

10-423/10-623 Generative AI

Machine Learning Department School of Computer Science Carnegie Mellon University

Course Overview + RNN-LMs + Automatic Differentiation

Matt Gormley & Pat Virtue Lecture 1 Jan. 11, 2025

WHAT IS GENERATIVE AI?

The basic goal of AI is to develop intelligent machines.

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



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"Deep Style" from https://deepdreamgenerator.com/#gallery

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Q: What does Generative AI have to do with any of these goals?

Artificial Intelligence

Machine Learning

Deep Learning

GenAl

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

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 Communication comprises the comprehension and generation of human language.

Artificial Intelligence

Machine Learning

Deep Learning

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- 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)

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Artificial Intelligence

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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

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 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?

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.

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

Machine Learning

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 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]

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Multimodal foundation models learn to answer questions about images (and text in images)

Diffusion models can be used as zero-shot classifiers

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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



Artificial Intelligence

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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

Uncropping



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 This is the demo for <u>MusicGen</u> , a simple and controllable m Ouplicate.Space for longer sequences, more control a	odel for music generation presented at: <u>"Simple and Controlla</u> nd no queue.	ble Music Generation".
Describe your music Condition on a melody (optional) File or Mic		
ion slow upm electro chili with organic samples	A File	Generated Music (wav)
	Drop Audio Here - or - Click to Upload	► 0:15/0:15

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) \overbrace{e}^{-} f(t) holds for every s \overbrace{e}^{-} t. Consider the formula: limit_{x goes to 0} {limit when n approaches infinite} underscore{ \matrix[[sum of i from 1 to n (f(nx) - integral from 0 to x sin(nx) dx), ((x + 2/8)² - 5)/((4x-1/x²) /(n xor 3)), \\ , ..., partial f(x/n) over partial x * (e²(-i*omega n x) + 3(x#7)), f inverse of (x mod n)]] multiply \matrix[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:



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 \$
- -- 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:

def step(self): for group in self.param_groups: for p in group['params']: if p.grad is None: continue grad = p.grad.data # reshape grad to 2D grad_2d = grad.reshape(-1, group['d_dim']) # SVD decomposition U, S, V = torch.svd(grad_2d) # keep top k singular vectors G_k = U[:, :group['k']] d torch.diag(S[:group['k']]) a V[:, :group['k']].T # keep top 2k singular vectors G_2k = U[:, :2*group['k']] torch.diag(S[:2*group['k']]) V[:, :2*group['k']].T # normalize G_k G_k /= torch.norm(G_2k, p=2) # truncate G_k threshold = torch.quantile(torch.abs(G_k), group['alpha']) G_k[torch.abs(G_k) < threshold] = 0 # apply momentum if 'momentum_buffer' not in group:

```
if "momentum_outrer" not in group:
    group['momentum_buffer'] = torch.zeros_like(G_k)
    group['momentum_buffer'] = group['momentum'] =
    group['momentum_buffer'] + G_k
# update parameters
```

```
# upate parameters
p.data.add_(-group['lr'] * group['momentum_buffer'])
# apply weight decay
if group['weight_decay'] != 0:
```

p.data.add_(-group['weight_decay'] * group['lr'], p.data)

ChatGPT:

def step(self):
 for group in self.param_groups:
 for p in group['params']:
 if p.grad is None:
 continue

grad = p.grad.data
grad = grad.reshape(-1, grad.shape[-1]) # reshape to 2D

```
# SVD decomposition
u, s, v = torch.svd(grad)
```

Keep top k and 2k singular vectors k = group['k'] u_k = u[:;tk] s_k = s[:k] u_2k = u[:;tk] u_2k = u[:;:2*k] s_2k = s[:2*k] v_2k = v[:;:2*k]

Normalize according to momentum of F-norm of G_2k
grad_k = u_k 0 torch.diag(s_k) 0 v_k.t()
norm_2k = s_2k.norm()
grad_k = grad_k + group['nomentum'] / norm_2k

Truncate to top alpha percentile

alpha = group['alpha']
percentile = grad_k.abs().flatten().kthvalue(int(alpha *
grad_k.numel()))
grad_k[grad_k.abs() < percentile] = 0</pre>

Apply weight decay

p.data.add_(-group['lr'], grad_k + group['weight_decay']
* p.data)

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

Composition of the Pile by Category

Academic Internet Prose Dialogue Misc



The Pile:

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

RLHF

Step 2

- InstructGPT uses Reinforcement Learning with Human Feedback (RLHF) to fine-tune a pretrained 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."

Step 1

Collect demonstration data, and train a supervised policy.



Collect comparison data,

and train a reward model.

Step 3

Optimize a policy against

the reward model using

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.

Figure from <u>https://arxiv.org/pdf/2203.02155.pdf</u>

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." <u>from Pytorch docs</u>

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

Device 2

Layer 3 part 1

Layer 2 part 1

Device 5

Device 4

Device 3

Device 2

Device 1



(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)

Device 1

Layer 3 part 1

Layer 2 part 1

- Matrix multiplication comprises most Transformer LM computation and can be divided along rows/columns of the respective matrices.
- (c) Microbatch-based pipeline parallelism (GPipe)

Transformer layer 5

Transformer layer 4

Transformer layer 3

Transformer layer 2

Transformer layer 1

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)




Figure from https://earthobservatory.nasa.gov/images/149321/2021-continued-earths-warming-trend

2021 ties 2018 for Sixth Warmest Year on Record

Global Temperature Anomaly (°C compared to the 1951-1980 average)



Figure from https://www.energy.gov/eere/vehicles/fact-617-april-5-2010-changes-vehicles-capita-around-world





GENERATIVE AI IS PROBABILISTIC MODELING

GenAl is Probabilistic Modeling



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



<u>Key Idea:</u>

(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 $\sqrt{473}$ (6 $\sqrt{623}$)
 - 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 use of found code / past work
 - No use of AI tools to complete HW
 - (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-40: 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...?

Home FAQ Syllabus	Generative Al				10-423 + 10-623, School of Computer Science Carnegie Mellon University		
People Schedule Office Hours Coursework Links	✤ Jump to Latest Important N This schedule is ter Tentative Sc	(Lecture 1) Notes ntative and s chedule	Open Latest Poll ubject to change. Please	e check back	often.		
	Date	Date Lecture Reading		Readings		Announcements	
	Generative models of text						
	Wed, 17-Jan	Lecture 1 : RN	N LMs / Autodiff				HW0 out
	Fri, 19-Jan	Recitation: HW	/0				
	Mon, 22-Jan	Lecture 2 : Tra	nsformer LMs				
	Wed, 24-Jan	Lecture 3 : Pre	-training, fine-tuning, evaluat	ion, decoding			HW0 due HW1 out (L1-L3)
	Fri, 26-Jan	Recitation: HW	/1				

60

Where can I find...?



Where can I find...?



Reminders

- Homework 0: PyTorch + Weights & Biases
 - Out: Wed, Jan 擵 汚
 - 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...

- 1. 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.
- 6. 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.



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



The Chain Rule of Probability









Learning an n-Gram Model

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



Learning an n-Gram Model

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

<u>Answer</u>: 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-1} = eat)
w _t	p(• •, •)
corn	4/11
grass	3/11
hay	2/11
if	1/11
which	1/11

 $p(w_{+} | w_{+}) = cows.$

Sampling from a Language Model

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

Answer:

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



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)	5-Gram Model		
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.	Approacheth, denay. dungy Thither! Julius think: grant,O Yead linens, sheep's Ancient, Agreed: Petrarch plaguy Resolved pear! observingly honourest adulteries wherever scabbard guess; affirmationhis 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)



The Chain Rule of Probability

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



Recall...

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



<u>Key Idea</u>:

(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



Key Idea:



Key Idea:



Key Idea:



Key Idea:



Key Idea:



Key Idea:



Why E TR 50k × 1024 by E TR 50k

<u>Key Idea:</u>



Key Idea:



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

Sampling from a Language Model

12 Control of the cost of the

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

Answer:

- Treat each probability distribution like a (50k-sided) weighted die 1.
- Pick the die corresponding to $p(w_t | w_{t-2}, w_{t-1})$ 2.

Dr. Start The

bat

Roll that die and generate whichever word w_t lands face up 3.

m

Repeat 4.

START

PC:/SZAPY)

The

The same approach to sampling we used for an **n**-Gram Language Model also works here for an RNN Language Model

(10, 0, 0, 1)

??

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 more to give thee but so much service in the noble bondman here, Would Shake her wine.

KING LEAR: O, if you were a feeble show, 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 <u>some broken limb</u> shall acquit him well. Your brother is

Which is the real Shakespeare?!

ender; and, for your love, I would be , as I must, for my own honour, if he pre, out of my love to you, I came hither withal, that either you might stay him

from his intender of the brook such disgrace well as he shall run into, in the is a thing of his own search and altogether against my will.

Shakespeare's As You Like It

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RNN-LM Sample

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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")
- Visit each node in **topological order**. For variable u_i with inputs v_1, \dots, v_N a. Compute $u_i = g_i(v_1, \dots, v_N)$ b. Store the result at the node

Backward Computation (Version A)

- Initialize dy/dy = 1. 1.
- 2.
- Visit each node v_j in **reverse topological order**. Let u_1, \ldots, u_M denote all the nodes with v_j as an input
 - Assuming that $y = h(\mathbf{u}) = h(u_1, ..., u_M)$ and $\mathbf{u} = g(\mathbf{v})$ or equivalently $u_i = g_i(v_1, ..., v_j, ..., v_N)$ for all i a. We already know dy/du_i for all i

 - Compute dy/dvi as below (Choice of algorithm ensures computing b. (du_i/dv_i) is easy) $\int_{-\infty}^{M} dy du_i$

 $\frac{du_i}{dv_j}$

Return partial derivatives dy/du_i for all variables

 \mathbf{V}

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, \dots, v_N a. Compute $u_i = g_i(v_1, \dots, v_N)$ b. Store the result at the node

Backward Computation (Version B)

- **Initialize** all partial derivatives dy/du_i to 0 and dy/dy = 1. 1.
- Visit each node in reverse topological order. 2. For variable $u_i = g_i(v_1, \dots, v_N)$
 - 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_j) is easy)

Return partial derivatives dy/du_i for all variables

Backpropagation: Procedural Method

Algorithm 1 Forward Computation

- 1: **procedure** NNFORWARD(Training example (x, y), Params α, β)
- 2: $\mathbf{a} = \boldsymbol{\alpha} \mathbf{x}$
- 3: $\mathbf{z} = \sigma(\mathbf{a})$
- 4: $\mathbf{b} = \boldsymbol{\beta} \mathbf{z}$

5:
$$\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{b})$$

6:
$$J = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

- 7: $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J)$
- 8: **return** intermediate quantities **o**

Algorithm 2 Backpropagation

- 1: **procedure** NNBACKWARD(Training example (x, y), Params α, β , Intermediates 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: $\mathbf{g}_{\mathbf{b}} = \mathbf{g}_{\hat{\mathbf{y}}}^T \left(\mathsf{diag}(\hat{\mathbf{y}}) - \hat{\mathbf{y}}\hat{\mathbf{y}}^T \right)$

5:
$$\mathbf{g}_{\boldsymbol{\beta}} = \mathbf{g}_{\mathbf{j}}^T \mathbf{z}^T$$

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

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 $\mathbf{g}_{\boldsymbol{\alpha}}, \mathbf{g}_{\boldsymbol{\beta}}$

Drawbacks of Procedural Method

- 1. Hard to reuse / adapt for other models
- 2. (Possibly) harder to make individual steps more efficient
- 3. Hard to find source 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 $\mathbf{b} = f(\mathbf{a})$.





Module-based AutoDiff

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

Sigmoid Module The sigmoid layer has only one input vector **a**. Below σ is the sigmoid applied elementwise, and \odot is element-wise multiplication s.t. **u** \odot **v** = $[u_1v_1, \ldots, u_Mv_M]$. 1: procedure SIGMOIDFORWARD(a) 2: **b** = σ (**a**) 3: return **b** 4: procedure SIGMOIDBACKWARD(**a**, **b**, **g**_b)

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

6: return g_a

Softmax Module The softmax layer has only one input vector **a**. For any vector $\mathbf{v} \in \mathbb{R}^D$, we have that 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.

1: **procedure** SOFTMAXFORWARD(a)

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

3: return b

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

5:
$$\mathbf{g}_{\mathbf{a}} = \mathbf{g}_{\mathbf{b}}^T \left(\mathsf{diag}(\mathbf{b}) - \mathbf{b}\mathbf{b}^T \right)$$

6: return g_a

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

- 1: **procedure** LinearForward (a, ω)
- 2: $\mathbf{b} = \boldsymbol{\omega} \mathbf{a}$
- 3: return b
- 4: **procedure** LinearBackward($\mathbf{a}, \omega, \mathbf{b}, \mathbf{g}_{\mathbf{b}}$)

5:
$$\mathbf{g}_{\boldsymbol{\omega}} = \mathbf{g}_{\mathbf{b}} \mathbf{a}^T$$

$$\mathbf{s}: \mathbf{g}_{\mathbf{a}} = oldsymbol{\omega}^T \mathbf{g}_{\mathbf{b}}$$

7: return
$$\mathbf{g}_{\boldsymbol{\omega}}, \mathbf{g}_{\mathbf{a}}$$

Cross-Entropy Module The cross-entropy layer has two inputs: a gold one-hot vector a and a predicted probability distribution \hat{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 (a, \hat{a})

2:
$$b = -\mathbf{a}^T \log \hat{\mathbf{a}}$$

3: return b

4: **procedure** CROSSENTROPYBACKWARD($\mathbf{a}, \hat{\mathbf{a}}, b, g_b$)

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

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

Module-based AutoDiff

Algorithm 1 Forward Computation

- 1: procedure NNFORWARD (Training example (x, y), Parameters α ,
- β)
- $\mathbf{a} = \mathsf{LinearForward}(\mathbf{x}, \boldsymbol{\alpha})$ 2:
- $\mathbf{z} = \mathsf{SigmoidForward}(\mathbf{a})$ 3:
- $\mathbf{b} = \text{LinearForward}(\mathbf{z}, \boldsymbol{\beta})$ 4:
- $\hat{\mathbf{y}} = \mathsf{SoftmaxForward}(\mathbf{b})$ 5:
- $J = CROSSENTROPYFORWARD(\mathbf{y}, \hat{\mathbf{y}})$ 6:
- $\mathbf{o} = \texttt{object}(\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J)$ 7:
- **return** intermediate quantities o 8:

Algorithm 2 Backpropagation

- 1: **procedure** NNBACKWARD(Training example (x, y), Parameters α, β , Intermediates o)
- Place intermediate quantities $\mathbf{x}, \mathbf{a}, \mathbf{z}, \mathbf{b}, \hat{\mathbf{y}}, J$ in \mathbf{o} in scope 2: $g_J = \frac{dJ}{dJ} = 1$ ▷ Base case 3:
- $\mathbf{g}_{\hat{\mathbf{y}}} = \mathsf{CROSSENTROPYBACKWARD}(\mathbf{y}, \hat{\mathbf{y}}, J, g_J)$ 4:
- $\mathbf{g}_{\mathbf{b}} = \mathsf{SOFTMAXBACKWARD}(\mathbf{b}, \hat{\mathbf{y}}, \mathbf{g}_{\hat{\mathbf{v}}})$ 5:
- $\mathbf{g}_{m{eta}}, \mathbf{g}_{\mathbf{z}} = \mathsf{LinearBackward}(\mathbf{z}, \mathbf{b}, \mathbf{g}_{\mathbf{b}})$ 6:
- $\mathbf{g}_{\mathbf{a}} = \mathsf{SigmoidBackward}(\mathbf{a}, \mathbf{z}, \mathbf{g}_{\mathbf{z}})$ 7:
- $\mathbf{g}_{m{lpha}}, \mathbf{g}_{\mathbf{x}} = \mathsf{LinearBackward}(\mathbf{x}, \mathbf{a}, \mathbf{g}_{\mathbf{a}})$ \triangleright We discard $\mathbf{g}_{\mathbf{x}}$ 8:
- **return** parameter gradients $\mathbf{g}_{\alpha}, \mathbf{g}_{\beta}$ 9:

Advantages of **Module-based** AutoDiff

- Easy to reuse / 1. adapt for other models
- Encapsulated 2. layers are easier to optimize (e.g. implement in C++ or CUDA)
- Easier to find 3. bugs because we can run a finitedifference check on each layer separately

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 Linear (Module)	
1	class Sigmoid (Module)	\mathbf{method} forward (a,	$\omega)$
2	method forward(a)	$\mathbf{b}=oldsymbol{\omega}\mathbf{a}$	
3	$\mathbf{b} = \sigma(\mathbf{a})$	return b	
4	return b	method backward(a	ω , b, g _b)
5	method backward(\mathbf{a} , \mathbf{b} , $\mathbf{g}_{\mathbf{b}}$)	$\mathbf{g}_{oldsymbol{\omega}} = \mathbf{g}_{\mathbf{b}} \mathbf{a}^T$	
6	$\mathbf{g_a} = \mathbf{g_b} \odot \mathbf{b} \odot (1 - \mathbf{b})$	$\mathbf{g}_{\mathbf{a}} = oldsymbol{\omega}^T \mathbf{g}_{\mathbf{b}}$	
7	$return g_a$	$\mathbf{return} \ \mathbf{g}_{\boldsymbol{\omega}}, \mathbf{g}_{\mathbf{a}}$	
1	class Softmax (Module)	class CrossEntropy(Modu	le)
2	method forward(a)	method forward(a,	â)
3	$\mathbf{b} = \mathtt{softmax}(\mathbf{a})$	$b = -\mathbf{a}^T \log \hat{\mathbf{a}}$	
4	return b	return b	
5	method backward(\mathbf{a} , \mathbf{b} , $\mathbf{g}_{\mathbf{b}}$)	method backward(a,	$\hat{\mathbf{a}}$, b , g_b)
6	$\mathbf{g_a} = \mathbf{g_b}^T \left(\mathtt{diag}(\mathbf{b}) - \mathbf{b} \mathbf{b}^T ight)$	$\mathbf{g}_{\hat{\mathbf{a}}} = -g_b(\mathbf{a} \div \hat{\mathbf{a}})$	
7	return g_a	return g_a	

1	class NeuralNetwork(Module):
2	
3	method init()
4	$lin1_layer = Linear()$
5	$sig_layer = Sigmoid()$
6	$lin2_layer = Linear()$
7	$soft_layer = Softmax()$
8	$ce_{layer} = CrossEntropy()$
9	
0	method forward (Tensor x, Tensor y, Tensor α , Tensor β)
11	$\mathbf{a} = \text{lin1} _ \text{layer.apply} _ \text{fwd}(\mathbf{x}, \boldsymbol{\alpha})$
2	$z = sig_layer.apply_fwd(a)$
3	$\mathbf{b} = \text{lin2} _ \text{layer.apply} _ \text{fwd}(\mathbf{z}, \boldsymbol{\beta})$
4	$\hat{\mathbf{y}} = \mathbf{s}_{oft} \text{layer.apply}_{fwd}(\mathbf{b})$
5	$J = ce_layer.apply_fwd(\mathbf{y}, \hat{\mathbf{y}})$
6	return J.out_tensor
7	
8	method backward (Tensor x, Tensor y, Tensor α , Tensor β)
9	tape_bwd()
0	return lin1_layer.in_gradients[1], lin2_layer.in_gradients[1]

class Module:

1 global tape = stack()

2
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4
5
6
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8
9
10
ensor ¹¹
12
13
14
15
16
17
18
Tensc ¹⁹
20
n2_le ²¹
22
23

```
method init()
   out tensor = null
   out gradient = 1
method apply_fwd(List in_modules)
   in tensors = [x.out tensor for x in in modules]
   out tensor = forward(in tensors)
   tape.push(self)
   return self
method apply_bwd():
   in_gradients = backward(in_tensors, out_tensor, out_gradient)
   for i in 1,..., len(in_modules):
       in modules[i].out gradient += in gradients[i]
   return self
```

```
21 function tape_bwd():
22 while len(tape) > 0
23 m = tape.pop()
24 m.apply_bwd()
```

1 global tape = stack()

1	class NeuralNetwork(Module):	2	ologa Madula.
2		3	class module:
3	method init()	4	41 1 .
4	$lin1_layer = Linear()$	5	method 11
5	$sig_layer = Sigmoid()$	6	out_te
6	$lin2_layer = Linear()$	7	out_gr
7	$soft_layer = Softmax()$	8	
8	ce_layer = CrossEntropy()	9	method a
9		10	in_ten
10	method forward (Tensor \mathbf{x} , Tensor \mathbf{y} , Tensor	11	out_te
11	$\mathbf{a} = \text{lin1}$ layer.apply $\text{fwd}(\mathbf{x}, \boldsymbol{\alpha})$	12	tape.p
12	$\mathbf{z} = sig layer.apply fwd(\mathbf{a})$	13	return
13	$\mathbf{b} = \lim_{z \to 0} 1 \lim_{z \to 0}$	14	
14	$\hat{\mathbf{v}} = \text{soft}$ layer apply fwd(\mathbf{b})	15	method a
15	$J = ce$ laver.apply $fwd(\mathbf{v}, \hat{\mathbf{v}})$	16	in_gra
16	return J .out tensor	17	for i i
17		18	in_{-}
18	method backward (Tensor \mathbf{x} , Tensor \mathbf{v} , Tensor	19	return
10	tape bwd()	20	
פי סכ	return lin1 layer in gradients[1] lin2 la	21	function tape
20		22	while len(
		23	m = ta

```
method init()
   out tensor = null
   out gradient = 1
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   in tensors = [x.out tensor for x in in modules]
   out tensor = forward(in tensors)
   tape.push(self)
   return self
method apply_bwd():
   in_gradients = backward(in_tensors, out_tensor, out_gradient)
   for i in 1,..., len(in_modules):
       in modules[i].out gradient += in gradients[i]
   return self
```

```
ction tape_bwd():
      while len(tape) > 0
          m = tape.pop()
          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):
 3
          super(NeuralNetwork, self). init ()
 4
 5
          self.flatten = nn.Flatten()
          self.linear1 = nn.Linear(28*28, 512)
 6
 7
          self.sigmoid = nn.Sigmoid()
          self.linear2 = nn.Linear(512,512)
 8
 9
      def forward(self, x):
10
11
          x = self.flatten(x)
          a = self.linearl(x)
12
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
29
      optimizer.step()
```

Example adapted from https://pytorch.org/tutorials/beginner/basics/quickstart_tutorial.html

PyTorch

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

A: 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)
```

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

0	method forward (Tensor x, Tensor y, Tensor α , Tensor β)
11	$\mathbf{a} = \text{lin1_layer.apply_fwd}(\mathbf{x}, \boldsymbol{\alpha})$
2	$\mathbf{z} = sig_layer.apply_fwd(\mathbf{a})$
3	$\mathbf{b} = \text{lin1_layer.apply_fwd}(\mathbf{z}, \boldsymbol{\beta})$
4	$\hat{\mathbf{y}} = \text{soft_layer.apply_fwd}(\mathbf{b})$
5	$J = ce_layer.apply_fwd(\mathbf{y}, \hat{\mathbf{y}})$
6	return $J.out_tensor$

7	
10	<pre>def forward(self, x):</pre>
11	x = self.flatten(x)
12	<pre>a = self.linearl(x)</pre>
13	<pre>z = self.sigmoid(a)</pre>
14	<pre>b = self.linear2(z)</pre>
15	return b