18-661 Introduction to Machine Learning

Neural Networks-III

Spring 2025

ECE – Carnegie Mellon University

Outline

1. Language Models and RNNs
2. Transformer Language Models
3. Stochastic Gradient Descent Convergence

Language Models and RNNs

What is Generative AI?

- So far, we have considered supervised learning tasks where we are given a training dataset of feature-label pairs $(\mathbf{x}_n, y_n)$, for $n = 1, \ldots, N$. Our goal is to learn a function $f(\mathbf{x}_n) \approx y_n$ that maps features to targets/labels
- In generative AI, we do not have explicit labels. Given a sequence of inputs $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_t$ our goal is to predict the next element of the sequence $\mathbf{x}_{t+1}$.

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- Examples:
    - Next word prediction
    - Text generation given a prompt
    - Machine translation
    - Image/video generation from a description

How does Generative AI work?

- We model the conditional distribution of the next token given the previous tokens:

$$\Pr(\mathbf{x}_{t+1}|\mathbf{x}_t, \ldots \mathbf{x}_1)$$

  using a neural network such as an RNN or transformer
- Then we sample from this probability distribution to generate $\mathbf{x}_{t+1}$

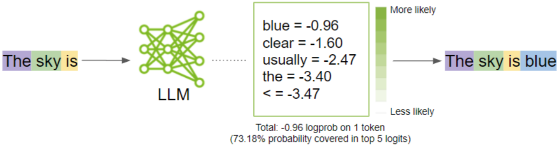
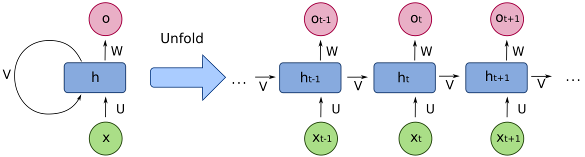


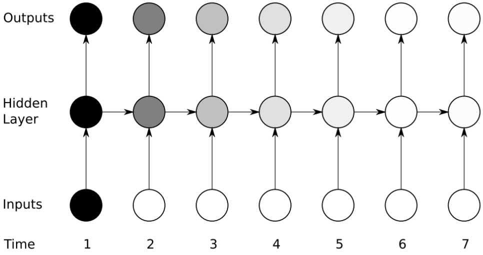
Figure source: NVIDIA technical blog

Recurrent Neural Networks (RNNs)



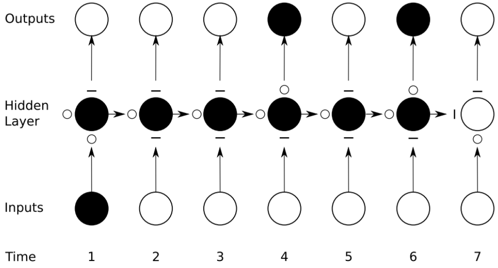
- Precursors to transformers, RNNs were widely used to model temporal or sequential data (e.g., natural language).
- Sequence of hidden states $\mathbf{h}_t$ that depend on the current input $\mathbf{x}_t$ and the previous hidden state $\mathbf{h}_{t-1}$
- Output computation: $\mathbf{o}_t = \psi(\mathbf{W}\mathbf{h}_t + b)$
- Hidden state computation: $\mathbf{h}_t = \phi(\mathbf{V}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + c)$
- The weight matrices $\mathbf{W}, \mathbf{V}, \mathbf{U}$ and biases b and c are trained using backpropagation on a dataset of sequences of varying lengths
- The predicted output $\mathbf{o}_t$ becomes the next input $\mathbf{x}_{t+1}$

RNNs and Forgetting



- RNNs tend to forget information as they progress forward through the sequence
- This is due to weak or vanishing gradients as we move longer distance through the model
- For a long sentence where the beginning of the sentence has information about the subject, such forgetfulness can be catastrophic

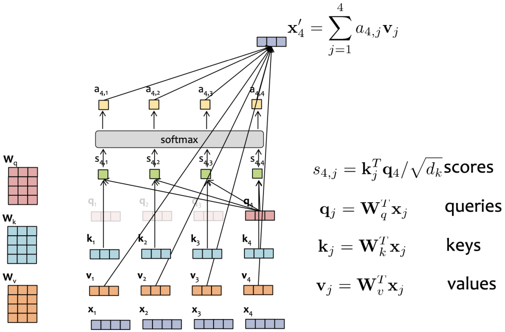
Long and Short-term Memory (LSTM)



- They combat the RNN forgetting issue via gates that decide whether to remember or forget information about the hidden states.
- But they still have drawbacks such as:
  - Difficulty with long-range dependencies (albeit less than RNNs)
  - Even though they solve the vanishing gradient problem, they suffer from exploding gradients
  - Inherently serial computation makes it harder to train

Transformer Language Models

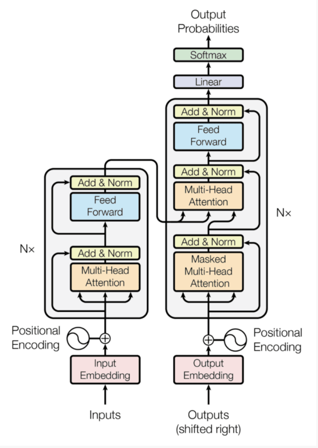
Transformers: Attention Mechanism



- RNNs and LSTM maintain a fixed length hidden state to represent the history of a sequence.
- Instead, the attention mechanism in Transformers looks at all previous token when predicting the next token
- The 'attention' that it pays to each token is computed using the attention mechanism

Transformers

- Encoder-decoder architecture: learn a representation of each input in the sequence, then decode to predict next entry in the output sequence
  - Autoregressive structure: takes previously generated outputs as inputs
  - Attach an attention weight to each entry of each input representation
  - Self-attention between each layer
- Much larger and slower to train, but usually gives good performance



Large Language Models

- "Generative pre-trained transformer" models: *generate* language outputs based on *pre-training* of *transformer*-based architectures on a massive corpus of language data
- Classification task: next-word prediction (run many times)
  - Tokenization: divide text into 'tokens of similar length/information
  - Predict the next token based on the preceding sequence of tokens (typically 1M long)
- Self-/semi-supervised models: generate supervisory signals ("labels") based on output of currently trained model
- Other generative models can generate images, videos, etc. Multi-modal models can, e.g., use a text input to generate an image.

Pre-Training and Finetuning

- Modern deep learning models are too expensive to train from scratch (GPT-4 likely cost millions of dollars to train!) As an example, Llama-7B, 13-B, etc. have billions of parameters.
- Pre-trained foundation models capture essential patterns and can be finetuned to specific datasets
  - Types of language, e.g., coding tools or translation tasks
  - Types of images, e.g., generating images of a certain style
- Foundation models can be trained further on a new dataset
  - Layer freezing or prompt engineering
  - "Warm start" initialization to the usual SGD-based training steps
- Prune, quantize, or compress foundation models to fit them or train them on smaller devices.

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Stochastic Gradient Descent Convergence

SGD is at the core of Machine Learning!

We use it to train the model parameters $\mathbf{w}$ in

- Linear Regression: $y = \mathbf{w}^\top \mathbf{x}$
- Logistic Regression: $y = \sigma(\mathbf{w}^\top \mathbf{x})$
- Neural Networks: $y = NN(\mathbf{x}; \mathbf{w})$

For each problem, we define a loss function $F(\mathbf{w})$ to measure the error in the predicted output, and then update $\mathbf{w}$ according to:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta g(\mathbf{w})$$

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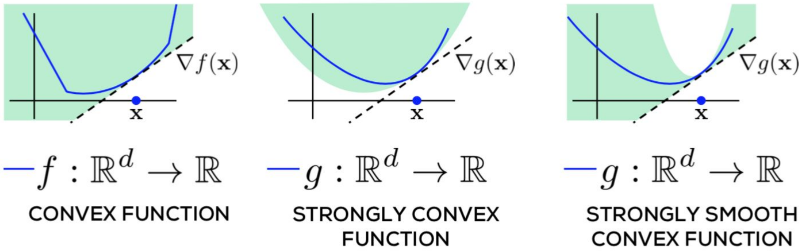
The gradient $g(\mathbf{w})$ can be

- Full gradient, $\nabla F(\mathbf{w}_t) = \frac{1}{N}\sum_{i=1}^{N} \nabla f(\mathbf{w}_t; \xi)$ computed over the whole dataset
- Stochastic gradient $\nabla f(\mathbf{w}_t; \xi)$ for a randomly chosen sample ξ
- Mini-batch stochastic gradient $g(\mathbf{w}; \xi) = \frac{1}{b}\sum_{i=1}^{b} \nabla f(\mathbf{w}; \xi_i)$, computed using a batch ξ of b samples chosen at random

Let us analyze the time SGD takes to reach an ϵ error

A c-strongly Convex and L-Smooth Function



Satisfies the upper and lower bounds given by

$$F(\mathbf{w}) \leq F(\mathbf{y}) + \nabla F(\mathbf{y})^\top(\mathbf{w} - \mathbf{y}) + \frac{L}{2}\|\mathbf{w} - \mathbf{y}\|^2$$

$$F(\mathbf{w}) \geq F(\mathbf{y}) + \nabla F(\mathbf{y})^\top(\mathbf{w} - \mathbf{y}) + \frac{1}{2}c\|\mathbf{w} - \mathbf{y}\|^2 \text{ for all } \mathbf{w}, \mathbf{y} \in \mathbb{R}^d$$

Convergence Analysis of GD

Convergence of GD

For a c-strongly convex and L-smooth function, if the learning rate $\eta < \frac{1}{L}$ and the starting point is $\mathbf{w}_0$ then $F(\mathbf{w}_t)$ after t gradient descent iterations is bounded as

$$F(\mathbf{w}_t) - F(\mathbf{w}^*) \leq (1 - \eta c)^t (F(\mathbf{w}_0) - F(\mathbf{w}^*))$$

How many iterations do we need to converge to reach error $F(\mathbf{w}_t) - F(\mathbf{w}^*) = \epsilon$?

$$\begin{aligned}
(1 - \eta c)^t (F(\mathbf{w}_0) - F(\mathbf{w}^*)) &\leq \epsilon \\
t \log(1 - \eta c) + \log(F(\mathbf{w}_0) - F(\mathbf{w}^*)) &\leq \log(\epsilon) \\
t \log(1/(1 - \eta c)) - \log(F(\mathbf{w}_0) - F(\mathbf{w}^*)) &\geq \log(\frac{1}{\epsilon}) \\
t &= O(\log(\frac{1}{\epsilon}))
\end{aligned}$$

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How does the convergence speed depend on

- Learning rate η – Converges faster for larger η as long as $\eta < \frac{1}{L}$
- Lipschitz smoothness L – Converges faster for smaller L because we can set a higher η
- Strong convexity parameter c – Converges faster for larger c

Convergence Analysis of Mini-batch SGD

Assumptions on the Stochastic Gradients

Since we are using noisy gradients, we need the following assumptions on them

- Unbiased Gradients: The stochastic gradient $\nabla f(\mathbf{w};\xi)$ is an unbiased estimate of $\nabla F(\mathbf{w})$, that is,

$$\mathbb{E}_{\xi}[\nabla f(\mathbf{w};\xi)] = \nabla F(\mathbf{w})$$

- Bounded Variance: The stochastic gradient $\nabla f(\mathbf{w};\xi)$ has bounded variance, that is,

$$\mathrm{Var}(\nabla f(\mathbf{w};\xi)) \leq \sigma^2$$

  which implies that the variance of a mini-batch gradient is:

$$\mathrm{Var}(g(\mathbf{w};\xi)) \leq \frac{\sigma^2}{b}$$

Convergence Analysis of Mini-batch SGD

Convergence of Mini-batch SGD

For a c-strongly convex and L-smooth function, if the learning rate $\eta < \frac{1}{L}$ and the starting point is $\mathbf{w}_0$ then $F(\mathbf{w}_t)$ after t gradient descent iterations is bounded as

$$\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \leq (1 - \eta c)^t \left(\mathbb{E}[F(\mathbf{w}_0)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \right)$$

- For batch *GD*, as $t \to \infty$, the objective $F(\mathbf{w}_t) \to F(\mathbf{w}^*)$
- For mini-batch SGD, as $t \to \infty$, we will be left with an error floor $\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) \to \frac{\eta L \sigma^2}{2cb}$.
- This is the price that we pay for noisy gradients, that is the variance bound being $\sigma^2 \geq 0$

Effect of Mini-batch Size on the Error Floor

Convergence of Mini-batch SGD

For a c-strongly convex and L-smooth function, if the learning rate $\eta < \frac{1}{L}$ and the starting point is $\mathbf{w}_0$ then $F(\mathbf{w}_t)$ after t gradient descent iterations is bounded as

$$\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \leq (1 - \eta c)^t \left(\mathbb{E}[F(\mathbf{w}_0)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2bc} \right)$$

- Recall that

$$g(\mathbf{w}, \xi) = \frac{1}{b} \sum_{n \in S} \nabla f(\mathbf{w}),$$

- And the bounded variance assumption is $\mathrm{Var}(g(\mathbf{w}; \xi)) \leq \sigma^2 / b$
- When we increase the mini-batch size b, the error floor $\frac{\eta L \sigma^2}{2cb}$ reduces.

Effect of Learning Rate on Convergence Speed and Error Floor

Convergence of Mini-batch SGD

For a c-strongly convex and L-smooth function, if the learning rate $\eta < \frac{1}{L}$ and the starting point is $\mathbf{w}_0$ then $F(\mathbf{w}_t)$ after t gradient descent iterations is bounded as

$$\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \leq (1 - \eta c)^t \left(\mathbb{E}[F(\mathbf{w}_0)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \right)$$

- The convergence speed, represents by $(1 - \eta c)$ only depends on the strong convexity parameter c and learning rate η, not on the mini-batch size b
- As η increases, the algorithm converges faster
- But, as η increases, the error floor $\frac{\eta L \sigma^2}{2cb}$ also increases

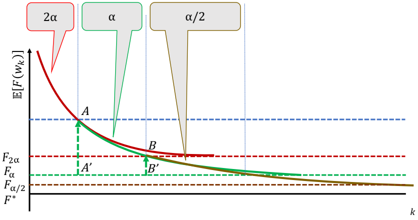
How do we achieve zero error floor?

Convergence of Mini-batch SGD

For a c-strongly convex and L-smooth function, if the learning rate $\eta < \frac{1}{L}$ and the starting point is $\mathbf{w}_0$ then $F(\mathbf{w}_t)$ after t mini-batch SGD iterations is bounded as

$$\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb} \leq (1-\eta c)^t \left(\mathbb{E}[F(\mathbf{w}_0)] - F(\mathbf{w}^*) - \frac{\eta L \sigma^2}{2cb}\right)$$

KEY IDEA: Decay the learning rate η (denoted by α in the figure below) by 2 whenever F is 2 times its error floor $\frac{\eta L \sigma^2}{2cb}$.



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Convergence of Mini-batch SGD

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KEY IDEA: Decay the learning rate η

- If $\eta = \eta_0 / t$, then we can show that $\mathbb{E}[F(\mathbf{w}_t)] - F(\mathbf{w}^*) \leq O(1/t)$
- Thus, the number of iterations required an error ϵ is $O(1/\epsilon)$
- In contrast, with GD we need only $O(\log(1/\epsilon))$ iterations to reach an ϵ error

Summary

You should know:

- Language models and RNNs
- Transformer language models