CSCI567 Machine Learning (Fall 2025)

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University of Southern California

Nov 14, 2025

Administration

HW4 is due on Nov 26th.

Outline

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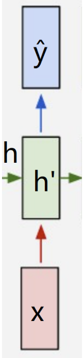
A recurrent layer



from $\widehat{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{x})$ to $(\widehat{\boldsymbol{y}}, \boldsymbol{h}') = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{h})$

- $\boldsymbol{h}$ is "hidden state" (like HMM), updated via

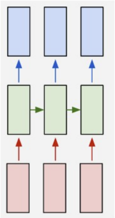
$$\boldsymbol{h}' = \boldsymbol{\sigma}(\boldsymbol{W}\boldsymbol{h} + \boldsymbol{U}\boldsymbol{x} + \boldsymbol{b}_h)$$

  where $\boldsymbol{\sigma}$ is an activation function

- $\widehat{\boldsymbol{y}} = \boldsymbol{V}\boldsymbol{h}' + \boldsymbol{b}_y$ is the output

Recurrent layer applied recursively

Given a **sequence** $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots$, can apply $\boldsymbol{f}$ recursively:

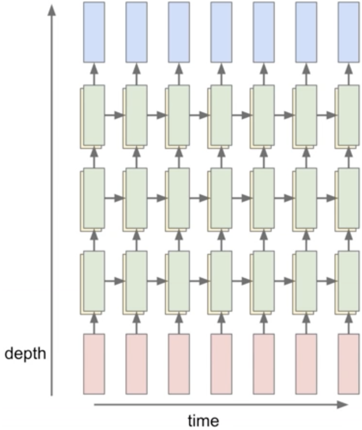


- $\boldsymbol{h}_0 = \mathbf{0}$
- $(\widehat{\boldsymbol{y}}_1, \boldsymbol{h}_1) = \boldsymbol{f}(\boldsymbol{x}_1, \boldsymbol{h}_0)$
- $(\widehat{\boldsymbol{y}}_2, \boldsymbol{h}_2) = \boldsymbol{f}(\boldsymbol{x}_2, \boldsymbol{h}_1)$
- $\cdots$

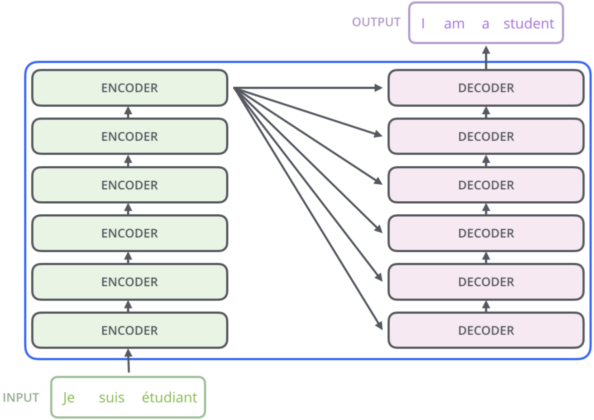
Making it "deep"

Stack multiple recurrent layers:

- hidden states become the inputs of the next layer
- different layers learn different $\boldsymbol{W}, \boldsymbol{U}, \boldsymbol{b}_h$
- last layer learns $\boldsymbol{V}, \boldsymbol{b}_y$ and output $\widehat{\boldsymbol{y}}$



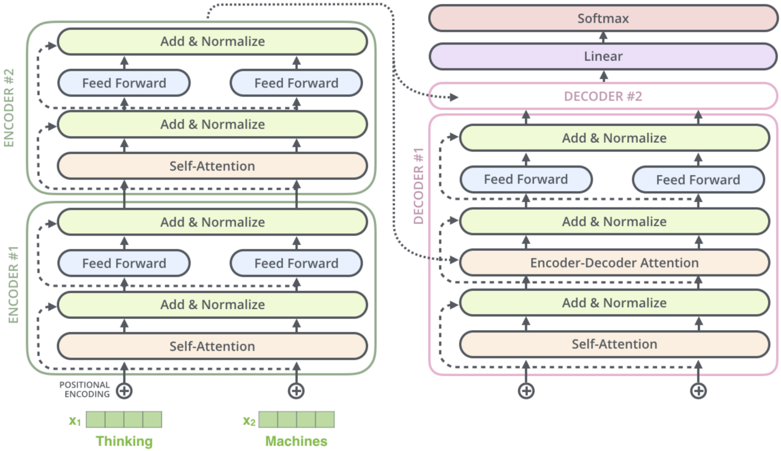
Transformer: overview



Encoder: summarizes the input into a useful representation

Decoder: generates outputs

Transformer: a closer look



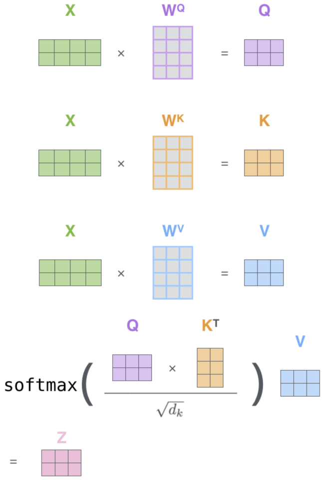
Transformer: a closer look at self-attention

Matrix notation:

- input matrix $\boldsymbol{X} \in \mathbb{R}^{T \times d}$, obtained by stacking $\boldsymbol{x}_1^\top, \ldots, \boldsymbol{x}_T^\top$
- query matrix $\boldsymbol{Q} = \boldsymbol{X}\boldsymbol{W}_Q \in \mathbb{R}^{T \times d_k}$
- key matrix $\boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}_K \in \mathbb{R}^{T \times d_k}$
- value matrix $\boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}_V \in \mathbb{R}^{T \times d_v}$
- attention score matrix $\boldsymbol{Q}\boldsymbol{K}^\top \in \mathbb{R}^{T \times T}$
- output matrix $\boldsymbol{Z} \in \mathbb{R}^{T \times d_v}$ is

$$\text{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d_k}}\right)\boldsymbol{V}$$

  where softmax is *applied row-wise*



$O(T^2)$ complexity (ignoring d, d_k, d_v)

Outline

1. Review of last lecture
2. Multi-Armed Bandits
   - Online decision making
   - Motivation and setup
   - Exploration vs. Exploitation
3. Dueling Bandits
4. Learning in Games

Decision making

Problems we have discussed so far:

- start with a training dataset
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Broadly, these are called **online decision making problems**.

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- discuss general reinforcement learning next week

Mulit-armed bandits: motivation

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- like a bandit with multiple arms (hence the name)
- **if I can play for 10 times, which machines should I play?**

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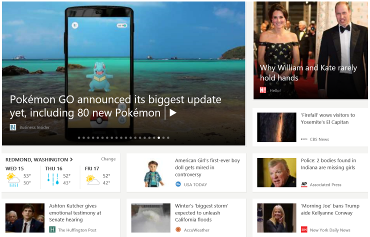

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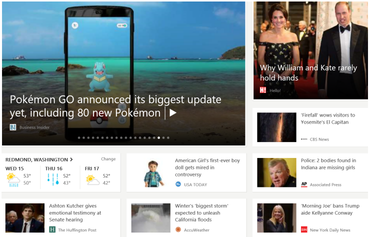

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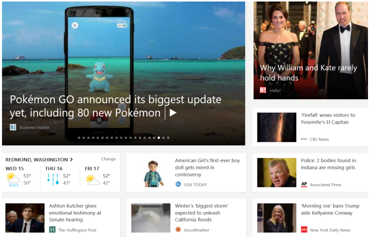
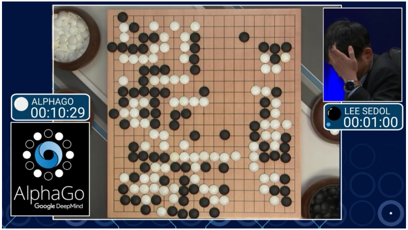
- game playing, each possible move is an arm (AlphaGo indeed has a bandit algorithm as one of the components)





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This kind of limited feedback is now usually referred to as bandit feedback

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$$\max_{a\in[K]} \sum_{t=1}^T r_{t,a} - \sum_{t=1}^T r_{t,a_t}$$

This is called the **regret**: *how much I regret for not sticking with the best fixed arm in hindsight?*

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We first focus on a simple setting:

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- each arm has a different mean $(\mu_1, \ldots, \mu_K)$; the problem is essentially about finding the best arm $\mathrm{argmax}_a \, \mu_a$ as quickly as possible

Empirical means

Let $\hat{\mu}_{t,a}$ be the **empirical mean** of arm a up to time t:

$$\hat{\mu}_{t,a} = \frac{1}{n_{t,a}} \sum_{\tau \leq t : a_\tau = a} r_{\tau,a}$$

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Concentration: $\hat{\mu}_{t,a}$ should be close to μ_a if $n_{t,a}$ is large

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- the algorithm will never pick arm 1 again!

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We next discuss **three ways** to trade off exploration and exploitation for our simple multi-armed bandit setting.

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Explore–then–Exploit

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Parameter T_0 clearly controls the exploration/exploitation trade-off

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- clearly it won't work if the environment is changing

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Is there a *more adaptive* way to explore?

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- the bonus term is large if the arm is not pulled often enough, which encourages exploration (adaptive due to the first term)

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More adaptive exploration

A simple modification of "Greedy" leads to the well-known:

Upper Confidence Bound (UCB) algorithm

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picture link

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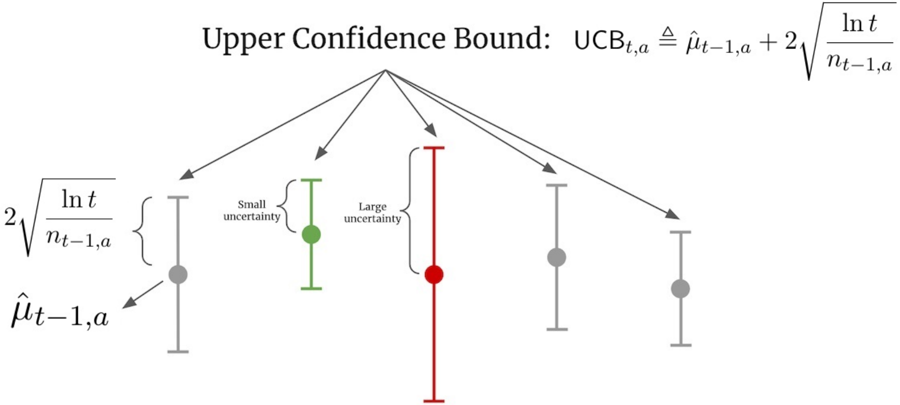

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Does not work: pessimism discourages exploration!

Outline

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We focus on the special case of multi-armed bandits, i.e., **dueling bandits**.

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Intuitively, the goal is to find $a^\star$ as quickly as possible.

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- usually apply two copies of the **same** algorithm to select a_t and b_t; hence the name **self-play**.

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- in fact, b_t can be completely arbitrary $\Rightarrow$ need an **"adversarial" multi-armed bandit algorithm**

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- with the right choice of η, Exp3 ensures regret $\lesssim \sqrt{KT}$ (**optimal**) even against an adversarial exponent

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Losses versus rewards (cont.)

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- after a_t wins one round, the algorithm increases its weight and decreases all other arms' weights aggressively

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- sample a_t from arm distribution $\boldsymbol{p}_t = \text{softmax}\left(-\eta \sum_{\tau=1}^{t-1} \boldsymbol{\ell}_\tau\right)$
- observe reward feedback $\mathbb{I}[a_t \succ b_t]$ (b_t selected by opponent)
- construct estimator $\boldsymbol{\ell}_t \in \mathbb{R}_+^K$ where for each a: $\boldsymbol{\ell}_{t,a} = \frac{\mathbb{I}[a_t=a]\mathbb{I}[a \prec b_t]}{p_{t,a}}$

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Losses versus rewards (cont.)

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What does low regret mean here?

Using Exp3 to select a_t guarantees

$$\sum_{t=1}^{T} \mathbb{I}[a^\star \succ b_t] - \sum_{t=1}^{T} \mathbb{I}[a_t \succ b_t] \precsim \sqrt{KT}$$

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Taking expectation and using $P_{a,b} + P_{b,a} = 1$ shows

$$\sum_{t=1}^{T} (P_{a^\star, a_t} + P_{a^\star, b_t} - 1) \lesssim \sqrt{KT},$$

so can only pick suboptimal actions a negligible fraction ($\sqrt{K/T}$) of times

Outline

Self-play in general games

Dueling bandits can be seen as a **game** between two players

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- self-play: use the same learning algorithm for all players

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- canonical examples: **rock-paper-scissors**

$$\begin{array}{c} \\ \text{Rock} \\ \text{Paper} \\ \text{Scissors} \end{array} \begin{array}{c} \begin{array}{ccc} \text{Rock} & \text{Paper} & \text{Scissors} \end{array} \\ \begin{pmatrix} 0.5 & 0 & 1 \\ 1 & 0.5 & 0 \\ 0 & 1 & 0.5 \end{pmatrix} \end{array}$$

More interesting examples

Figure: chess

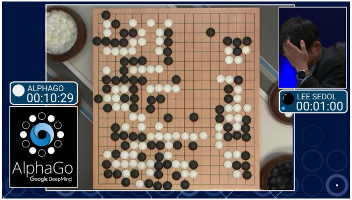

Figure: Go

Figure: poker

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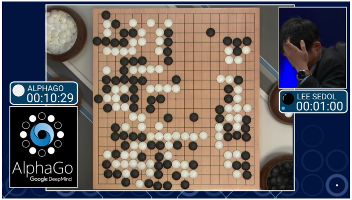

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Figure: StarCraft

Extremely large action space; still, all can be *"solved" by self-play*

Solving Go via self-play

Mastering the game of Go with deep neural networks and tree search

David Silver, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George van den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, Sander Dieleman, Dominik Grewe, John Nham, Nal Kalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, Koray Kavukcuoglu, Thore Graepel & Demis Hassabis

Nature **529**, 484–489 (2016) | Cite this article

Abstract

The game of Go has long been viewed as the most challenging of classic games for artificial intelligence owing to its enormous search space and the difficulty of evaluating board positions and moves. Here we introduce a new approach to computer Go that uses 'value networks' to evaluate board positions and 'policy networks' to select moves. These deep neural networks are trained by a novel combination of supervised learning from human expert games, and reinforcement learning from games of self-play. Without any lookahead search, the neural networks play Go at the level of state-of-the-art Monte Carlo tree search programs that simulate thousands of random games of self-play. We also introduce a new search algorithm that combines Monte Carlo simulation with value and policy networks.

Solving poker games via self-play

Description of Pluribus

The core of Pluribus's strategy was computed through self-play, in which the AI plays against copies of itself, without any data of human or prior AI play used as input. The AI starts from scratch by playing randomly and gradually improves as it determines which actions, and which probability distribution over those actions, lead to better outcomes against earlier versions of its strategy. Forms of self-play have previously been used to generate powerful AIs in two-player zero-sum games such as backgammon (18), Go (9, 19), Dota 2 (20), StarCraft 2 (21), and two-player poker (4–6), though the precise algorithms that were used have varied widely. Although it is easy to construct toy games with more than two players in which commonly used self-play algorithms fail to converge to a meaningful solution (22), in practice self-play has nevertheless been shown to do reasonably well in some games with more than two players (23).

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- so no player has incentive to deviate from an NE
- they are also the best strategies assuming the worst opponent:

$$p^\star = \operatorname*{argmax}_p \min_q p^\top M q \quad \text{and} \quad q^\star = \operatorname*{argmin}_q \max_p p^\top M q$$

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- observe M_{a_t,b_t} (plus noise), feed it as reward to $\mathcal{A}$ and as loss to $\mathcal{B}$

Low regret means convergence to NE

Suppose $\mathcal{A}$ and $\mathcal{B}$ have at most $\sqrt{T}$ regret:

$$\max_{a\in[K]} \sum_{t=1}^{T} M_{a,b_t} - \sum_{t=1}^{T} M_{a_t,b_t} \precsim \sqrt{T}$$

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and thus

$$\max_{p} p^\top M \bar{q} - \min_{q} \bar{p}^\top M q \lesssim \frac{1}{\sqrt{T}}$$

for $\bar{p}$ and $\bar{q}$ being the **empirical distribution** of $a_{1:T}$ and $b_{1:T}$

Low regret means convergence to NE (cont.)

$$\max_p p^\top M \bar{q} - \min_q \bar{p}^\top M q \precsim \frac{1}{\sqrt{T}}$$

means

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meaning that $(\bar{p}, \bar{q})$ **converges to NE as** $T \to \infty$

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- **self-play** with **Exp3** for preference feedback (dueling bandits)
- self-play for solving games (low regret $\Rightarrow$ convergence to NE)