frac{\partial J}{\partial a_i} = \sum_{j=1}^J \frac{\partial J}{\partial b_j} \frac{db_j}{da_i}$ for all $i \in \{1, \ldots, A\}$.

Module-based AutoDiff

Dimensions: input $\mathbf{a} \in \mathbb{R}^A$, output $\mathbf{b} \in \mathbb{R}^B$, gradient of output $\mathbf{g_a} \triangleq \nabla_{\mathbf{a}} J \in \mathbb{R}^A$, and gradient of input $\mathbf{g_b} \triangleq \nabla_{\mathbf{b}} J \in \mathbb{R}^B$.

```
Sigmoid Module The sigmoid layer has only one input vector \mathbf{a}. Below \sigma is the sigmoid applied elementwise, and \odot is element-wise multiplication s.t. \mathbf{u}\odot \mathbf{v}=[u_1v_1,\ldots,u_Mv_M].

1: procedure SIGMOIDFORWARD(a)

2: \mathbf{b}=\sigma(\mathbf{a})

3: return \mathbf{b}

4: procedure SIGMOIDBACKWARD(a, b, \mathbf{g}_\mathbf{b})

5: \mathbf{g}_\mathbf{a}=\mathbf{g}_\mathbf{b}\odot\mathbf{b}\odot(1-\mathbf{b})

6: return \mathbf{g}_\mathbf{a}
```

Softmax Module The softmax layer has only one input vector \mathbf{a} . For any vector $\mathbf{v} \in \mathbb{R}^D$, we have that $\operatorname{diag}(\mathbf{v})$ returns a $D \times D$ diagonal matrix whose diagonal entries are v_1, v_2, \ldots, v_D and whose non-diagonal entries are zero.

```
diagonal entries are zero.

1: procedure SOFTMAXFORWARD(a)

2: \mathbf{b} = \operatorname{softmax}(\mathbf{a})

3: return \mathbf{b}

4: procedure SOFTMAXBACKWARD(a, b, \mathbf{g_b})

5: \mathbf{g_a} = \mathbf{g_b}^T \left( \operatorname{diag}(\mathbf{b}) - \mathbf{bb}^T \right)

6: return \mathbf{g_a}
```

Linear Module The linear layer has two inputs: a vector \mathbf{a} and parameters $\omega \in \mathbb{R}^{B \times A}$. The output \mathbf{b} is not used by LINEARBACKWARD, but we pass it in for consistency of form.

```
1: procedure LINEARFORWARD(\mathbf{a}, \boldsymbol{\omega})
2: \mathbf{b} = \boldsymbol{\omega}\mathbf{a}
3: return \mathbf{b}
4: procedure LINEARBACKWARD(\mathbf{a}, \boldsymbol{\omega}, \mathbf{b}, \mathbf{g_b})
5: \mathbf{g}_{\boldsymbol{\omega}} = \mathbf{g_b}\mathbf{a}^T
6: \mathbf{g_a} = \boldsymbol{\omega}^T\mathbf{g_b}
7: return \mathbf{g}_{\boldsymbol{\omega}}, \mathbf{g_a}
```

Cross-Entropy Module The cross-entropy layer has two inputs: a gold one-hot vector \mathbf{a} and a predicted probability distribution $\hat{\mathbf{a}}$. It's output $b \in \mathbb{R}$ is a scalar. Below \div is element-wise division. The output b is not used by CrossEntropyBackward, but we pass it in for consistency of form.

```
1: procedure CROSSENTROPYFORWARD(\mathbf{a}, \hat{\mathbf{a}})
2: b = -\mathbf{a}^T \log \hat{\mathbf{a}}
3: return \mathbf{b}
4: procedure CROSSENTROPYBACKWARD(\mathbf{a}, \hat{\mathbf{a}}, b, g_b)
5: \mathbf{g}_{\hat{\mathbf{a}}} = -g_b(\mathbf{a} \div \hat{\mathbf{a}})
6: return \mathbf{g}_{\mathbf{a}}
```

Module-based AutoDiff

Algorithm 1 Forward Computation

```
1: procedure NNFORWARD(Training example (x, y), Parameters \alpha, \beta)

2: \mathbf{a} = \text{LINEARFORWARD}(\mathbf{x}, \alpha)

3: \mathbf{z} = \text{SIGMOIDFORWARD}(\mathbf{a})

4: \mathbf{b} = \text{LINEARFORWARD}(\mathbf{z}, \beta)

5: \hat{\mathbf{y}} = \text{SOFTMAXFORWARD}(\mathbf{b})

6: J = \text{CROSSENTROPYFORWARD}(\mathbf{y}, \hat{\mathbf{y}})

7: \mathbf{o} = \text{object}(\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J)

8: return intermediate quantities \mathbf{o}
```

Algorithm 2 Backpropagation

```
1: procedure NNBACKWARD(Training example (\mathbf{x}, \mathbf{y}), Parameters \alpha, \beta, Intermediates \mathbf{o})

2: Place intermediate quantities \mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J in \mathbf{o} in scope

3: g_J = \frac{dJ}{dJ} = 1 \triangleright Base case

4: \mathbf{g}_{\hat{\mathbf{y}}} = \mathsf{CROSSENTROPYBACKWARD}(\mathbf{y}, \hat{\mathbf{y}}, J, g_J)

5: \mathbf{g}_{\mathbf{b}} = \mathsf{SOFTMAXBACKWARD}(\mathbf{b}, \hat{\mathbf{y}}, \mathbf{g}_{\hat{\mathbf{y}}})

6: \mathbf{g}_{\beta}, \mathbf{g}_{\mathbf{z}} = \mathsf{LINEARBACKWARD}(\mathbf{z}, \mathbf{b}, \mathbf{g}_{\mathbf{b}})

7: \mathbf{g}_{\mathbf{a}} = \mathsf{SIGMOIDBACKWARD}(\mathbf{a}, \mathbf{z}, \mathbf{g}_{\mathbf{z}})

8: \mathbf{g}_{\alpha}, \mathbf{g}_{\mathbf{x}} = \mathsf{LINEARBACKWARD}(\mathbf{x}, \mathbf{a}, \mathbf{g}_{\mathbf{a}}) \triangleright We discard \mathbf{g}_{\mathbf{x}}

9: return parameter gradients \mathbf{g}_{\alpha}, \mathbf{g}_{\beta}
```

Advantages of Module-based AutoDiff

- Easy to reuse / adapt for other models
- Encapsulated layers are easier to optimize (e.g. implement in C++ or CUDA)
- 3. Easier to find bugs because we can run a finitedifference check on each layer separately

Module-based AutoDiff (OOP Version)

Object-Oriented Implementation:

- Let each module be an object
- Then allow the control flow dictate the creation of the computation graph
- No longer need to implement NNBackward(\cdot), just follow the computation graph in **reverse topological order**

```
class Sigmoid(Module)

method forward(a)

\mathbf{b} = \sigma(\mathbf{a})

return \mathbf{b}

method backward(\mathbf{a}, \mathbf{b}, \mathbf{g_b})

\mathbf{g_a} = \mathbf{g_b} \odot \mathbf{b} \odot (1 - \mathbf{b})

return \mathbf{g_a}
```

```
class Softmax(Module)

method forward(a)

b = softmax(a)

return b

method backward(a, b, g_b)

g_a = g_b^T (diag(b) - bb^T)

return g_a
```

```
class Linear(Module)

method forward(\mathbf{a}, \boldsymbol{\omega})

\mathbf{b} = \boldsymbol{\omega} \mathbf{a}

return \mathbf{b}

method backward(\mathbf{a}, \boldsymbol{\omega}, \mathbf{b}, \mathbf{g}_{\mathbf{b}})

\mathbf{g}_{\boldsymbol{\omega}} = \mathbf{g}_{\mathbf{b}} \mathbf{a}^{T}

\mathbf{g}_{\mathbf{a}} = \boldsymbol{\omega}^{T} \mathbf{g}_{\mathbf{b}}

return \mathbf{g}_{\boldsymbol{\omega}}, \mathbf{g}_{\mathbf{a}}
```

```
class CrossEntropy(Module)

method forward(\mathbf{a}, \hat{\mathbf{a}})

b = -\mathbf{a}^T \log \hat{\mathbf{a}}

return \mathbf{b}

method backward(\mathbf{a}, \hat{\mathbf{a}}, b, g_b)

\mathbf{g}_{\hat{\mathbf{a}}} = -g_b(\mathbf{a} \div \hat{\mathbf{a}})

return \mathbf{g}_{\mathbf{a}}
```

Module-based AutoDiff (OOP Version)

```
class NeuralNetwork (Module):
2
         method init()
3
               lin1_layer = Linear()
               sig_layer = Sigmoid()
               lin2 layer = Linear()
               soft layer = Softmax()
               ce layer = CrossEntropy()
         method forward (Tensor x, Tensor y, Tensor \alpha, Tensor \beta)
10
               \mathbf{a} = \text{lin1}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{x}, \boldsymbol{\alpha})
11
               z = sig_layer.apply_fwd(a)
12
               \mathbf{b} = \text{lin2}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{z}, \boldsymbol{\beta})
13
               \hat{\mathbf{y}} = \text{soft layer.apply fwd}(\mathbf{b})
               J = \text{ce}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{y}, \hat{\mathbf{y}})
15
               return J. out tensor
17
         method backward (Tensor x, Tensor y, Tensor \alpha, Tensor \beta)
18
               tape bwd()
               return lin1_layer.in_gradients[1], lin2_layer.in_gradients[1]
```

Module-based Auto Diff (OOP Version)

```
global tape = stack()
  class NeuralNetwork (Module):
                                                                          class Module:
2
        method init()
3
                                                                               method init()
             lin1_layer = Linear()
                                                                                    out tensor = null
             sig layer = Sigmoid()
                                                                                    out_gradient = 1
             lin2 layer = Linear()
             soft layer = Softmax()
                                                                               method apply_fwd(List in_modules)
                                                                      9
             ce layer = CrossEntropy()
                                                                      10
9
                                                                                    out tensor = forward(in tensors)
                                                                      11
        method forward (Tensor x, Tensor y, Tensor
10
                                                                                    tape.push(self)
                                                                      12
             \mathbf{a} = \text{lin1}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{x}, \boldsymbol{\alpha})
11
                                                                                    return self
                                                                      13
             z = sig_layer.apply_fwd(a)
12
                                                                      14
             \mathbf{b} = \lim_{\mathbf{z}} \operatorname{layer.apply\_fwd}(\mathbf{z}, \boldsymbol{\beta})
13
                                                                               method apply bwd():
                                                                      15
             \hat{\mathbf{y}} = \text{soft layer.apply fwd}(\mathbf{b})
                                                                      16
             J = \text{ce}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{y}, \hat{\mathbf{y}})
15
                                                                                    for i in 1,..., len(in_modules):
                                                                      17
             return J. out tensor
16
                                                                      18
17
                                                                                    return self
                                                                     19
         method backward (Tensor x, Tensor y, Tensor
18
                                                                     20
             tape bwd()
                                                                          function tape_bwd():
             return lin1_layer.in_gradients[1], lin2_la
                                                                               while len(tape) > 0
                                                                      22
```

```
in tensors = [x.out tensor for x in in modules]
          in gradients = backward(in tensors, out tensor, out gradient)
              in modules[i].out gradient += in gradients[i]
          m = tape.pop()
23
          m.apply bwd()
24
```

Module-based Auto Diff (OOP Version)

```
global tape = stack()
  class NeuralNetwork (Module):
                                                                          class Module:
2
        method init()
3
                                                                               method init()
             lin1_layer = Linear()
                                                                                    out tensor = null
             sig layer = Sigmoid()
                                                                                    out_gradient = 1
             lin2 layer = Linear()
             soft layer = Softmax()
                                                                               method apply_fwd(List in_modules)
                                                                      9
             ce layer = CrossEntropy()
                                                                      10
9
                                                                                    out tensor = forward(in tensors)
                                                                      11
        method forward (Tensor x, Tensor y, Tensor
10
                                                                                    tape.push(self)
                                                                      12
             \mathbf{a} = \text{lin1}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{x}, \boldsymbol{\alpha})
11
                                                                                    return self
                                                                      13
             z = sig_layer.apply_fwd(a)
12
                                                                      14
             \mathbf{b} = \lim_{\mathbf{z}} \operatorname{layer.apply\_fwd}(\mathbf{z}, \boldsymbol{\beta})
13
                                                                               method apply bwd():
                                                                      15
             \hat{\mathbf{y}} = \text{soft layer.apply fwd}(\mathbf{b})
                                                                      16
             J = \text{ce}_{\text{layer.apply}_{\text{fwd}}}(\mathbf{y}, \hat{\mathbf{y}})
15
                                                                                    for i in 1,..., len(in_modules):
                                                                      17
             return J. out tensor
16
                                                                      18
17
                                                                                    return self
                                                                     19
         method backward (Tensor x, Tensor y, Tensor
18
                                                                     20
             tape bwd()
                                                                          function tape_bwd():
             return lin1_layer.in_gradients[1], lin2_la
                                                                               while len(tape) > 0
                                                                      22
```

```
in tensors = [x.out tensor for x in in modules]
          in gradients = backward(in tensors, out tensor, out gradient)
              in modules[i].out gradient += in gradients[i]
          m = tape.pop()
23
          m.apply bwd()
24
```

PyTorch

The same simple neural network we defined in pseudocode can also be defined in PyTorch.

```
1 # Define model
 2 class NeuralNetwork(nn.Module):
      def init (self):
          super(NeuralNetwork, self). init ()
          self.flatten = nn.Flatten()
          self.linear1 = nn.Linear(28*28, 512)
          self.sigmoid = nn.Sigmoid()
          self.linear2 = nn.Linear(512,512)
      def forward(self, x):
11
          x = self.flatten(x)
          a = self.linearl(x)
13
          z = self.sigmoid(a)
14
          b = self.linear2(z)
15
          return b
16
17 # Take one step of SGD
18 def one step of sgd(X, y):
      loss fn = nn.CrossEntropyLoss()
19
      optimizer = torch.optim.SGD(model.parameters(), lr=1e-3)
20
21
22
      # Compute prediction error
      pred = model(X)
23
      loss = loss fn(pred, y)
24
25
26
      # Backpropagation
      optimizer.zero grad()
27
      loss.backward()
28
      optimizer.step()
```

PyTorch

Q: Why don't we call linear.forward() in PyTorch?

This is just syntactic sugar. There's a special method in Python __call__ that allows you to define what happens when you treat an object as if it were a function. In other words, running the following: linear(x)is equivalent to running: $linear._call__(x)$ which in PyTorch is (nearly) the same as running: linear.forward(x) This is because PyTorch defines every Module's __call__ method to be something like this: def __call__(self): self.forward()

PyTorch

Q: Why don't we pass in the parameters to a PyTorch Module?

A: This just makes your code cleaner.

In PyTorch, you store the parameters inside the Module and "mark" them as parameters that should contribute to the eventual gradient used by an optimizer

```
method forward (Tensor \mathbf{x}, Tensor \mathbf{y}, Tensor \boldsymbol{\alpha}, Tensor \boldsymbol{\beta})

a = lin1_layer.apply_fwd(\mathbf{x}, \boldsymbol{\alpha})

z = sig_layer.apply_fwd(\mathbf{z})

b = lin1_layer.apply_fwd(\mathbf{z}, \boldsymbol{\beta})

\hat{\mathbf{y}} = soft_layer.apply_fwd(\mathbf{b})

J = ce_layer.apply_fwd(\mathbf{y}, \hat{\mathbf{y}})

return J.out_tensor
```