

Machine Learning

V12a: Learning Games from Selfplay

Learning to act
Example: DeepMind's Alpha Zero
Training the policy/value network

Based on material by

- David Silver, DeepMind
- David Foster, Applied Data Science
- Surag Nair, Stanford University



Teaser (See <https://youtu.be/tXIM99xPQC8>)



Educational objectives for today

- **Know** what **reinforcement learning** is and how it differs from supervised learning
- **Know** real-world applications of **reinforcement learning**
- **Explain** how **Alpha Zero** works in principle, apart from the neural network details
- **Be able** to **start working** on a simple **self-play example** yourself



1. LEARNING TO ACT

Reinforcement learning (RL)

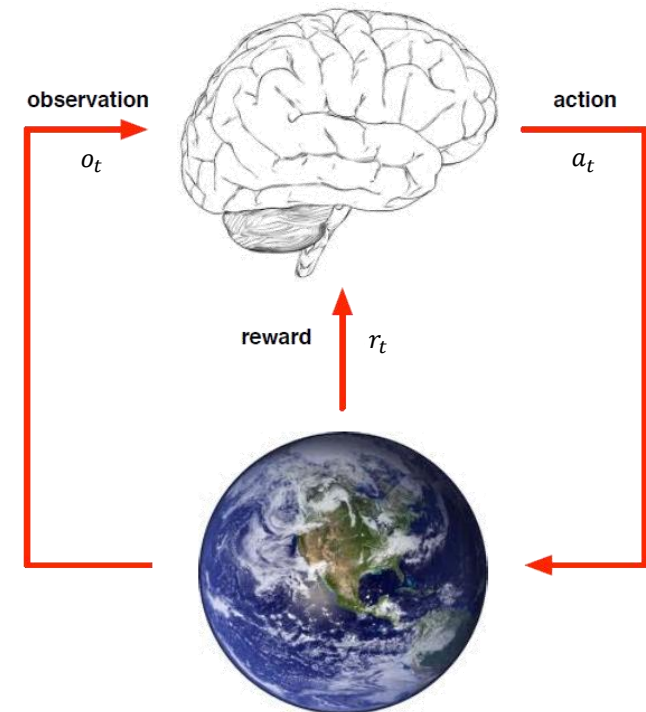
Agent learns by **interacting** with a stochastic environment
→ Science of **sequential decision making**

Many faces of reinforcement learning

- Optimal control (Engineering)
- Dynamic Programming (Operations Research)
- Reward systems (Neuro-science)
- Classical/Operant Conditioning (Psychology)

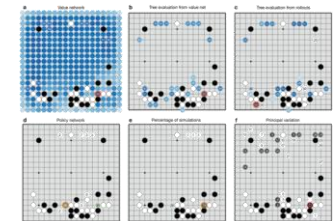
Characteristics

- No supervisor, only **reward** signals
- Objective: maximize cumulative reward
- Feedback is **delayed**
- Trade-off between **exploration & exploitation**
- Sequential decisions: actions effect observations (non i.i.d.)

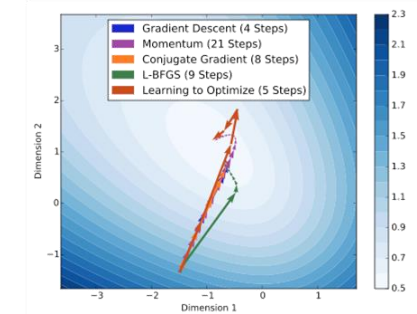


Application areas

- Automated vehicle control
→ An unmanned helicopter learning to fly and perform stunts
- Chat bots
→ Agent figuring out how to make a conversation
- Medical treatment planning
→ Planning a sequence of treatments based on the effect of past treatments
- **Game playing**
→ Playing backgammon, Atari Breakout, Tetris, Tic Tac Toe
- Data Center Cooling
→ <https://deepmind.com/blog/deepmind-ai-reduces-google-data-centre-cooling-bill-40/>
- Database query optimization
→ J. Ortiz et al., “Learning State Representations for Query Optimization with Deep Reinforcement Learning”, DEEM’2018
- Learning new machine learning algorithms
→ <https://bair.berkeley.edu/blog/2017/09/12/learning-to-optimize-with-rl/>



AlphaGo



...and more

- see <https://www.oreilly.com/ideas/practical-applications-of-reinforcement-learning-in-industry>,
<https://www.meetup.com/de-DE/Reinforcement-Learning-Zurich/>

2. EXAMPLE: DEEPMIND'S ALPHA ZERO



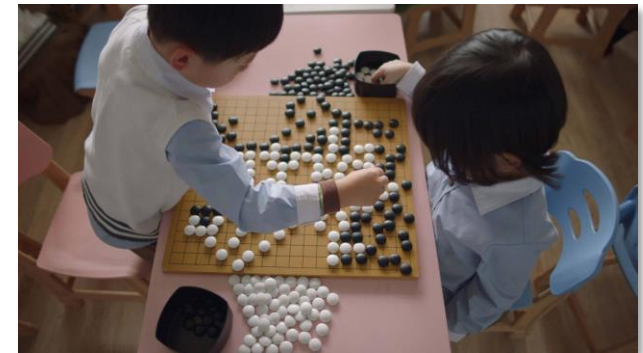
The game of Go

Properties

- **Perfect-information, deterministic**, two-player, turn-based, zero-sum game
- Played on a 19x19 board, alternate moves between black and white
- Two possible results: win or loss
- Considered a grand challenge for AI due to **vast search space** ($\sim 10^{170}$ states; chess: 10^{50})

Rules

- Each turn, a **stone** of the player's color is **put on** an **intersection** of the board (or “**pass**”)
- A stone (or **connected group** of stones) fully and **directly surrounded** by stones of the other color **is removed** from the board (“captured”)
- It is not allowed to recreate a former board position
- **Two consecutive passes end the game**
- The player having **more “area” wins**



AlphaGo, AlphaGo Zero & Alpha Zero



ARTICLE

Mastering the game of Go without human knowledge

David Silver^{1,2}, Julian Schrittwieser^{1,2}, Karen Simonyan^{1,2}, Ioannis Antonoglou¹, Aja Huang¹, Arthur Guez¹, Thomas Hubert¹, Lucas Baker¹, Matthew Lai¹, Adrian Hui¹, Yutian Chen¹, Timothy Lillicrap¹, Fan Hui¹, Laurent Sifre¹, George van den Driessche¹, Thore Graepel¹ & Demis Hassabis¹

A long-standing goal of artificial intelligence is an algorithm that learns, *tabula rasa*, superhuman proficiency in challenging domains. Recently, AlphaGo became the first program to defeat a world champion in the game of Go. The tree search in AlphaGo evaluated positions and selected moves using deep neural networks. These neural networks were trained by supervised learning from human expert moves, and by reinforcement learning from self-play. Here we introduce an algorithm based solely on reinforcement learning, without human data, guidance or domain knowledge beyond game rules. AlphaGo becomes its own teacher: a neural network is trained to predict AlphaGo's own move selections and also the winner of AlphaGo's games. This neural network improves the strength of the tree search, resulting in higher quality move selection and stronger self-play in the next iteration. Starting *tabula rasa*, our new program AlphaGo Zero achieved superhuman performance, winning 100–0 against the previously published, champion-defeating AlphaGo.

Much progress towards artificial intelligence has been made using supervised learning systems that are trained to replicate the decisions of human experts^{1–5}. However, expert data sets are often expensive, unreliable or simply unavailable. Even when reliable data sets are available, they may impose a ceiling on the performance of systems trained in this manner^{6–8}. By contrast, reinforcement learning systems are trained from their own experience, in principle allowing them to exceed human capabilities, and to operate in domains where human expertise is lacking. Recently, there has been rapid progress towards this goal, using deep neural networks trained by reinforcement learning. These systems have outperformed humans in computer games, such as Atari^{9–10} and 3D virtual environments^{11–13}. However, the most challenging domains in terms of human intellect—such as the game of Go, widely viewed as a grand challenge for artificial intelligence¹⁴—require a precise and sophisticated lookahead in vast search spaces. Fully general methods have not previously achieved human-level performance in these domains.

AlphaGo was the first program to achieve superhuman performance in Go. The published version¹⁵, which we refer to as AlphaGo Fan, defeated the European champion Fan Hui in October 2015. AlphaGo Fan used two deep neural networks: a policy network that outputs move probabilities and a value network that outputs a position evaluation. The policy network was trained initially by supervised learning to accurately predict human expert moves, and was subsequently refined by policy gradient reinforcement learning. The value network was trained to predict the winner of games played by the policy network against itself. Once trained, these networks were combined with a Monte Carlo tree search (MCTS)^{16–17} to provide a lookahead search, using the policy network to narrow down the search to high-probability moves, and using the value network (in conjunction with Monte Carlo rollouts using a fast rollout policy) to evaluate positions in the tree. A subsequent version, which we refer to as AlphaGo Lee, used a similar approach (see Methods), and defeated Lee Sedol, the winner of 18 international titles, in March 2016.

Our program, AlphaGo Zero, differs from AlphaGo Fan and AlphaGo Lee¹⁵ in several important aspects. First and foremost, it is

trained solely by self-play reinforcement learning, starting from random play, without any supervision or use of human data. Second, it uses only the black and white stones from the board as input features. Third, it uses a single neural network, rather than separate policy and value networks. Finally, it uses a simpler tree search that relies upon this single neural network to evaluate positions and sample moves, without performing any Monte Carlo rollouts. To achieve these results, we introduce a new reinforcement learning algorithm that incorporates lookahead search inside the training loop, resulting in rapid improvement and precise and stable learning. Further technical differences in the search algorithm, training procedure and network architecture are described in Methods.

Reinforcement learning in AlphaGo Zero

Our new method uses a deep neural network f_θ with parameters θ . This neural network takes as an input the raw board representation s of the position and its history, and outputs both move probabilities and a value, $(p, v) = f_\theta(s)$. The vector of move probabilities p represents the probability of selecting each move a (including pass), $p_a = \text{Pr}(s|a)$. The value v is a scalar evaluation, estimating the probability of the current player winning from position s . This neural network combines the roles of both policy network and value network¹⁸ into a single architecture. The neural network consists of many residual blocks¹⁹ of convolutional layers^{20,21} with batch normalization²² and rectified nonlinearities²³ (see Methods).

The neural network in AlphaGo Zero is trained from games of self-play by a novel reinforcement learning algorithm. In each position s , an MCTS search is executed, guided by the neural network f_θ . The MCTS search outputs probabilities p of playing each move. These search probabilities usually select much stronger moves than the raw move probabilities p of the neural network $f_\theta(s)$. MCTS may therefore be viewed as a powerful policy improvement operator^{24–26}. Self-play with search—using the improved MCTS-based policy to select each move, then using the game winner w as a sample of the value—may be viewed as a powerful policy evaluation operator²⁷. The main idea of our reinforcement learning algorithm is to use these search operators

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Mastering Chess and Shogi by Self-Play with a General Reinforcement Learning Algorithm

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Abstract

The game of chess is the most widely-studied domain in the history of artificial intelligence. The strongest programs are based on a combination of sophisticated search techniques, domain-specific adaptations, and handcrafted evaluation functions that have been refined by human experts over several decades. In contrast, the AlphaGo Zero program recently achieved superhuman performance in the game of Go, by *tabula rasa* reinforcement learning from games of self-play. In this paper, we generalise this approach into a single AlphaZero algorithm that can achieve, *tabula rasa*, superhuman performance in many challenging domains. Starting from random play, and given no domain knowledge except the game rules, AlphaZero achieved within 24 hours a superhuman level of play in the games of chess and shogi (Japanese chess) as well as Go, and convincingly defeated a world-champion program in each case.

The study of computer chess is as old as computer science itself. Babbage, Turing, Shannon, and von Neumann devised hardware, algorithms and theory to analyse and play the game of chess. Chess subsequently became the grand challenge task for a generation of artificial intelligence researchers, culminating in high-performance computer chess programs that perform at superhuman level (9, 13). However, these systems are highly tuned to their domain, and cannot be generalised to other problems without significant human effort.

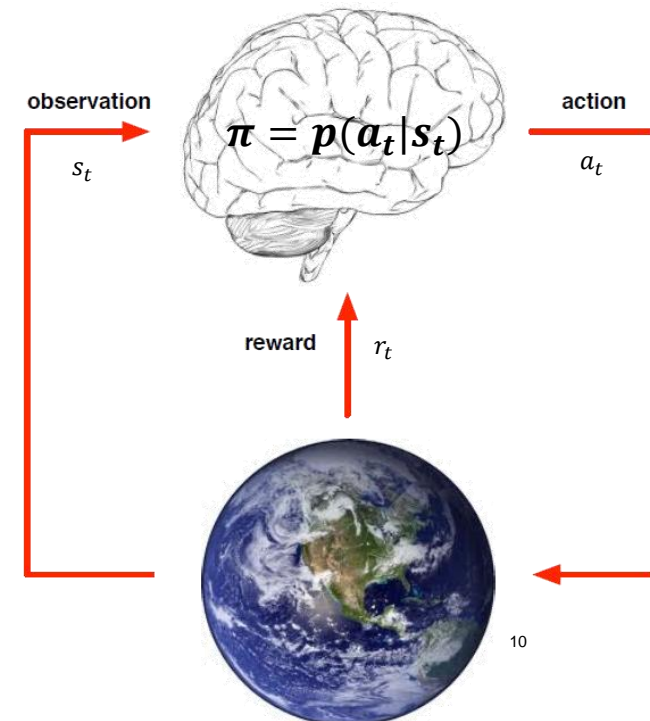
A long-standing ambition of artificial intelligence has been to create programs that can instead learn for themselves from first principles (26). Recently, the AlphaGo Zero algorithm achieved superhuman performance in the game of Go, by representing Go knowledge using deep convolutional neural networks (22, 28), trained solely by reinforcement learning from games of self-play (29). In this paper, we apply a similar but fully generic algorithm, which we

Interesting: playing strength ↑, generality ↑, complexity ↓ (over time)

Goal: a policy

Policy

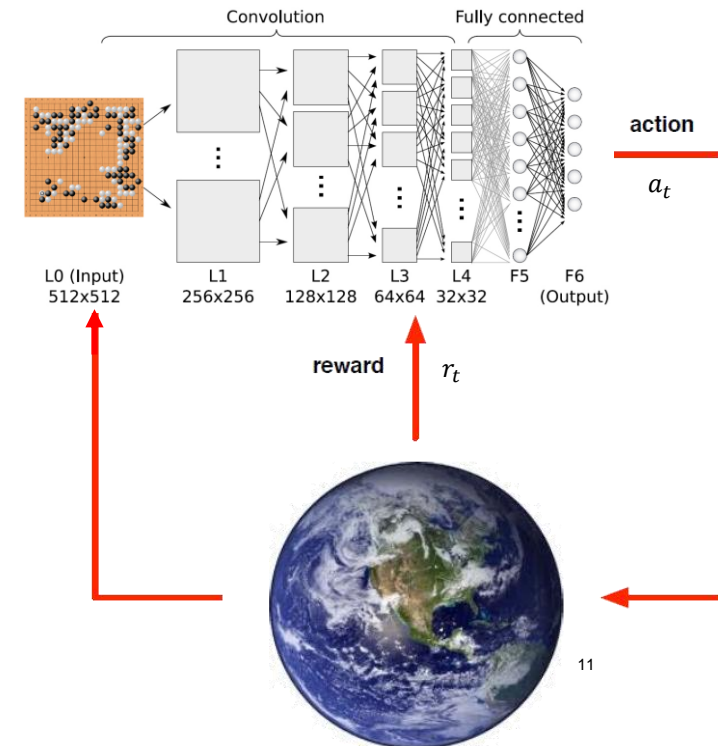
- Policy $\pi = p(a_t | s_t)$ maps (probabilistically) from the current state s_t to action a_t
→ can be represented by a **function approximator** (e.g., a neural network)
- Given the optimal policy π^* , one can behave optimally in the environment
→ but optimality in complex strategic situations is difficult to achieve
→ **lookahead search** makes **tactical** behavior easier



Goal: a policy

Policy

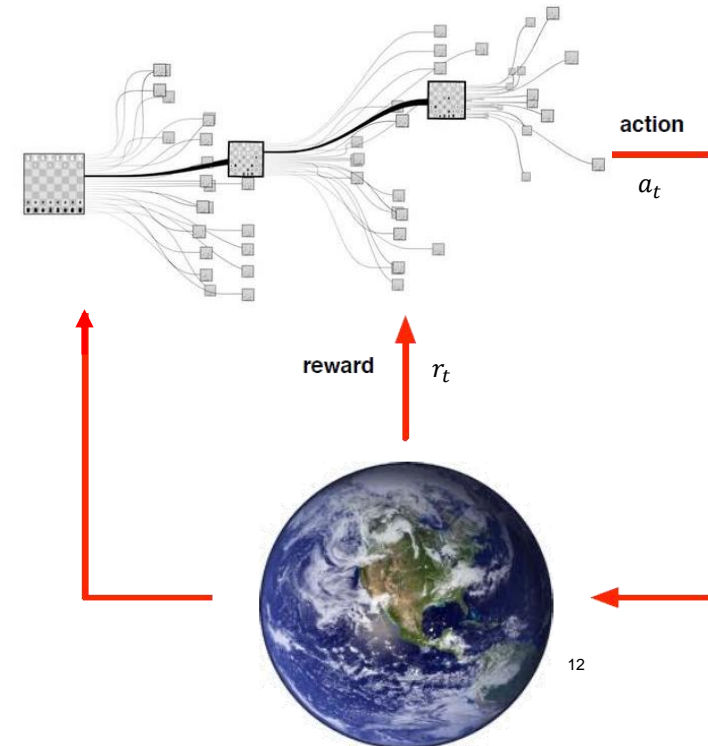
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Goal: a policy

Policy

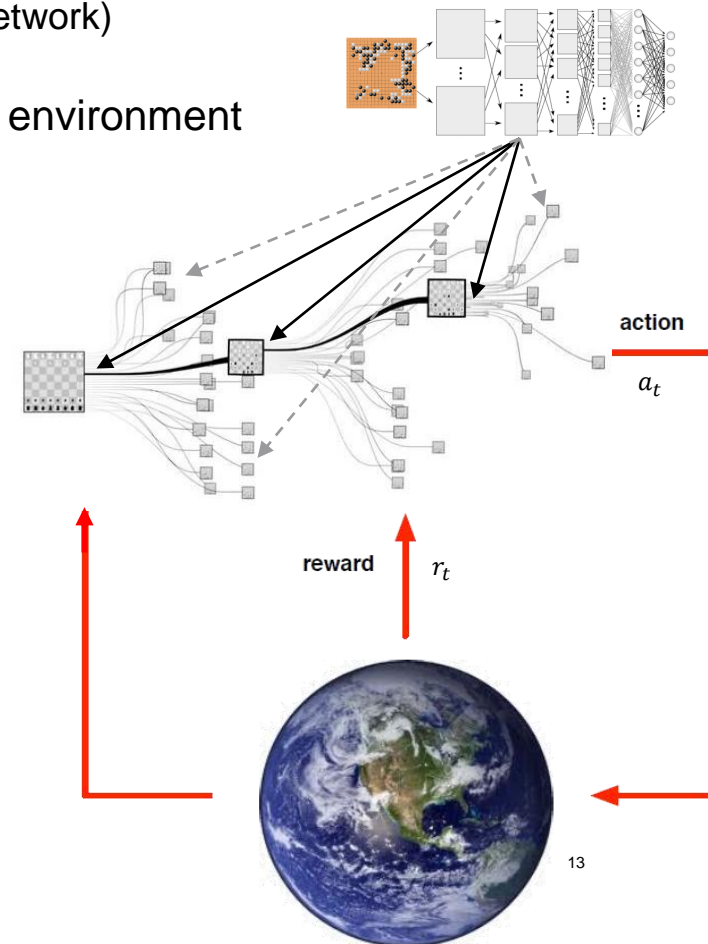
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Goal: a policy

Policy

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Using a learned policy in Alpha Zero

I.e., play a move given a policy

Goal

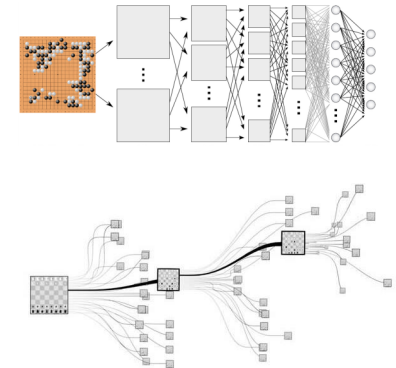
- In state s_t , chose next move a_t

Ingredients

- **Neural network** $\vec{p}, v = f_{\theta}(s_t)$ that outputs two quantities
 - Policy vector \vec{p} (a distribution over all possible actions)
 - Value v (an estimate of the probability of winning from this state)

→ **intuition**
- **Monte Carlo Tree Search (MCTS)** to build ad hoc search tree
 - MC: tree not fully grown → only **likely branches** get explored
 - (Chosen branch can be reused for next move for computational savings)

→ **tactics**



How to chose each move

- Perform MCTS search on ad-hoc built tree
(using neural network for initial intuition if a move is good → see next slide)
- Play move most often taken by search ($\max(N)$)



Perform a MCTS search

I.e., provide the basis for a move

- Create (empty or partly re-used) tree with root s_t
- Perform 1,600 simulations:
(one simulation = one traversal of current tree until yet unexpanded leaf node or terminal node is hit)

1. Start at $s = s_t$

2. Traverse tree:

while s is not a leaf node: choose a that maximizes $Q + U$

(Q is the current mean value of s over all simulations in this search;

U is high if s has high prior probability p from the neural net, or hasn't been explored much (small N);

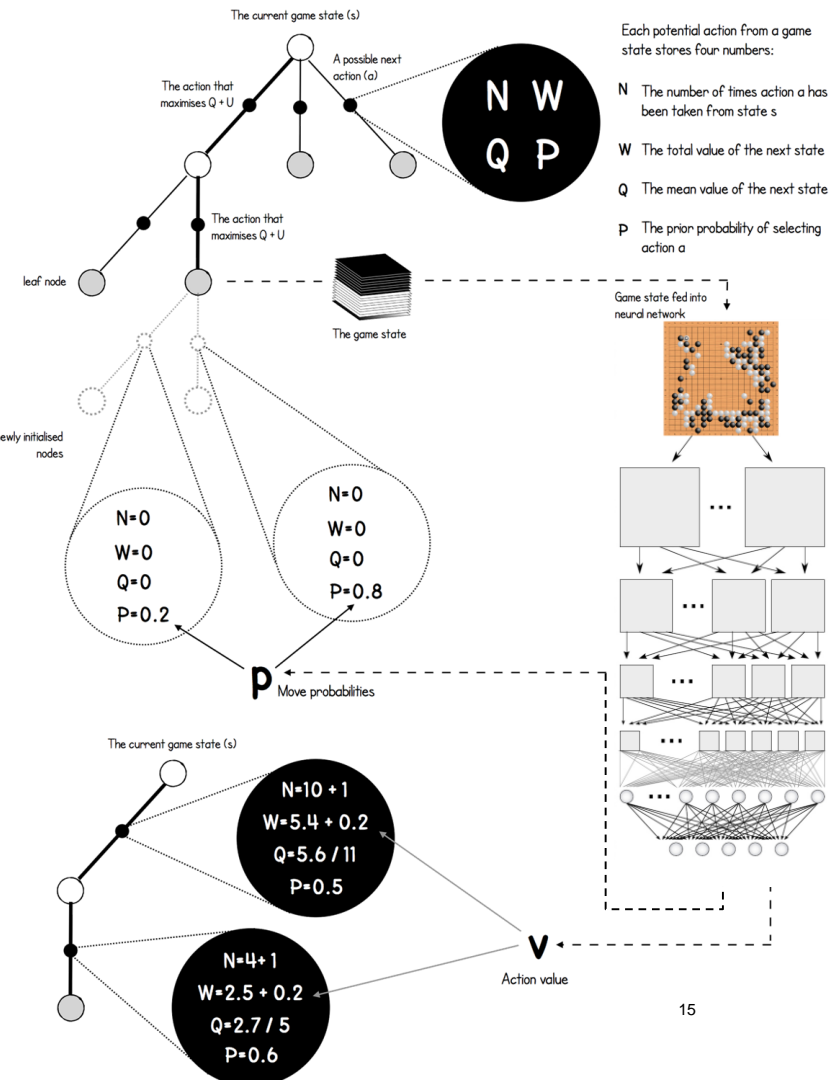
→ U dominates at the beginning of a search; as the branch gets explored, Q becomes important)

3. Expand tree: query neural net for $\vec{p}, v = f_{\theta}(s)$

$N = 0, W = 0, Q = 0, p = \vec{p}_a$

4. Backup: update statistics of each visited node:

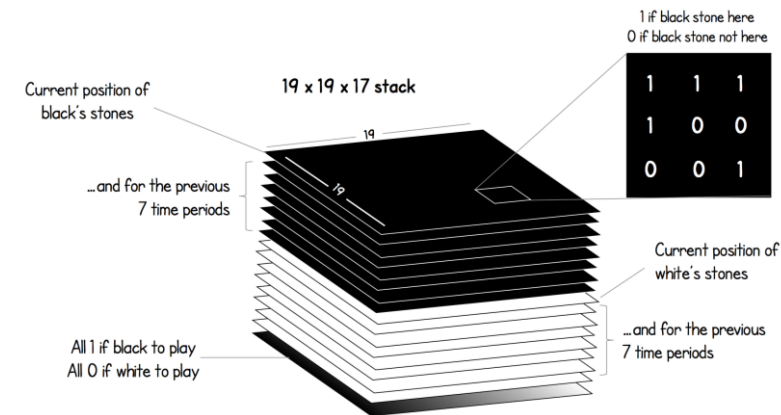
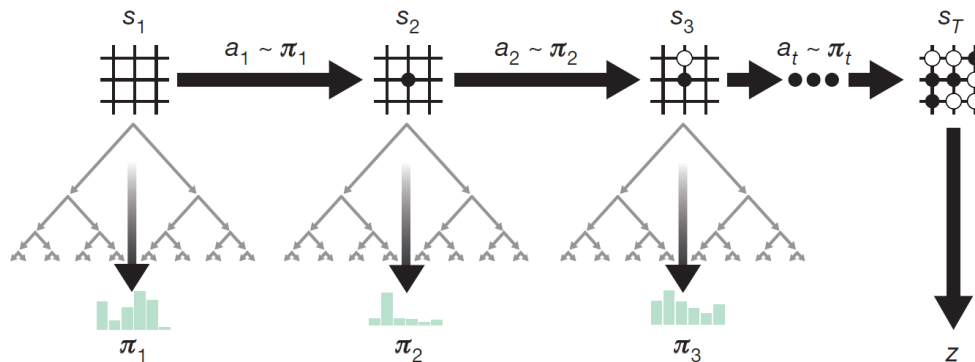
$N = N + 1, W = W + v, Q = W/N$



3. TRAINING THE POLICY/VALUE NETWORK

Create experience by selfplay (=Evaluate the current policy)

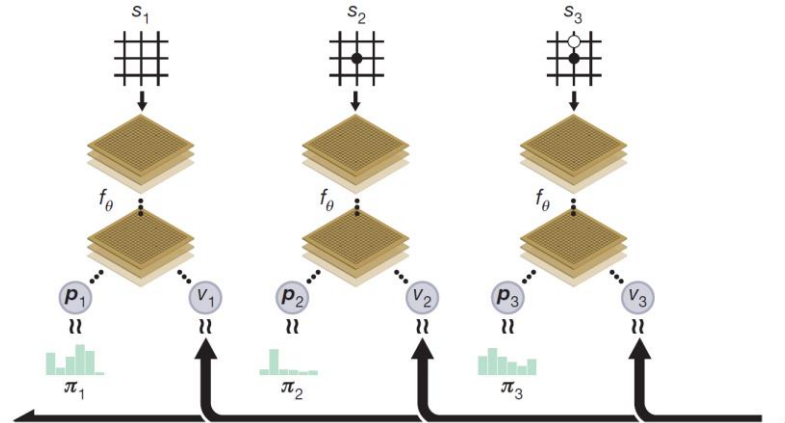
1. Initialize f_θ randomly
2. Play 25,000 games against yourself
 - Use MCTS and current best f_θ for both player's moves
 - **For each move, store**
 - **game state** (see figure →),
 - **search probabilities** from MCTS ($\pi_t \sim N$ for all actions of s_t),
 - **winner** ($z = \pm 1$ from perspective of current player)



3. Trigger retraining (→ see next slide), goto 2

Retrain neural network (=Improve the current policy)

1. Experience replay: sample mini-batch of 2,048 positions from last 500,000 self-play games
2. Retrain f_θ on this batch using **supervised learning**:
 - **Input:** game states
 - **Output:** move-probabilities p (dropping vector notation for simplicity), value v
 - **Labels:** search-probabilities π , actual winner z
 - **Loss:** cross-entropy between p, π + MSE between v, z + L_2 -regularization of θ



3. Trigger evaluation (→ see next slide) after 1,000 training loops, goto 2

Evaluate current network

1. Play 400 games between current best vs. latest f_θ
 - **Choose each move by MCTS** and respective network
 - **Play deterministically** (no additional exploration → see below)

After 1,600 simulations, the move can either be chosen:

Deterministically (for competitive play)

Choose the action from the current state with greatest N

Stochastically (for exploratory play)

Choose the action from the current state from the distribution

$$\pi \sim N^{1/\tau}$$

where τ is a temperature parameter; controlling exploration

2. Replace best network with latest f_θ if the latest wins $\geq 55\%$ of matches

Source: <https://medium.com/applied-data-science/alphago-zero-explained-in-one-diagram-365f5abf67e0>

The diagram illustrates the AlphaGo Zero training pipeline, which is divided into three main stages:

- SELF PLAY:** Create a 'training set'. The best current player plays 25,000 games against itself. See MCTS section to understand how AlphaGo Zero selects each move. At each move, the following information is stored:
 - The game state (See 'What is a Game State' section)
 - The search probabilities (From the MCTS)
 - The winner (+1 if this player won, -1 if this player lost - added once the game has finished)
- RETRAIN NETWORK:** Optimise the network weights. A TRAINING LOOP: Sample a new batch of 2048 positions from the last 500,000 games. Retrain the current neural network on these positions. The game states are the input (See 'Deep Neural Network Architecture'). Loss function: Compares predictions from the neural network with the search probabilities and actual winner.

PREDICTIONS: $\begin{bmatrix} P \\ V \end{bmatrix}$ Cross-entropy + Mean squared error + Regularisation. ACTUAL: π (trophy icon)

After every 1,000 training loops, evaluate the network.
- EVALUATE NETWORK:** Test to see if the new network is stronger. Play 400 games between the latest neural network and the current best neural network. Both players use MCTS to select their moves, with their respective neural networks to evaluate leaf nodes. Latest player must win 55% of games to be declared the new best player.

On the right, a detailed view of the game state input to the deep neural network is shown. It consists of a 19 x 17 stack of boards. The current position of black's stones is indicated by a black dot on the top board. The current position of white's stones is indicated by a white dot on the top board. The stack is labeled 'Current position of black's stones' and 'Current position of white's stones'. The stack is also labeled '19 x 17 stack'. The stack is labeled 'All 1 if black to play All 0 if white to play'. The stack is labeled '...and for the previous 7 time periods'. The stack is labeled 'This stack is the input to the deep neural network'.

THE DEEP NEURAL NETWORK ARCHITECTURE

How AlphaGo Zero assesses new positions

The network learns "tabula rasa" (from a blank slate)
At no point is the network trained using human knowledge or expert moves

The value head

task non-linearity
Fully connected layer
Rectifier non-linearity
Fully connected layer
Batch normalization
1 convoluted filter (x3)
Input

game value for current player
1-1, 0
header
Hidden layer size 256

The policy head

task non-linearity
Fully connected layer
Rectifier non-linearity
Batch normalization
2 convoluted filters (x3)
Input

96 x 96 x 1 filter pool
move logit probabilities

A residual layer

Residual connection
Batch normalization
256 convoluted filters (3x3)
Rectifier non-linearity
Batch normalization
256 convoluted filters (3x3)
Input

A convolutional layer

Batch normalization
256 convoluted filters (3x3)
Input

The network

18 residual layers
Value head
Policy head
Input: The game state (see below)

Each performed action from a game state stores four numbers:

- N** The number of times action has been taken from state s
- W** The total value of the next state
- Q** The mean value of the next state
- p** The prior probability of selecting action a

The diagram illustrates the MCTS process. It shows a game tree with nodes and edges. A path is highlighted from the root to a leaf node, representing a selected action. The leaf node is labeled "leaf node". The path is labeled "The action that maximizes $Q = 0$ ". The root node is labeled "The action that maximizes $Q = 0$ ". A stack of cards is labeled "The game state". A vertical stack of cards is labeled "Game state that record networks". A legend defines the variables: **N** (Number of times action has been taken from state), **W** (Total value of the next state), **Q** (Mean value of the next state), and **p** (Prior probability of selecting action). The diagram shows the calculation of the action value V for a leaf node. The leaf node has $N=0$, $W=0$, $Q=0$, and $p=0.2$. The parent node has $N=10$, $W=5.4$, $Q=5.6/11$, and $p=0.5$. The action value V is calculated as $V = (W + 0.2) / (N + 1) = 5.6 / 11$. The action value V is then used to update the parent node's statistics.

- The rest of the tree is discarded

Important RL concepts showcased here

To be detailed elsewhere

- Formal framework: **Markov decision processes** (MPDs)
- The RL problem: observations vs. **states**, learning vs. **planning, prediction & control**
- Ingredients to a solution: **model**, **value function** (v: state-value / q: action-value), **policy**
- Methods: **dynamic programming (policy iteration)**, **Monte Carlo**, temporal difference learning
- RL & function approximation: general instability, **experience replay**, **target networks**
- Exploration vs. exploitation: **optimistic initialization (upper confidence bounds)**, noise on priors



Where's the intelligence?

Man vs. machine

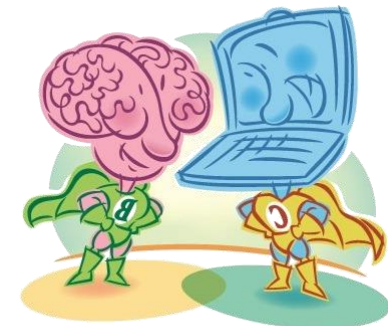
- Alpha(Go) Zero **learns** without human intervention **from scratch** (pure selfplay & the rules)
→ strong point for capabilities of RL
- Alpha(Go) Zero is considerably more **simple/principled** than previous approaches
→ good ideas are usually simple and intuitively right (the reverse is not necessarily true!)
- Recently*, OpenAI showed similar **fascinating performance** on Dota2, and DeepMind on Quake III Arena**
→ RL has made big progress and seems fit for real applications beyond simulations
- Yet***, solutions are still hand-crafted per use case and suffer from extreme **sample inefficiency** and **training instabilities**
→ Training takes very long even on server hardware, debugging is frustrating, success is fragile
- And: Go was an easy and exceptional target, difficult to repeat elsewhere****

*) See <https://blog.openai.com/openai-five/> and <https://blog.openai.com/learning-dexterity/>

**) See <https://deepmind.com/blog/capture-the-flag/>

***) See <https://www.alexirpan.com/2018/02/14/rl-hard.html> and <http://amid.fish/reproducing-deep-rl>

****) See <https://medium.com/@karpathy/alphago-in-context-c47718cb95a5>



Review

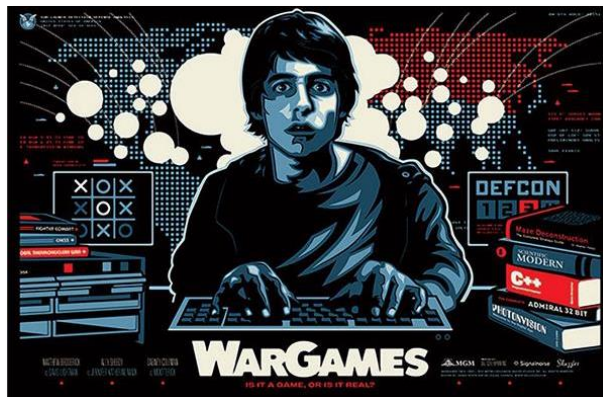
- **Reinforcement learning (RL)** is “**learning to act**” – a general method for “**sequential decision making**”
- Most notable **differences** from unsupervised & supervised **ML**:
 - **no “data set”**
 - agent learns from interaction with environment and sparse rewards
 - less learning signal
 - **experience** is highly correlated and **not i.i.d.!**; but:
- **Alpha Zero** uses an elegant RL algorithm based on
 - **Selfplay** (for experience generation)
 - **MCTS** tree search (to plan ahead in a principled way)
 - Function approximation using **deep learning** (to use intuition as guide for tree search)
- Read the original publication, it is worth it (clear, concise, precise, complete):
<https://www.nature.com/articles/nature24270>



P12: Selfplay for Tic Tac Toe

Work through P12:

1. Background research: acquaint yourself with the thoughts of Peter Abbeel and others on selfplay and contrast it with David Silver et al.'s work.
2. Build an agent that learns to play Tic Tac Toe purely from selfplay using the simple TD(0) approach outlined in the introductory chapter of Sutton & Barto's RL book*.



*) See <http://incompleteideas.net/book/bookdraft2017nov5.pdf>



APPENDIX

Pseudo code – training π

Source: <https://web.stanford.edu/~surag/posts/alphazero.html>

```
def policyIterSP(game):
    nnet = initNNet() #initialise random neural network
    examples = []
    for i in range(numIters):
        for e in range(numEps):
            #collect examples from this game
            examples += executeEpisode(game, nnet)
        new_nnet = trainNNet(examples)
        #compare new net with previous net
        frac_win = pit(new_nnet, nnet)
        if frac_win > threshold:
            nnet = new_nnet #replace with new net
    return nnet

def executeEpisode(game, nnet):
    examples = []
    s = game.startState()
    mcts = MCTS() #initialise search tree

    while True:
        for _ in range(numMCTSSims):
            mcts.search(s, game, nnet)
            #rewards can not be determined yet
            examples.append([s, mcts.pi(s), None])
            #sample action from improved policy
            a = random.choice(len(mcts.pi(s)), p=mcts.pi(s))
            s = game.nextState(s,a)
        if game.gameEnded(s):
            examples = assignRewards(examples, game.gameReward(s))
            return examples
```

```
def search(s, game, nnet):
    if game.gameEnded(s): return -game.gameReward(s)

    if s not in visited:
        visited.add(s)
        P[s], v = nnet.predict(s)
        return -v

    max_u, best_a = -float("inf"), -1
    for a in range(game.getValidActions(s)):
        u = Q[s][a] + c_puct*P[s][a]*sqrt(sum(N[s]))/(1+N[s][a])
        if u>max_u:
            max_u = u
            best_a = a
    a = best_a

    sp = game.nextState(s, a)
    v = search(sp, game, nnet)

    Q[s][a] = (N[s][a]*Q[s][a] + v)/(N[s][a]+1)
    N[s][a] += 1
    return -v
```