A final modification of standard Q-learning was also found to improve stability. They clipped the error term $R_{t+1} + \gamma \max_a \tilde{q}(S_{t+1}, a, \mathbf{w}_t) - \hat{q}(S_t, A_t, \mathbf{w}_t)$ so that it remained in the interval $[-1, 1]$.

Mnih et al. conducted a large number of learning runs on 5 of the games to gain insight into the effect that various of DQN's design features had on its performance. They ran DQN with the four combinations of experience replay and the duplicate target network being included or not included. Although the results varied from game to game, each of these features alone significantly improved performance, and very dramatically improved performance when used together. Mnih et al. also studied the role played by the deep convolutional ANN in DQN's learning ability by comparing the deep convolutional version of DQN with a version having a network of just one linear layer, both receiving the same stacked preprocessed video frames. Here, the improvement of the deep convolutional version over the linear version was particularly striking across all 5 of the test games.

Creating artificial agents that excel over a diverse collection of challenging tasks has been an enduring goal of artificial intelligence. The promise of machine learning as a means for achieving this has been frustrated by the need to craft problem-specific representations. DeepMind's DQN stands as a major step forward by demonstrating that a single agent can learn problem-specific features enabling it to acquire human-competitive skills over a range of tasks. This demonstration did not produce one agent that simultaneously excelled at all the tasks (because learning occurred separately for each task), but it showed that deep learning can reduce, and possibly eliminate, the need for problem-specific design and tuning. As Mnih et al. point out, however, DQN is not a complete solution to the problem of task-independent learning. Although the skills needed to excel on the Atari games were markedly diverse, all the games were played by observing video images, which made a deep convolutional ANN a natural choice for this collection of tasks. In addition, DQN's performance on some of the Atari 2600 games fell considerably short of human skill levels on these games. The games most difficult for DQN—especially Montezuma's Revenge on which DQN learned to perform about as well as the random player—require deep planning beyond what DQN was designed to do. Further, learning control skills through extensive practice, like DQN learned how to play the Atari games, is just one of the types of learning humans routinely accomplish. Despite these limitations, DQN advanced the state-of-the-art in machine learning by impressively demonstrating the promise of combining reinforcement learning with modern methods of deep learning.

16.6 Mastering the Game of Go

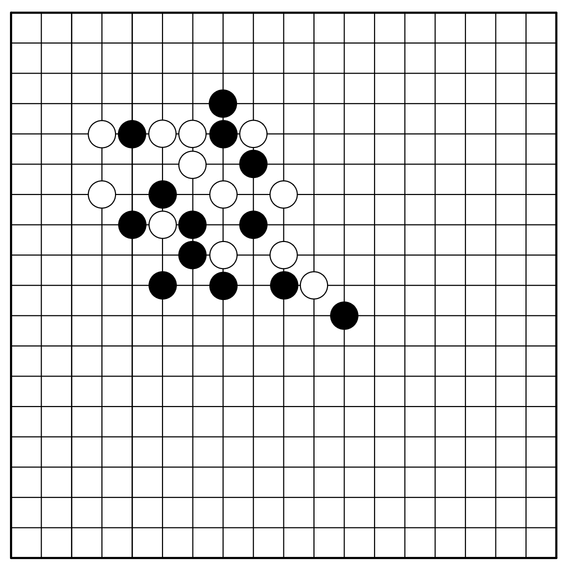
The ancient Chinese game of Go has challenged artificial intelligence researchers for many decades. Methods that achieve human-level skill, or even superhuman-level skill, in other games have not been successful in producing strong Go programs. Thanks to a very active community of Go programmers and international competitions, the level of Go program play has improved significantly over the years. Until recently, however, no Go program had been able to play anywhere near the level of a human Go master.

A team at DeepMind (Silver et al., 2016) developed the program *AlphaGo* that broke this barrier by combining deep ANNs (Section 9.6), supervised learning, Monte Carlo tree search (MCTS, Section 8.11), and reinforcement learning. By the time of Silver et al.'s 2016 publication, *AlphaGo* had been shown to be decisively stronger than other current Go programs, and it had defeated the European Go champion Fan Hui 5 games to 0. These were the first victories of a Go program over a professional human Go player without handicap in full Go games. Shortly thereafter, a similar version of *AlphaGo* won stunning victories over the 18-time world champion Lee Sedol, winning 4 out of a 5 games in a challenge match, making worldwide headline news. Artificial intelligence researchers thought that it would be many more years, perhaps decades, before a program reached this level of play.

Here we describe *AlphaGo* and a successor program called *AlphaGo Zero* (Silver et al. 2017a). Where in addition to reinforcement learning, *AlphaGo* relied on supervised learning from a large database of expert human moves, *AlphaGo Zero* used only reinforcement learning and no human data or guidance beyond the basic rules of the game (hence the *Zero* in its name). We first describe *AlphaGo* in some detail in order to highlight the relative simplicity of *AlphaGo Zero*, which is both higher-performing and more of a pure reinforcement learning program.

In many ways, both *AlphaGo* and *AlphaGo Zero* are descendants of Tesauro's TD-Gammon (Section 16.1), itself a descendant of Samuel's checkers player (Section 16.2). All these programs included reinforcement learning over simulated games of self-play. *AlphaGo* and *AlphaGo Zero* also built upon the progress made by DeepMind on playing Atari games with the program DQN (Section 16.5) that used deep convolutional ANNs to approximate optimal value functions.

Go is a game between two players who alternately place black and white 'stones' on unoccupied intersections, or 'points,' on a board with a grid of 19 horizontal and 19 vertical lines to produce positions like that shown to the right. The game's goal is to capture an area of the board larger than that captured by the opponent. Stones are captured according to simple rules. A player's stones are captured if they are completely surrounded by the other player's stones, meaning that there is no horizontally or vertically adjacent point that is unoccupied. For example, Figure 16.5 shows on the left three white stones with an unoccupied adjacent point (labeled X). If player black places a stone on X, the three white stones are captured and taken off the board (Figure 16.5 middle). However, if player white were to place a stone on point X first, then the possibility of this capture would be blocked (Figure 16.5 right). Other rules are needed to prevent infinite capturing/re-capturing loops. The game ends when neither player wishes to place another stone. These rules are simple, but they produce a very complex game that has had wide



A Go board configuration

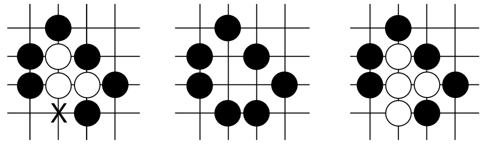


Figure 16.5: Go capturing rule. Left: the three white stones are not surrounded because point X is unoccupied. Middle: if black places a stone on X, the three white stones are captured and removed from the board. Right: if white places a stone on point X first, the capture is blocked.

appeal for thousands of years.

Methods that produce strong play for other games, such as chess, have not worked as well for Go. The search space for Go is significantly larger than that of chess because Go has a larger number of legal moves per position than chess (≈ 250 versus ≈ 35) and Go games tend to involve more moves than chess games (≈ 150 versus ≈ 80). But the size of the search space is not the major factor that makes Go so difficult. Exhaustive search is infeasible for both chess and Go, and Go on smaller boards (e.g., 9×9) has proven to be exceedingly difficult as well. Experts agree that the major stumbling block to creating stronger-than-amateur Go programs is the difficulty of defining an adequate position evaluation function. A good evaluation function allows search to be truncated at a feasible depth by providing relatively easy-to-compute predictions of what deeper search would likely yield. According to Müller (2002): "No simple yet reasonable evaluation function will ever be found for Go." A major step forward was the introduction of MCTS to Go programs. The strongest programs at the time of *AlphaGo*'s development all included MCTS, but master-level skill remained elusive.

Recall from Section 8.11 that MCTS is a decision-time planning procedure that does not attempt to learn and store a global evaluation function. Like a rollout algorithm (Section 8.10), it runs many Monte Carlo simulations of entire episodes (here, entire Go games) to select each action (here, each Go move: where to place a stone or to resign). Unlike a simple rollout algorithm, however, MCTS is an iterative procedure that incrementally extends a search tree whose root node represents the current environment state. As illustrated in Figure 8.10, each iteration traverses the tree by simulating actions guided by statistics associated with the tree's edges. In its basic version, when a simulation reaches a leaf node of the search tree, MCTS expands the tree by adding some, or all, of the leaf node's children to the tree. From the leaf node, or one of its newly added child nodes, a rollout is executed: a simulation that typically proceeds all the way to a terminal state, with actions selected by a rollout policy. When the rollout completes, the statistics associated with the search tree's edges that were traversed in this iteration are updated by backing up the return produced by the rollout. MCTS continues this process, starting each time at the search tree's root at the current state, for as many iterations as possible given the time constraints. Then, finally, an action from the root node (which still represents the current environment state) is selected according to statistics accumulated in the root node's outgoing edges. This is the action the agent takes. After the environment transitions to its next state, MCTS is executed again with the root node set to represent the new current state. The search tree at the start of this next execution might be just this new root node, or it might include descendants of this node left over from MCTS's previous execution. The remainder of the tree is discarded.

16.6.1 AlphaGo

The main innovation that made *AlphaGo* such a strong player is that it selected moves by a novel version of MCTS that was guided by both a policy and a value function learned by reinforcement learning with function approximation provided by deep convolutional ANNs. Another key feature is that instead of reinforcement learning starting from random network weights, it started from weights that were the result of previous supervised learning from a large collection of human expert moves.

The DeepMind team called *AlphaGo*'s modification of basic MCTS "asynchronous policy and value MCTS," or APV-MCTS. It selected actions via basic MCTS as described above but with some twists in how it extended its search tree and how it evaluated action edges. In contrast to basic MCTS, which expands its current search tree by using stored action values to select an unexplored edge from a leaf node, APV-MCTS, as implemented in *AlphaGo*, expanded its tree by choosing an edge according to probabilities supplied by a 13-layer deep convolutional ANN, called the *SL-policy network*, trained previously by supervised learning to predict moves contained in a database of nearly 30 million human expert moves.

Then, also in contrast to basic MCTS, which evaluates the newly-added state node solely by the return of a rollout initiated from it, APV-MCTS evaluated the node in two ways: by this return of the rollout, but also by a value function, v_θ, learned previously by a reinforcement learning method. If s was the newly-added node, its value became

$$v(s) = (1-\eta)v_\theta(s) + \eta G, \tag{16.4}$$

where G was the return of the rollout and η controlled the mixing of the values resulting from these two evaluation methods. In *AlphaGo*, these values were supplied by the *value network*, another 13-layer deep convolutional ANN that was trained as we describe below to output estimated values of board positions. APV-MCTS's rollouts in *AlphaGo* were simulated games with both players using a fast *rollout policy* provided by a simple linear network, also trained by supervised learning before play. Throughout its execution, APV-MCTS kept track of how many simulations passed through each edge of the search tree, and when its execution completed, the most-visited edge from the root node was selected as the action to take, here the move *AlphaGo* actually made in a game.

The value network had the same structure as the deep convolutional SL policy network except that it had a single output unit that gave estimated values of game positions instead of the SL policy network's probability distributions over legal actions. Ideally, the value network would output optimal state values, and it might have been possible to approximate the optimal value function along the lines of TD-Gammon described above: self-play with nonlinear TD(λ) coupled to a deep convolutional ANN. But the DeepMind team took a different approach that held more promise for a game as complex as Go. They divided the process of training the value network into two stages. In the first stage, they created the best policy they could by using reinforcement learning to train an *RL* *policy network*. This was a deep convolutional ANN with the same structure as the SL policy network. It was initialized with the final weights of the SL policy network that were learned via supervised learning, and then policy-gradient reinforcement learning was used to improve upon the SL policy. In the second stage of training the value network, the team used Monte Carlo policy evaluation on data obtained from a large number of simulated self-play games with moves selected by the RL policy network.

Figure 16.6 illustrates the networks used by *AlphaGo* and the steps taken to train them in what the DeepMind team called the "*AlphaGo* pipeline." All these networks were trained before any live game play took place, and their weights remained fixed throughout live play.

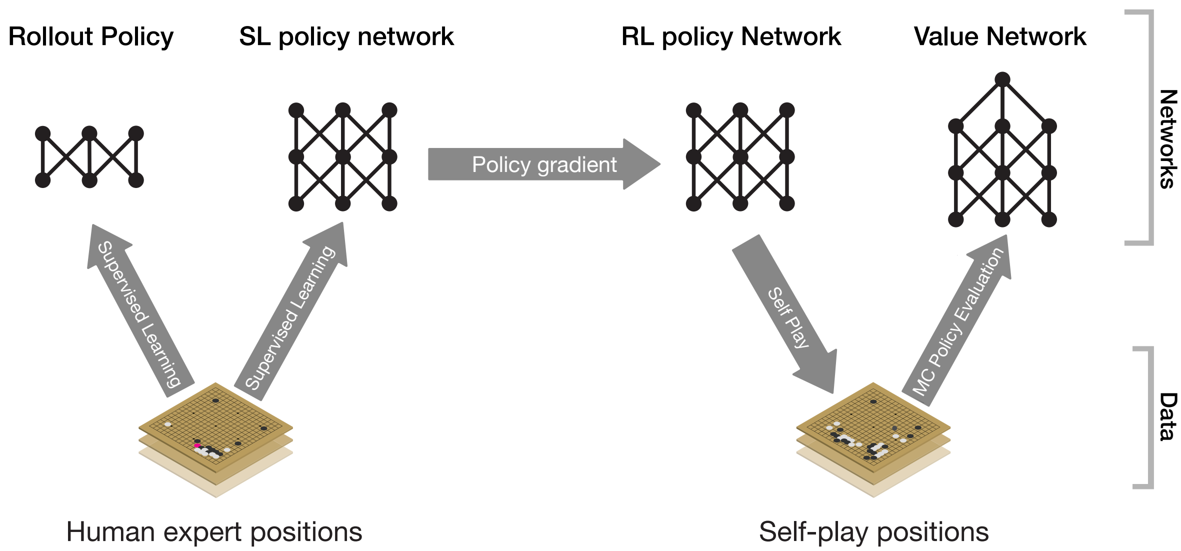


Figure 16.6: *AlphaGo* pipeline. Adapted with permission from Macmillan Publishers Ltd: *Nature*, vol. 529(7587), p. 485, ©2016.

Here is some more detail about *AlphaGo*'s ANNs and their training. The identically-structured SL and RL policy networks were similar to DQN's deep convolutional network described in Section 16.5 for playing Atari games, except that they had 13 convolutional layers with the final layer consisting of a soft-max unit for each point on the 19×19 Go board. The networks' input was a $19 \times 19 \times 48$ image stack in which each point on the Go board was represented by the values of 48 binary or integer-valued features. For example, for each point, one feature indicated if the point was occupied by one of *AlphaGo*'s stones, one of its opponent's stones, or was unoccupied, thus providing the "raw" representation of the board configuration. Other features were based on the rules of Go, such as the number of adjacent points that were empty, the number of opponent stones that would be captured by placing a stone there, the number of turns since a stone was placed there, and other features that the design team considered to be important.

Training the SL policy network took approximately 3 weeks using a distributed implementation of stochastic gradient ascent on 50 processors. The network achieved 57% accuracy, where the best accuracy achieved by other groups at the time of publication was 44.4%. Training the RL policy network was done by policy gradient reinforcement learning over simulated games between the RL policy network's current policy and opponents using policies randomly selected from policies produced by earlier iterations of the learning algorithm. Playing against a randomly selected collection of opponents prevented overfitting to the current policy. The reward signal was +1 if the current policy won, −1 if it lost, and zero otherwise. These games directly pitted the two policies against one another without involving MCTS. By simulating many games in parallel on 50 processors, the DeepMind team trained the RL policy network on a million games in a single day. In testing the final RL policy, they found that it won more than 80% of games played against the SL policy, and it won 85% of games played against a Go program using MCTS that simulated 100,000 games per move.

The value network, whose structure was similar to that of the SL and RL policy networks except for its single output unit, received the same input as the SL and RL policy networks with the exception that there was an additional binary feature giving the current color to play. Monte Carlo policy evaluation was used to train the network from data obtained from a large number of self-play games played using the RL policy. To avoid overfitting and instability due to the strong correlations between positions encountered in self-play, the DeepMind team constructed a data set of 30 million positions each chosen randomly from a unique self-play game. Then training was done using 50 million mini-batches each of 32 positions drawn from this data set. Training took one week on 50 GPUs.

The rollout policy was learned prior to play by a simple linear network trained by supervised learning from a corpus of 8 million human moves. The rollout policy network had to output actions quickly while still being reasonably accurate. In principle, the SL or RL policy networks could have been used in the rollouts, but the forward propagation through these deep networks took too much time for either of them to be used in rollout simulations, a great many of which had to be carried out for each move decision during live play. For this reason, the rollout policy network was less complex than the other policy networks, and its input features could be computed more quickly than the features used for the policy networks. The rollout policy network allowed approximately 1,000 complete game simulations per second to be run on each of the processing threads that *AlphaGo* used.

One may wonder why the SL policy was used instead of the better RL policy to select actions in the expansion phase of APV-MCTS. These policies took the same amount of time to compute because they used the same network architecture. The team actually found that *AlphaGo* played better against human opponents when APV-MCTS used as the SL policy instead of the RL policy. They conjectured that the reason for this was that the latter was tuned to respond to optimal moves rather than to the broader set of moves characteristic of human play. Interestingly, the situation was reversed for the value function used by APV-MCTS. They found that when APV-MCTS used the value function derived from the RL policy, it performed better than if it used the value function derived from the SL policy.

Several methods worked together to produce *AlphaGo*'s impressive playing skill. The DeepMind team evaluated different versions of *AlphaGo* in order to assess the contributions made by these various components. The parameter η in (16.4) controlled the mixing of game state evaluations produced by the value network and by rollouts. With $\eta = 0$, *AlphaGo* used just the value network without rollouts, and with $\eta = 1$, evaluation relied just on rollouts. They found that *AlphaGo* using just the value network played better than the rollout-only *AlphaGo*, and in fact played better than the strongest of all other Go programs existing at the time. The best play resulted from setting $\eta = 0.5$, indicating that combining the value network with rollouts was particularly important to *AlphaGo*'s success. These evaluation methods complemented one another: the value network evaluated the high-performance RL policy that was too slow to be used in live play, while rollouts using the weaker but much faster rollout policy were able to add precision to the value network's evaluations for specific states that occurred during games.

Overall, *AlphaGo*'s remarkable success fueled a new round of enthusiasm for the promise of artificial intelligence, specifically for systems combining reinforcement learning with deep ANNs, to address problems in other challenging domains.

16.6.2 AlphaGo Zero

Building upon the experience with *AlphaGo*, a DeepMind team developed *AlphaGo Zero* (Silver et al. 2017a). In contrast to *AlphaGo*, this program used *no human data or guidance beyond the basic rules of the game* (hence the *Zero* in its name). It learned exclusively from self-play reinforcement learning, with input giving just "raw" descriptions of the placements of stones on the Go board. *AlphaGo Zero* implemented a form of policy iteration (Section 4.3), interleaving policy evaluation with policy improvement. Figure 16.7 is an overview of *AlphaGo Zero*'s algorithm. A significant difference between *AlphaGo Zero* and *AlphaGo* is that *AlphaGo Zero* used MCTS to select moves throughout self-play reinforcement learning, whereas *AlphaGo* used MCTS for live play after—but not during—learning. Other differences besides not using any human data or human-crafted features are that *AlphaGo Zero* used only one deep convolutional ANN and used a simpler version of MCTS.

AlphaGo Zero's MCTS was simpler than the version used by *AlphaGo* in that it did not include rollouts of complete games, and therefore did not need a rollout policy. Each iteration of *AlphaGo Zero*'s MCTS ran a simulation that ended at a leaf node of the current search tree instead of at the terminal position of a complete game simulation. But as in *AlphaGo*, each iteration of MCTS in *AlphaGo Zero* was guided by the output of a deep convolutional network, labeled f_θ in Figure 16.7, were θ is the network's weight vector. The input to the network, whose architecture we describe below, consisted of raw representations of board positions, and its output had two parts: a scalar value, v, an estimate of the probability that the current player will win from from the current board position, and a vector, $\mathbf{p}$, of move probabilities, one for each possible stone placement on the current board, plus the pass, or resign, move.

Instead of selecting self-play actions according to the probabilities $\mathbf{p}$, however, *AlphaGo Zero* used these probabilities, together with the network's value output, to direct each execution of MCTS, which returned new move probabilities, shown in Figure 16.7 as the policies π_i. These policies benefitted from the many simulations that MCTS conducted

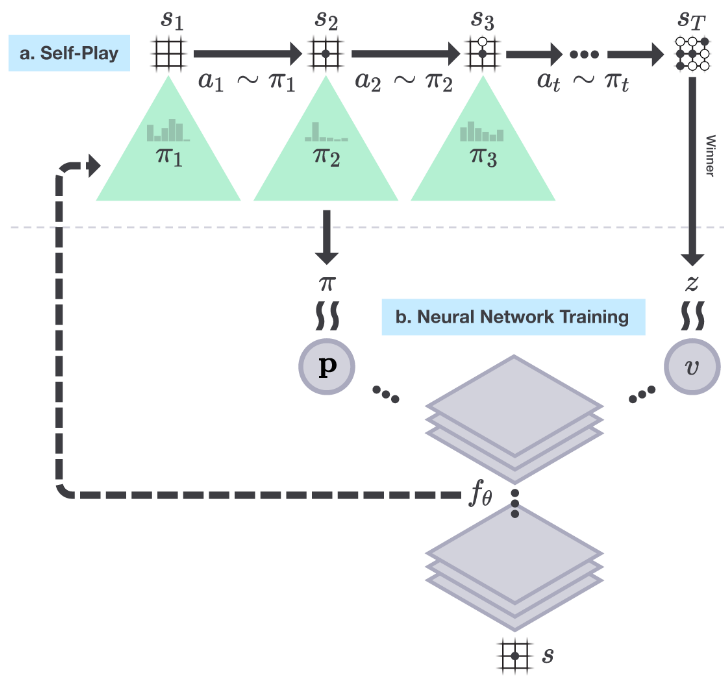


Figure 16.7: *AlphaGo Zero* self-play reinforcement learning. a) The program played many games against itself, one shown here as a sequence of board positions s_i, $i = 1, 2, \ldots, T$, with moves a_i, $i = 1, 2, \ldots, T$, and winner z. Each move a_i was determined by action probabilities π_i returned by MCTS executed from root node s_i and guided by a deep convolutional network, here labeled f_θ, with latest weights θ. Shown here for just one position s but repeated for all s_i, the network's inputs were raw representations of board positions s_i (together with several past positions, though not shown here), and its outputs were vectors $\mathbf{p}$ of move probabilities that guided MCTS's forward searches, and scalar values v that estimated the probability of the current player winning from each position s_i. b) Deep convolutional network training. Training examples were randomly sampled steps from recent self-play games. Weights θ were updated to move the policy vector $\mathbf{p}$ toward the probabilities π returned by MCTS, and to include the winners z in the estimated win probability v. Reprinted from draft of Silver et al. (2017a) with permission of the authors and DeepMind.

each time it executed. The result was that the policy actually followed by *AlphaGo Zero* was an improvement over the policy given by the network's outputs $\mathbf{p}$. Silver et al. (2017a) wrote that "MCTS may therefore be viewed as a powerful *policy improvement* operator."

Here is more detail about *AlphaGo Zero*'s ANN and how it was trained. The network took as input a $19 \times 19 \times 17$ image stack consisting of 17 binary feature planes. The first 8 feature planes were raw representations of the positions of the current player's stones in the current and seven past board configurations: a feature value was 1 if a player's stone was on the corresponding point, and was 0 otherwise. The next 8 feature planes similarly coded the positions of the opponent's stones. A final input feature plane had a constant value indicating the color of the current play: 1 for black; 0 for white. Because repetition is not allowed in Go and one player is given some number of "compensation points" for not getting the first move, the current board position is not a Markov state of Go. This is why features describing past board positions and the color feature were needed.

The network was "two-headed," meaning that after a number of initial layers, the network split into two separate "heads" of additional layers that separately fed into two sets of output units. In this case, one head fed 362 output units producing $19^2 + 1$ move probabilities $\mathbf{p}$, one for each possible stone placement plus pass; the other head fed just one output unit producing the scalar v, an estimate of the probability that the current player will win from the current board position. The network before the split consisted of 41 convolutional layers, each followed by batch normalization, and with skip connections added to implement residual learning by pairs of layers (see Section 9.6). Overall, move probabilities and values were computed by 43 and 44 layers respectively.

Starting with random weights, the network was trained by stochastic gradient descent (with momentum, regularization, and step-size parameter decreasing as training continues) using batches of examples sampled uniformly at random from all the steps of the most recent 500,000 games of self-play with the current best policy. Extra noise was added to the network's output $\mathbf{p}$ to encourage exploration of all possible moves. At periodic checkpoints during training, which Silver et al. (2017a) chose to be at every 1,000 training steps, the policy output by the ANN with the latest weights was evaluated by simulating 400 games (using MCTS with 1,600 iterations to select each move) against the current best policy. If the new policy won (by a margin set to reduce noise in the outcome), then it became the best policy to be used in subsequent self-play. The network's weights were updated to make the network's policy output $\mathbf{p}$ more closely match the policy returned by MCTS, and to make its value output, v, more closely match the probability that the current best policy wins from the board position represented by the network's input.

The DeepMind team trained *AlphaGo Zero* over 4.9 million games of self-play, which took about 3 days. Each move of each game was selected by running MCTS for 1,600 iterations, taking approximately 0.4 second per move. Network weights were updated over 700,000 batches each consisting of 2,048 board configurations. They then ran tournaments with the trained *AlphaGo Zero* playing against the version of *AlphaGo* that defeated Fan Hui by 5 games to 0, and against the version that defeated Lee Sedol by 4 games to 1. They used the Elo rating system to evaluate the relative performances of the programs. The difference between two Elo ratings is meant to predict the outcome of games between the players. The Elo ratings of *AlphaGo Zero*, the version of *AlphaGo* that played against Fan Hui, and the version that played against Lee Sedol were respectively 4,308, 3,144, and 3,739. The gaps in these Elo ratings translate into predictions that *AlphaGo Zero* would defeat these other programs with probabilities very close to one. In a match of 100 games between *AlphaGo Zero*, trained as described, and the exact version of *AlphaGo* that defeated Lee Sedol held under the same conditions that were used in that match, *AlphaGo Zero* defeated *AlphaGo* in all 100 games.

The DeepMind team also compared *AlphaGo Zero* with a program using an ANN with the same architecture but trained by supervised learning to predict human moves in a data set containing nearly 30 million positions from 160,000 games. They found that the supervised-learning player initially played better than *AlphaGo Zero*, and was better at predicting human expert moves, but played less well after *AlphaGo Zero* was trained for a day. This suggested that *AlphaGo Zero* had discovered a strategy for playing that was different from how humans play. In fact, *AlphaGo Zero* discovered, and came to prefer, some novel variations of classical move sequences.

Final tests of *AlphaGo Zero*'s algorithm were conducted with a version having a larger ANN and trained over 29 million self-play games, which took about 40 days, again starting with random weights. This version achieved an Elo rating of 5,185. The team pitted this version of *AlphaGo Zero* against a program called *AlphaGo Master*, the strongest program at the time, that was identical to *AlphaGo Zero* but, like *AlphaGo*, used human data and features. *AlphaGo Master*'s Elo rating was 4,858, and it had defeated the strongest human professional players 60 to 0 in online games. In a 100 game match, *AlphaGo Zero* with the larger network and more extensive learning defeated *AlphaGo Master* 89 games to 11, thus providing a convincing demonstration of the problem-solving power of *AlphaGo Zero*'s algorithm.

AlphaGo Zero soundly demonstrated that superhuman performance can be achieved by pure reinforcement learning, augmented by a simple version of MCTS, and deep ANNs with very minimal knowledge of the domain and no reliance on human data or guidance. We will surely see systems inspired by the DeepMind accomplishments of both *AlphaGo* and *AlphaGo Zero* applied to challenging problems in other domains.

Recently, yet a better program, *AlphaZero*, was described by Silver et al. (2017b) that does not even incorporate knowledge of Go. *AlphaZero* is a general reinforcement learning algorithm that improves over the world's hitherto best programs in the diverse games of Go, chess, and shogi.

16.7 Personalized Web Services

Personalizing web services such as the delivery of news articles or advertisements is one approach to increasing users' satisfaction with a website or to increase the yield of a marketing campaign. A policy can recommend content considered to be the best for each particular user based on a profile of that user's interests and preferences inferred from their history of online activity. This is a natural domain for machine learning, and in particular, for reinforcement learning. A reinforcement learning system can improve a recommendation policy by making adjustments in response to user feedback. One way to obtain user feedback is by means of website satisfaction surveys, but for acquiring feedback in real time it is common to monitor user clicks as indicators of interest in a link.

A method long used in marketing called *A/B testing* is a simple type of reinforcement learning used to decide which of two versions, A or B, of a website users prefer. Because it is non-associative, like a two-armed bandit problem, this approach does not personalize content delivery. Adding context consisting of features describing individual users and the content to be delivered allows personalizing service. This has been formalized as a contextual bandit problem (or an associative reinforcement learning problem, Section 2.9) with the objective of maximizing the total number of user clicks. Li, Chu, Langford, and Schapire (2010) applied a contextual bandit algorithm to the problem of personalizing the Yahoo! Front Page Today webpage (one of the most visited pages on the internet at the time of their research) by selecting the news story to feature. Their objective was to