# Diversifying AI: <br> Towards Creative Chess with AlphaZero 

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In recent years, Artificial Intelligence (AI) systems have surpassed human intelligence in a variety of computational tasks. However, AI systems, like humans, make mistakes, have blind spots, hallucinate, and struggle to generalize to new situations. This work explores whether AI can benefit from creative decision-making mechanisms when pushed to the limits of its computational rationality. In particular, we investigate whether a team of diverse AI systems can outperform a single AI in challenging tasks by generating more ideas as a group and then selecting the best ones. We study this question in the game of chess, the so-called "drosophila of AI". We build on AlphaZero (AZ) and extend it to represent a league of agents via a latent-conditioned architecture, which we call $A Z_{d b}$. We train $A Z_{d b}$ to generate a wider range of ideas using behavioral diversity techniques and select the most promising ones with sub-additive planning. Our experiments suggest that $\mathrm{AZ}_{\mathrm{db}}$ plays chess in diverse ways, solves more puzzles as a group and outperforms a more homogeneous team. Notably, $\mathrm{AZ}_{\mathrm{db}}$ solves twice as many challenging puzzles as AZ, including the challenging Penrose positions. When playing chess from different openings, we notice that players in $\mathrm{AZ}_{\mathrm{db}}$ specialize in different openings, and that selecting a player for each opening using sub-additive planning results in a 50 Elo improvement over AZ. Our findings suggest that diversity bonuses emerge in teams of AI agents, just as they do in teams of humans and that diversity is a valuable asset in solving computationally hard problems.


Figure 1 | Left: an illustration of diverse AI systems playing chess. Right: AZ ${ }_{d b}$ architecture. For each player $i$, a matchmaker selects an opponent $j$. A latent variable $l^{i}$ associated with the player conditions the network outputs $p, v, v_{d}$. A score for each position is computed using $v, v_{d}$ and the diversity intrinsic reward $r^{i}$ and used with the prior $p$ for MCTS.

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## 1. Introduction

Artificial Intelligence (AI) systems have achieved superhuman performance in a variety of fields, including playing games like chess, Go, poker, and Atari (Schrittwieser et al., 2020), and more recently, in retrieving knowledge, reasoning over it and answering questions in medical, law, and business domains (Chowdhery et al., 2022; Katz et al., 2023; OpenAI, 2023; Singhal et al., 2023). AI can outperform humans in many ways; it has greater computational power and ability to experience and learn from more data. Nevertheless, AI is limited by the amount of data and compute available to it, as well as the quality of human feedback. Reinforcement learning (RL) can further improve AI systems by enabling them to learn from trial and error, explore new possibilities, and discover new knowledge.

AlphaZero (AZ; Silver et al., 2018a), an RL algorithm, learned to play Go, chess, and shogi from scratch, without any prior knowledge of the games. It not only outperformed human experts, but also played moves that were considered to be creative (Metz, 2016). Millions of people watched AZ play against StockFish (SF), (Agadmator, GothamChess), and books have been written about it (Sadler and Regan, 2019). AZ has influenced the style of professional chess players (González-Díaz and Palacios-Huerta, 2022) and is associated with increased novelty in the decision-making of Go players (Shin et al., 2023). Indeed, AZ has had a profound impact on the world of chess, inspiring most contemporary chess engines, such as Leela Chess Zero (Lc0) and SF, to incorporate neural networks into their evaluation functions. More recently, AZ has been extended beyond games to discover better algorithms to compress videos (Mandhane et al., 2022), for matrix multiplication (Fawzi et al., 2022), and similar techniques combining search and a neural network have been applied to other domains (Kemmerling et al., 2023).

Even though chess engines are very powerful, we have most likely not reached optimal play yet. For instance, in the related game of Go, superhuman AI has been shown to be vulnerable to adversarial attacks (Timbers et al., 2022; Wang et al., 2022). Other evidence includes the results of computer chess competitions like the Top Chess Engine Championship (TCEC), where the strength of the top engines continues to increase with each season. It is well known that the strength of modern chess engines depends on the amount of compute they have for search; for example, AZ's policy network, i.e., AZ without search, is rated at least 1000 Elo points lower than AZ. More evidence can be found in anti-computer tactics, which exploit blind spots in how computers reason about chess. We can find blind spots in chess puzzles, which computers struggle to solve for different reasons: they can be counterintuitive, may require long-term planning, were designed to trick specific chess engines, or involve querying a chess engine in positions that are different from what it was trained on (out-of-distribution (OOD)). Finding positions that computers don't understand attracted the interest of many chess players (Copeland, 2021a; Doggers, 2017; Penrose, 2020). While these positions become rarer over time, computers still can't solve all of them. In addition, despite being considered weaker players overall, humans can solve most of these puzzles, demonstrating a gap between human and machine thinking. Some scientists even ask if understanding these positions can "help to understand human consciousness" (Doggers, 2017).

This work aims to bridge the gap between human and artificial intelligence by investigating whether creative problem-solving mechanisms identified in human intelligence can be used to make artificial intelligence more creative. We acknowledge that there are different definitions of creativity, which vary across domains and disciplines, but broadly speaking there is "a general agreement that creativity involves the production of novel, useful products" (Mumford, 2003). In this work, we focus on creative problem-solving rather than creativity in other domains such as art or AI-generated art. Even within this narrower context, there is no agreed-upon definition of creativity. Chess players, for example, have difficulty describing their creative thinking process in words: "In my games I have sometimes found a combination intuitively, simply feeling that it must be there. Yet, I was not able to translate my thoughts into normal human language" (Michail Tal). Similarly, creativity in mathematical invention is considered spontaneous and unconscious (Hadamard, 2020). For these reasons, we have chosen to limit our discussion to a specific definition for creative-problem solving by Osborn: "searching for an original and previously unknown solution to a problem" (Osborn, 2012).

In particular, we ask if a team of diverse chess agents can become more creative than a single super human AI. We propose to measure this by looking at the number of challenging chess puzzles that the team solves as a group. These ideas are inspired by studies that have shown that diverse human thinkers outperform homogenous groups on complex tasks, producing "diversity bonuses" (Page, 2019): improved problem solving, increased innovation, and more accurate predictions-all of which lead to better results. One example is the story of the Netflix prize (Wired) - an open
competition to predict customers' movie ratings - where the top two teams worked together to beat the challenge by cleverly combining each other's algorithms. Other examples of the correlation between heterogeneous teams and diversity bonuses include: teams of three or more songwriters writing the majority of the Billboard 100 hits (Priceonomics), larger and diverse teams outperform individuals in scientific writing (Singh and Fleming, 2010), companies with diverse managements outperforming homogeneous ones (Dezsø and Ross, 2012; Hunt et al., 2015) and many more (Page, 2019, Chapter 5).

In the past, chess clubs used to collaborate and play each other via correspondence chess, which led to creative and impressive games. One notable mention is the "Kasparov versus the World" game (Kasparov and King, 2000), where a team of thousands played against Kasparov and decided on each move by plurality vote. The team demonstrated strong chess on which Kasparov wrote that he had "never expended as much effort on any other game in his life". In a similar vein, chess grandmasters (GMs) often prepare for important games or matches with a team, composed of strong players with diverse styles and qualities (e.g., GM Magnus Carlsen's team).

It might surprise some readers that RL can benefit from creative-problem solving mechanisms, since in principle, RL can solve any problem via trial and error. However, RL methods cannot find truly optimal policies in most problems of practical interest and hence find a particular (hopefully) near-optimal solution whose choice is determined by the nature of the agent's bounds (memory, compute, training experience). This singular sub-optimal choice can potentially generalise poorly when faced with situations it did not encounter during its training. Humans, on the other hand, seem capable of considering multiple good solutions when attempting to solve a new problem instance (Page, 2019), ruling out solutions that had worked before (Stokes, 2005), and accepting the notion of failure (Kasparov and King, 2000). This leads to a kind of creativity through diversity (of solutions) that is missing in current RL agents (see Appendix C for more details).

To test our hypothesis we designed an algorithm to train a league of high-quality, diverse AZ agents, which we call $\mathrm{AZ}_{\mathrm{db}}$. The league is represented as a single latent-conditioned architecture (Fig. 1) such that each player $i$ in the league is represented via a latent variable $l^{i}$. We encourage diversity via behavioral and response diversity techniques, which complemented each other in other domains (Liu et al., 2021). Behavioral diversity is implemented via intrinsic motivation: each player $i$ receives an intrinsic reward $r^{i}$ that motivates the agent to visit different positions from the others. Response diversity is implemented via a matchmaker that samples opponent $j$ for each player $i$.

We find that the players in the $A Z_{\mathrm{db}}$ league play chess differently: there's more variance in whether they castle long or short, develop different pawn structures, prefer different moves in common openings, and more. We collected puzzles from various sources and evaluated the performance of $\mathrm{AZ}_{\mathrm{db}}$ in these positions. We observed that different players solve different puzzles, that the $A Z_{d b}$ team can solve twice as many challenging puzzles as an individual player, and that diverse teams solve more puzzles than more homogeneous teams. We note that getting better at solving chess puzzles may not necessarily improve the overall strength of a chess program, but we believe that improving the creativity and generalization of machines to these human-made "questions" is of great importance to the AI and chess communities.

Lastly, we also see diversity bonuses in chess matchups: The best player in the $A Z_{d b}$ league is 30 ELO stronger than $A Z$ indicating that $A Z_{d b}$ benefits from diversity bonuses via its training pipeline. But even more importantly, we observe that different players in the league specialize to different openings: With sub-additive-planning $\mathrm{AZ}_{\mathrm{db}}$ is 50 ELO stronger than AZ .

## 2. Background

AZ uses a deep neural network $(p, v)=f_{\theta}(s)$ with parameters $\theta$. This neural network $f_{\theta}(s)$ takes the board position $s$ as an input and outputs a vector of move probabilities $p$ with components $p_{a}=\operatorname{Pr}(a \mid s)$ for each action $a$, and a scalar value $v$ estimating the expected outcome $z$ of the game from position $s(\mathbb{E}[z \mid s])$. AZ learns these move probabilities and value estimates entirely from self-play (playing vs. itself); these are then used to guide its search in future games. The board $s$ is represented as an image stack composed of a concatenation of planes of size $8 \times 8$, and also includes metadata about the position (e.g., history/castling rights, etc.). Further details can be found in Silver et al. (2018b, Representation section in the Appendix).

AZ uses a Monte Carlo tree search (MCTS) algorithm as described in Silver et al. (2017). Each state-action pair $(s, a)$ stores a set of statistics, $\{N(s, a), W(s, a), Q(s, a), P(s, a)\}$, where $N(s, a)$ is the visit count, $W(s, a)$ is the total action-value, $Q(s, a)$ is the mean action-value, and $P(s, a)$ is the prior probability of selecting $a$ in $s$. Each simulation begins at the root node of the search tree, $s_{0}$, and finishes when the simulation reaches a leaf node $s_{L}$ at time-step $L$. At each timestep, $t<L$, an action $a_{t}$ is selected using the PUCT algorithm (Rosin, 2011):

$$
\begin{equation*}
a_{t}=\arg \max _{a} Q\left(s_{t}, a\right)+U\left(s_{t}, a\right), \tag{1}
\end{equation*}
$$

where $U(s, a)=C(s) P(s, a) \sqrt{N(s)} /(1+N(s, a))$, where $N(s)$ is the parent visit count and $C(s)$ is the exploration rate, which grows slowly with search time, $C(s)=\log \left(\left(1+N(s)+c_{\text {base }}\right) / c_{\text {base }}\right)+c_{\text {init }}$. The leaf node $s_{L}$ is added to a queue for neural network evaluation, $(p, v)=f_{\theta}\left(s_{L}\right)$. The leaf node is expanded and each state-action pair $\left(s_{L}, a\right)$ is initialized to $\left\{N\left(s_{L}, a\right)=0, W\left(s_{L}, a\right)=0, Q\left(s_{L}, a\right)=0, P\left(s_{L}, a\right)=p_{a}\right\}$. The visit counts and values are then updated in a backward pass through each step $t \leq L, N\left(s_{t}, a_{t}\right)=$ $N\left(s_{t}, a_{t}\right)+1, Q\left(s_{t}, a_{t}\right)=W\left(s_{t}, a_{t}\right) / N\left(s_{t}, a_{t}\right)$ and

$$
\begin{equation*}
W\left(s_{t}, a_{t}\right)=W\left(s_{t}, a_{t}\right)+v . \tag{2}
\end{equation*}
$$

The search returns a vector $\pi$ representing a probability distribution over moves, $\pi_{a}=\operatorname{Pr}\left(a \mid s_{\text {root }}\right)$. Further details can be found in Silver et al. (2018b, see the pseudocode in the Appendix). Note that Eq. (2) is highlighted since the only change we make to MCTS is to the value estimate $v$. AZ is trained by RL from self-play games, starting from randomly initialized parameters $\theta$. Each game is played by running an MCTS from the current position $s_{\text {root }}=s_{t}$ at turn $t$, and then selecting a move, $a_{t} \sim \pi_{t}$, either proportionally (for exploration) or greedily (for exploitation) with respect to the visit counts at the root state. At the end of the game, the terminal position $s_{T}$ is scored according to the rules of the game to compute the game outcome $z \in\{-1,0,1\}$ (for loss, draw or win). The neural network parameters $\theta$ are adjusted by gradient descent to minimize the error between the predicted outcome $v$ and the game outcome $z$, and to maximize the similarity of policy vector $p$ to the probabilities $\pi$ :

$$
\begin{equation*}
(p, v)=f_{\theta}(s), \ell=(z-v)^{2}-\pi^{T} \log p . \tag{3}
\end{equation*}
$$

## 3. Methods

On a high level, $\mathrm{AZ}_{\mathrm{db}}$ is composed of a latent-conditioned architecture (Fig. 1), which is commonly used for modeling diverse policies, see for example, (Eysenbach et al., 2019; Gregor et al., 2017) for behavioral diversity and (Liu et al., 2022b) for response diversity. The architecture has a shared torso and three heads: policy, value, and intrinsic value. The policy and the value heads have identical architecture to the ones used by AZ and are trained in the same manner. The agent uses a single set of weights $\theta$ to represent the league by conditioning the network on a latent variable $l^{i}$ that is associated
with each player $i \in \Pi=\left\{0, \ldots, N_{\text {Players }}-1\right\}$. We represent these latent variables as one-hot vectors and concatenate them to the input as additional constant planes.

Our objective is to discover a set of Quality-Diverse (QD; Mouret and Clune, 2015; Pugh et al., 2016) policies - policies that play chess well but do so differently from each other. We use response and behavioral diversity techniques, which have been demonstrated to complement each other (Liu et al., 2021). The next section explains how we implemented behavioural diversity in $A Z_{d b}$ and how we combine the policies via sub additive planning. In Appendix B, we further provide details regarding match-making techniques for response diversity. Our results on different match makers were inconclusive and we discuss them in the Appendix for completeness.

Behavioral diversity. To optimize the diversity of the policies in $A Z_{\mathrm{db}}$ we focus on behavioural diversity. We refer to the behavior of a policy $\pi$ as the state-action occupancy measure $d_{\pi}$, which measures how often a policy visits each state-action pair when following $\pi$. We define a diversity objective Diversity $\left(d_{\pi^{1}}, \ldots, d_{\pi^{n}}\right)$ over the state occupancies of the policies in $A Z_{\mathrm{db}}$. To optimize this objective, we rely on the Reward is Enough principle (Silver et al., 2021), which states that any objective can be optimized by maximizing a local reward signal. Concretely, we rely on the intrinsic reward equation:

$$
\begin{equation*}
r_{d}(s, a)=\nabla_{d_{\pi}} f\left(d_{\pi}\right)(s, a), \tag{4}
\end{equation*}
$$

which states that one can optimise the function $f$ by locally maximizing its gradient as an intrinsic reward (Zahavy et al., 2021b). This approach allows us to use the AZ algorithm with only a few changes to maximize diversity. We will now provide more formal details.

Let $\mathbb{P}_{\pi}\left(s_{t}=\cdot\right)$ be the probability measure over states at time $t$ under policy $\pi$, then $d_{\pi}^{\text {avg }}(s, a)=$ $\lim _{T \rightarrow \infty} \frac{1}{T} \mathbb{E} \sum_{t=1}^{T} \mathbb{P}_{\pi}\left(s_{t}=s\right) \pi(s, a), d_{\pi}^{\gamma}(s, a)=(1-\gamma) \mathbb{E} \sum_{t=1}^{\infty} \gamma^{t} \mathbb{P}_{\pi}\left(s_{t}=s\right) \pi(s, a)$, for the average reward case and the discounted case respectively. It is worth noting that $d_{\pi}$ can be calculated for any stationary policy $\pi$, and that the RL problem of reward maximization can be written as finding a policy whose state occupancy has the largest inner product with the extrinsic reward $\left(r_{e}\right)$, i.e. $d_{\pi} \cdot r_{e}$, which is known as the dual formulation of RL.

We use $\phi(s, a)$ to denote the feature representation of a state-action pair, which represents the chess board after taking action $a$ from state $s$. It includes the locations of the pieces on the board as well as castling rights (see examples in Fig. 17). Note that the board representation $s$ used as input for AZ and $\mathrm{AZ}_{\mathrm{db}}$ is slightly different from $\phi$, and includes history, side to play and a 50 moves counter (see more details in the background section). We removed these features from $\phi$ because the first is redundant and the latter two occur in a predictable and relatively independent manner.

Given $\phi(s, a)$, we define $\psi=\mathbb{E}_{s, a \sim d_{\pi}}[\phi(s, a)]$ to be the expected features under the state occupancy $d_{\pi}$. With this notation, we define our objective as maximizing a non-linear quality-diversity objective over occupancies:

$$
\begin{equation*}
\max _{\Pi^{n}} \operatorname{Diversity}\left(d_{\pi^{1}}, \ldots, d_{\pi^{n}}\right)+\sum_{i} \lambda_{i} d_{\pi^{i}} \cdot r_{e}, \tag{5}
\end{equation*}
$$

where $\lambda_{i}$ is a policy-specific scalar, $r_{e}$ is the extrinsic reward vector and Diversity $\left(\Pi^{n}\right)$ is a non-linear utility function that we will soon define. To solve this problem, our agent maximizes a reward that combines the extrinsic reward $r_{e}$ (win/draw/loss) and a policy-specific diversity intrinsic reward $r_{d}^{i}$ :

$$
\begin{equation*}
r(s, a)=\left(1-\lambda_{i}\right) r_{d}^{i}(s, a)+\lambda_{i} r_{e}(s, a) . \tag{6}
\end{equation*}
$$

For simplicity, $\forall i>0$ we set $\lambda_{i}=\lambda$, but for policy $i=0$ we set $\lambda_{0}=1$ so it only maximizes extrinsic reward.

The non-linear diversity utility function is defined over the expected features $\psi$ of the policies in the set. Diverse policies, under this definition, are policies that have different piece occupancies:

$$
\begin{equation*}
\operatorname{Diversity}\left(\Pi^{n}\right)=\sum_{i=1}^{n}\left(1-\lambda_{i}\right)(\underbrace{0.5\left\|\psi^{i}-\psi^{j_{i}^{*}}\right\|_{2}^{2}-0.2\left(\left\|\psi^{i}-\psi^{j_{i}^{*}}\right\|_{2}^{5} / \ell_{0}^{3}\right)}_{\text {Repulsive }}) \text { Attractive }, \tag{7}
\end{equation*}
$$

where index $j_{i}^{*}$ refers to the player with the closest expected features to player i, i.e., $j_{i}^{*}=\arg \min _{j \neq i} \| \psi^{i}-$ $\psi^{j} \|_{2}^{2}$. The utility function, Diversity $\left(\Pi^{n}\right)$, is designed to balance the QD trade-off, i.e., to discover policies that are diverse and optimal. Simply maximizing a linear combination of a diversity objective and the extrinsic reward, often results in policies that are either optimal or diverse. Instead, Eq. (7) introduces a hyperparameter $\ell_{0}$ to control the QD trade-off. $\ell_{0}$ defines an equilibrium between two distance-dependent forces: one force that attracts the policies to behave similarly to each other and another that repulses them (Zahavy et al., 2023). According to the intrinsic reward equation (Eq. (4)), the gradient of Eq. (7) can be used as an intrinsic reward for maximising it. Differentiating it gives:

$$
\begin{equation*}
r_{d}^{i}(s, a)=\left(1-\left(\left\|\psi^{i}-\psi^{j_{i}^{*}}\right\|_{2} / \ell_{0}\right)^{3}\right) \phi(s, a) \cdot\left(\psi^{i}-\psi^{j_{i}^{*}}\right) . \tag{8}
\end{equation*}
$$

As we can see, once a set of policies satisfies a diversity degree of $\left\|\psi^{i}-\psi^{j_{i}^{*}}\right\|_{2}=\ell_{0}$, the intrinsic reward is zero, which allows the policies to focus on maximizing the extrinsic reward.

To maximize this reward, we learn an intrinsic value function $v_{d}$ (in addition to the policy and value functions) by first computing an intrinsic value target $z_{d}\left(s_{t}\right)$ and then adding a loss $\left(z_{d}-v_{d}\right)^{2}$ to Eq. (3). To compute the target we only take into account diversity rewards for the player that is currently playing. This is implemented by zeroing out the reward in all of the opponent transitions and using an even number of TD steps $N_{\text {TD }}$ when computing the intrinsic value target $z_{d}\left(s_{t}\right)=\sum_{i}^{N_{\mathrm{TD}} / 2} r_{d}\left(s_{t+2 i}\right)+v_{d}\left(s_{t+N_{\mathrm{TD}}}\right)$ (as black and white alternate moves in chess).

Similarly, during MCTS, the value estimate $v$ in Eq. (2) is modified in two ways. Firstly, each value estimate is replaced by a combined value estimate: $v=\lambda^{i} v^{i}+\left(1-\lambda^{i}\right) v_{d}^{i}$. Secondly, in each MCTS simulation, we accumulate all the intrinsic rewards from the root to the leaf and add them to $v$. We also zero out the intrinsic reward in states that correspond to the turn of the other player as we did for learning. Furthermore, during MCTS the same latent (associated with the player in the root) is used throughout the entire search, i.e., the planning agent searches against itself. This latent conditions the value, prior and intrinsic value as well as the intrinsic reward. Therefore, the planning player does not have access to privileged information about the opponent.

Sub-additive planning. To choose a player from its team to solve a chess puzzle, $\mathrm{AZ}_{\mathrm{db}}$ produces $N_{\text {Players }}$ moves, one for each player. The first method, which we call max-over-latents, is an oracle that selects the player who has successfully solved the puzzle. If at least one player has solved the puzzle, the score is one. Teams that propose diverse and creative ideas that are also useful have high max-over-latents scores.

The max-over-latents method is not always feasible, because we don't always know the solution and therefore cannot select the player who solved it. In these cases, we require a method that chooses a player without seeing the solution. We limit our discussion to sub-additive planning methods that involve two steps. (i) a planning step, in which each player $i \in \Pi=\left\{0, \cdots, N_{\text {Players }}-1\right\}$ performs MCTS and returns the following search-statistics:

$$
\eta^{\text {Players }}=\left\{N^{i}(s, a), Q^{i}(s, a), U^{i}(s, a)\right\}_{i=0}^{N_{\text {Players }}-1},
$$

where $N$ stands for visitation counts, $Q$ for value estimates, and $U$ for exploration terms (see the background section for more details). (ii) a selection step, in which a player is chosen based on the
search statistics $\eta^{\text {Players }}$. In other words, sub-additive planning uses a heuristic to decide which player has the best chances to solve the puzzle, similar to how humans use heuristics as a way of reducing the complexity of decision making Gigerenzer (1991). These two steps can be written together as:

$$
\left.i \text {, } \text { score }_{i} \leftarrow \text { sub-additive-fn( } \eta^{\text {Players }}\right),
$$

where sub-additive-fn outputs a player's index $i$ and its score in a puzzle $\operatorname{score}_{i}$. Let $V^{j}(s)=$ $\max _{a} Q^{j}(s, a)$, the player's selection is based on one of the following rules:

$$
\begin{align*}
& \text { (Visit) }: i \leftarrow \underset{j}{\arg \max } \max _{a} N^{j}(s, a) . \\
& \text { (Value) }: i \leftarrow \underset{j}{\arg \max _{j} V^{j}(s) .} \\
& \text { (LCB) }: i \leftarrow \underset{j}{\arg \max } \max _{a} Q^{j}(s, a)-U^{j}(s, a) . \\
& \left(\text { Gap) }: i \leftarrow \underset{j \in\left\{j: V^{j}(s) \geq V^{j}(s)-\operatorname{Gap}(s)\right\}}{\arg \min } V^{j}(s) .\right. \tag{9}
\end{align*}
$$

These equations correspond (top to bottom) for selecting a player using visit counts, values, and Lower-Confidence-Bound (LCB) values (Tirinzoni et al., 2023). The LCB is obtained by switching the sign of the exploration term in the PUCT action-selection formula in Eq. (1). The Gap method defines a set of candidate policies - all the policies whose value is within a $\operatorname{Gap}(s)$ from the optimal value and selects the policy with the lowest value in this set. The gap is usually a small number, so in most cases, this action selection is effectively the same as the Value. We set $\operatorname{Gap}(s)$ to be $\max _{a, j} U^{j}(s, a)$ in puzzles, and 2 /seeds in chess matchups (more details in the experiments). Selecting the arg min over the candidates can be viewed as a technique to reduce over estimation (Van Hasselt et al., 2016).

Note that the cumulative sum of solutions in the team (max-over-latents) always upper bounds the performance of any sub-additive planning method (it also explains why these methods are called sub-additive). In addition to that, a good sub-additive method should perform better than the best player in the team. In the case of $A Z_{d b}$ this is usually player 0 , which is trained without intrinsic reward ( $\lambda^{0}=1$ ). For these reasons, we will always compare sub-additive planning with max-over-latents and the performance of player 0 . Lastly, we note that in addition to the three sub-additive planning methods in Eq. (9), we tried other approaches such as selecting players based on their raw value estimates, on their entropy of the prior policy etc. The performance of these methods was lower than that of player 0 .

## 4. Experiments

Setup. We trained AZ and $\mathrm{AZ}_{\mathrm{db}}$ while keeping almost all the hyperparameters identical to those used in (Silver et al., 2018b). We now explain which hyperparameters were changed in each of our training configurations. Firstly, AZ's state representation includes history states, which are not available in puzzles (which typically only have a position to solve and not the preceding states). To address this, we trained AZ with history dropout, which randomly removes history states with a probability of 0.2 .

The full configuration trains a league of 10 players. It uses a batch size of 4096 during training and is trained for 1.6 M training steps. The agent is trained with a distributed actor-learner setup. It plays a number of asynchronous self-play games and these games are stored in a replay buffer, along with the policy and raw value targets for each state transition from the game. These targets are used to train their respective estimates. In this configuration, the agent only stores $10 \%$ of state transitions from those games (randomly chosen) in the replay buffer and discards the rest. The replay buffer
can store at most 1 M positions. At each training step, the agent samples a batch of 4096 samples to make one training update. $\mathrm{AZ}_{\mathrm{db}}$ uses PSRO-NASH matchmaking algorithm for response diversity and diversity rewards as described in the methods section. More details can be found in the Appendix.

The fast configuration is identical to the full configuration, except for the following three changes: the league is of size 5 , the batch size during training is reduced to 1024 and all positions generated from self-play games are stored in the replay buffer, i.e., no positions are discarded. This configuration allows an experiment with $\mathrm{AZ}_{\mathrm{db}}$ to complete in less than a day compared to a week with the full configuration, but has significantly weaker performance in both puzzles and matches. This configuration allows us to conduct a number of careful ablations on $\mathrm{AZ}_{\mathrm{db}}$. This configuration uses 1 million MCTS simulations in each position, unless otherwise specified.

To provide a proper AZ baseline, we retrained AZ using these configurations and provide its results when relevant. Concretely, AZ and $\mathrm{AZ}_{\mathrm{db}}$ in this paper play the same number of games and learn with the same algorithm. For $\mathrm{AZ}_{\mathrm{db}}$, those games are divided uniformly between the players. The winrate of AZ against reference players in this paper is the same as in (Silver et al., 2018b). We use the PSRO matchmaker throughout all of our experiments. In Appendix B we present a detailed study comparing the different matchmakers. However, we could not identify a single matchmaker that outperformed the other matchmakers across the puzzle data sets, and the decision to use PSRO is arbitrary. One potential explanation for this is that chess is a transitive game, and therefore, does not require clever matchmaking techniques. Our experiments are designed to answer the following questions:

1. Do $\mathrm{AZ}_{\mathrm{db}}$ 's policies play chess differently from each other?
2. What makes puzzles hard for $A Z$ and why?
3. Do diversity bonuses emerge in $\mathrm{AZ}_{\mathrm{db}}$ when solving puzzles and playing chess?

Do $A Z_{d b}$ policies play different chess? To answer this question, we examined the piece occupancies of the different $\mathrm{AZ}_{\mathrm{db}}$ policies and assessed their opening diversity. Recall that the expected feature vectors $\psi=\mathbb{E}_{s \sim d_{\pi}}[\phi(s)]$ represent the features that a policy $\pi$ observes on average when playing chess. The features $\phi$ represent the chess board and also include castling rights. Our diversity objective is designed to discover policies with different associated vectors $\psi$ (Eq. (8)). Therefore, we now inspect these vectors to gain insights on the behavior of $\mathrm{AZ}_{\mathrm{db}}$ 's policies.

In Fig. 2 we present standard deviation (across players) of vectors $\psi$. We also present the raw vectors for all the players and a mean subtracted visualization in the Appendix (Fig. 17 \& Fig. 18).


Figure 2 | Left: Standard deviation across players of the piece occupancies of $\mathrm{AZ}_{\mathrm{db}}$. Black rectangles highlight the starting position of each piece. Right: average Castling Rights of different players. x -axis corresponds to castling to the Queen (O-O-O) or King (O-O) side as White (W) and Black (B), y-axis corresponds to players. Color units (in the color bars) correspond to occupancy in $\%$ multiplied by the average number of moves in a game (65). For orientation, the chess coordinate system is displayed on the left top.

Figures show notable differences in the behavior of the players. Firstly we can see high variability in castling rights on Fig. 2, right. Players $2 \& 4$ have lower occupancy for castling, which means that they either castle earlier or move the king or rook so they lose their castling rights earlier in the game. Inspecting Fig. 18 in Appendix we can indeed see that when player 2 plays as white, its king occupies $g 1$ for more moves (the square where it gets to after castling kingside). Player 3 on the other hand, castles later, and occasionally castles queenside. In Fig. 18 we see that it spends more time on $e 1$.

Inspecting the pawn structure in Fig. 17, we can see that most players push the $e$ and $d$ pawns to take control over the center. Unlike the other players, player 5 favours the Fianchetto and pushes the $g$ pawn ( $g 2-g 3$ ) to get its kingside bishop to $g 2$ (Fig. 17). We can also see most players push the $a$ and $h$ pawns more than the $b, f, g$ pawns and that the $c$-pawn is pushed fairly frequently too (the $c 2$ square is often lighter than other squares).

There is also variability across players in the average time that each piece gets to stay on the board (see the black numbers above each sub-figure in Fig. 17). For example, the white queen stays on the board $48 \%$ of the game with player 0 as white and $52 \%$ with player 4 as black. The rook is the piece that survives the most, $62 \%$ with player 3 but only $60 \%$ with other players. We can also see that rooks tend to stay on the first rank and the second most common rank for them is the 7th (with lower occupancy). One exception is player 2 that has a rook at the 3rd rank.

To study the opening diversity of $A Z_{\mathrm{db}}$ we performed two analyses. Firstly, we study the diversity in 8 popular chess opening positions in Fig. 3. Inspecting the results, we can see that $\mathrm{AZ}_{\mathrm{db}}$ 's players play different moves. All of these moves are played by chess GMs at the highest levels, although some of them are considered niche (eg. 6. Bd3 in the Najdorf, 4. c3 in the Caro-Kann advanced variation). We report the percentage in which each move was played by GMs (black numbers) as well as their relative win rate (blue numbers).


Figure $3 \mid$ Opening diversity with $\mathrm{AZ}_{\mathrm{db}}$. We selected 8 popular openings where humans tend to play different moves and present with green arrows the moves chosen by $\mathrm{AZ}_{\mathrm{db}}$ policies with LCB action selection and 100 k simulations. For each move, we present in black numbers (top) the $\%$ in which this move was played by chess GMs (taken from the Lichess Masters database), and in blue numbers (below them) the relative win percentage ( $\%$ wins - $\%$ losses).

For a quantitative evaluation, we measured the number of different moves played by $\mathrm{AZ}_{\mathrm{db}}$ 's policies in 3233 openings from the Encyclopaedia of Chess Openings using lichess-org chess-openings (we excluded irregular openings ( A 00 )). $\mathrm{AZ} \mathrm{Z}_{\mathrm{db}}$ discovered $1.26 \pm 0.01,2.45 \pm 0.02$, and $1.65 \pm 0.01$ moves on average in each position, for $1,400,100 k$ simulations respectively. Note that $\mathrm{AZ}_{\mathrm{db}}$ discovered the most opening moves when it used 400 simulations, which is the number of simulations it used for training. We further discuss this finding at the end of this section.

Why are puzzles hard for AZ? In the previous section, we observed that the players in the $\mathrm{AZ}_{\mathrm{db}}$ league play chess differently from each other. We would like to evaluate these players on challenging puzzles and examine if diversity bonuses emerge. But before we do so, we examine why chess puzzles make a challenge for computer chess agents like AZ.

For this goal, we have collected two data sets of challenging puzzles that can trick modern chess engines. The Challenge set includes 15 multi-step puzzles that are challenging to modern chess engines, and the Penrose set includes 53 challenging puzzles including fortresses and Penrose positions to measure the value accuracy of AZ. More details about these data sets can be found in the Appendix.

In the first row of the top panel in Table 1 we can see the solve rate of AZ with $1 M$ MCTS simulations in these data sets; it only solved $11.76 \%$ of the Challenge set and $3.64 \%$ of the Penrose set. Although AZ is a very strong chess player, these puzzles confuse it. We now attempt to understand what makes these puzzles difficult for AZ through a few experiments and visualizations. Note that for all the experiments in this section, we used the fast configuration of AZ (see setup at the beginning of this section).

Our first hypothesis is that these puzzle sets present a hard generalization challenge for AZ, highlighting its weaknesses and blind spots. To verify this prediction, we allow AZ to begin self-play games from puzzle positions. It is important to note that the solution is not provided to AZ; only the starting position of the puzzle. By presenting the position to AZ, it can learn to solve the puzzle by trial and error and potentially improve at doing so via its RL pipeline. In the second row of the top panel in Table 1 we can see the solve rate of AZ when it begins self-play games from the puzzle positions. We can see that it solved most of the Penrose set and significantly improved its performance on the Challenge set (from 11.76\% to 76.47\%).

We further explore if this generalization challenge is in distribution generalization or OOD generalization in the middle panel of Table 1. For in distribution generalization, we randomly

|  | Challenge Set | Penrose Set |
| :--- | :--- | :--- |
| (1) AZ | $11.76 \%$ | $3.64 \%$ |
| (2) Self-play from puzzles | $76.47 \%$ | $96.23 \%$ |
| (3) In distribution | - | $88.24 \%$ |
| (4) Out of distribution | - | $11.76 \%$ |
| (5) + intermediate positions | $88.23 \%$ | $96.23 \%$ |
| (6) + exploration | $94.11 \%$ | $96.23 \%$ |
| (7) + half-move clock | $94.11 \%$ | $100 \%$ |

Table 1 | Self-play from puzzle positions. From top to bottom. (1) AZ. (2) AZ with self-play from puzzle positions. (3) Randomly splitting the Penrose set to train and test sets. (4) Training on the first Penrose position \& testing on the second (OOD). (5-7) AZ with self-play from puzzle positions and additional exploration techniques.
split the Penrose set to train and test sets. We allow AZ to begin self-play from the train set and evaluate its performance on the test set. In the OOD case, we split the Penrose set between variations of the two Penrose positions and evaluate on one of them (details in Appendix). We can see that AZ generalizes pretty well in distribution while it struggles to generalize to OOD positions.

However, it remains unclear what prevents AZ from reaching $100 \%$ solve rate when it begins self-play games from these puzzle positions. Recall that many of these puzzles involve a long sequence of actions and an incorrect action at any point results in the agent failing to solve the puzzle. Thus, we hypothesize that these positions also present an exploration challenge to AZ. To verify this second hypothesis, we performed three more experiments which we present in the lower panel of Table 1. We only briefly explain them here and refer the reader to Appendix C. 3 for more details. (1) we extended the puzzle positions from the Challenge set to also include intermediate positions ( $76.47 \% \rightarrow 88.23 \%$ on the Challenge set), (2) we change AZ's action selection mechanism to sample actions from a softmax distribution over the MCTS visits ( $88.23 \% \rightarrow 94.11 \%$ ) and (3) we manually augmented the half-move counter ( $100 \%$ in the Penrose set). Each one of these changes have improved AZ's performance on the challenging puzzles until it finally solve all but one of them.

We note that these puzzles were collected and composed by chess players deliberately to trick computers and it's not likely that AZ had seen such positions when it learned to play chess by playing against itself. Our findings in this section suggest that the challenges for AZ are OOD generalization and exploration. In the next section we will inspect if different players in the $A Z_{d b}$ league generalize differently and solve more puzzles as a result. However, we would like to emphasize that there is no fundamental or incomputable problem to solve these puzzle positions. The challenges are OOD generalization and exploration which are well known challenges in AI.

AZ's understanding of puzzles. In Fig. 4 and Fig. 19 in the Appendix, we visualize AZ's policy $p(s)$, raw value $v(s)$, and MCTS value estimates $Q(s, a)$ for four puzzle positions. We compare the estimates of AZ with the fast configuration with the variation of AZ that begins self-play games from the puzzle positions. Fig. 4 shows two Penrose positions from the Penrose set and Fig. 19 in the Appendix shows two steps from a puzzle from the Challenge set (recall that these are multi-step puzzles and to get a score of one the agent has to find the correct solution in all the steps). The right column in these figures shows three bar plots: the prior policy's probability $p$ of legal actions from the given position (top), the raw values $v$ (center), and the MCTS values $Q$ (bottom). We use blue arrows and blue x-ticks to indicate correct actions, and red for incorrect ones.

Inspecting the first row in Fig. 4, we see one of the Penrose positions. It is white's turn to play, and there are only two legal actions available ( Kb 2 and Kb 1 ). We can see that the prior is roughly uniform across the legal actions, which is fine since both of them are correct. However, when we inspect the raw values (shown in black bars) we see that AZ estimates the white player to win when it plays either of these two actions. After MCTS, the value estimate reduces and predicts a draw, which is the correct evaluation. The self-play from puzzles agent (blue) accurately predicts the position to be a draw in both raw and MCTS values indicating better understanding.

The second puzzle in Fig. 4 is the original Penrose position (white's turn to play). The solution to this puzzle is to move the white king to any of its neighboring white squares (blue color) so that it can eventually draw the game. Any other move leads to a losing position (red color). Inspecting the figure, we see similar findings to the previous puzzle: AZ is confused regarding the correct move to play. The prior puts an equal probability on any of the legal actions (c.f. prior barplot), raw value predicts a win (c.f. raw value barplot), and MCTS value predicts a loss (c.f. MCTS value barplot). The self-play from puzzles agent, on the other hand, have accurate raw and MCTS values for this position (a draw for the correct actions and a loss for the incorrect actions), demonstrating understanding.


Figure 4 | Left: Two Penrose puzzle positions from the Penrose set. Right: Visualizations of prior probability from a subset of legal actions, and its corresponding raw value and MCTS value estimates for $A Z$ and $A Z$ trained on puzzle sets. Correct and Incorrect moves are colored in Blue and Red respectively.

To summarize, in Fig. 4 (and Fig. 19 in the Appendix), we see that AZ fails to understand positions from the Penrose and the Challenge sets when trained with the fast configuration. AZ's ability to understand difficult chess positions (in terms of prior, raw value, and MCTS value) improves when it is allowed to train from those puzzle positions, which also translates to better performance on those puzzle sets.

Diversity bonuses in $A Z_{d b}$. In the previous sections we have seen that $A Z_{d b}$ trains a league of strong chess players that play chess differently. We have also seen that chess puzzles are a challenging problem for strong chess agents like AZ. In this section we examine if diversity bonuses emerge in $A Z_{d b}$ when solving chess puzzles. We then let $A Z_{d b}$ to play chess games against $A Z$ from different opening positions and see if diversity bonuses emerge there and conclude with ablative analysis on diversity bonuses. From this point on, the puzzle sets are not available to any of the agents and they are not allowed to start self-play games from them.

Diversity bonuses in solving puzzles. In this section we compare the performance of $A Z$ and $A Z_{d b}$ on four data sets. These include the Challenge and Penrose sets from before, and two larger scale data sets. The Strategic test suite (STS) composed of 1000 multiple choice puzzles and the Lichess data set, composed of 500 multi-step puzzles from lichess.org. More details about the data sets can be found in the Appendix.

We would like to see if diversity bonuses emerge in the upper limit of AZ's computational rationality. Therefore, in this section we use the full configuration of $A Z_{d b}$ and allow it to search for $100 M$ simulations per position - the largest search budget we could afford without running out of memory due to the size of the search tree. We also use the LCB action selection rule unless mentioned otherwise.

Inspecting Fig. 5, we can see $\mathrm{AZ}_{\mathrm{db}}$ 's player 0 performs roughly as well as AZ on most of the data


Figure 5 | Puzzle solve rates.
sets. More importantly, we can observe strong diversity bonuses on each one of the data sets: $\mathrm{AZ}_{\mathrm{db}}$ manages to solve many more puzzles as a team via sub-additive planning and max-over-latents. In particular, it solves more than twice more puzzles from Challenge set. In Penrose set, it solves the two notoriously hard Penrose positions and more generally, $56.6 \%$ of the puzzles. In Lichess and STS we observe that max-over-latents solves $3 \%$ more puzzles than player 0 , and that sub-additive planning is $0.5 \%$ better. Note that these data sets are relatively easier (taken from human games), and $A Z_{d b}$ is already solving them at high percentage, thus the relative gains are actually quite significant.

Diversity bonuses in chess matchups. In this section, we assess the impact of diversity bonuses on the performance of $A Z_{\mathrm{db}}$ in chess matches. We matched each player in the $A Z_{\mathrm{db}}$ league against $A Z$ and let them play chess from 74 opening positions. For each opening, AZ played one game as black and one as white. The opening positions were carefully chosen by GM Matthew Sadler to favor one player by giving them a strong opening advantage (up to 1500 centipawns). This was done in order to produce more decisive matches between agents, with one player winning rather than the match ending in a draw. The games were played in a bullet time control, where each agent used 400 MCTS simulations to select a move in a match. This roughly translates to 100 milliseconds of thinking time per move. Recall that the same amount of MCTS simulations were used in training $A Z_{\mathrm{db}}$.

Table 2 | Summary of chess matchups between $A Z_{d b}$ and $A Z$. The standard error, in winrate, is 0.34 (for each Player) up to quantization error of 0.01 .

|  | Player 0 | Sub-additive planning | Max-over-latents |
| :--- | :--- | :--- | :--- |
| Winrate | 54.25 | 57.18 | 58.6 |
| Elo | 29.6 | 50.3 | 60.3 |

Table 2 presents a summary of the games in terms of overall win rate and relative Elo score for player 0, Max-over-latents \& Sub-additive planning. Fig. 21 in the Appendix additionally presents the number of wins, draws and losses (as black and as white) for all the players. These statistics are obtained by averaging the results from each position over 500 random seeds. The win rate and relative Elo improvements show that most of the players in the $A Z_{\mathrm{db}}$ league are stronger than AZ .


Figure 6 | Results from a subset of chess openings between $\mathrm{AZ}_{\mathrm{db}}$ and AZ (scores averaged from 500 random seeds) where $\mathrm{AZ}_{\mathrm{db}}$ played as White and AZ as Black. Results from all openings are presented in the Appendix.

This is likely due to implicit diversity bonuses, such as seeing more diverse data during training and playing against each other. In particular, player 0, the strongest player, achieves a win rate of 54.25\% and a relative Elo of 29.6 compared to AZ . It makes sense that player 0 is the strongest in the league, as it is a "special player" that is trained without the diversity intrinsic reward.

We can also see that the max-over-latents method performs better than player 0. But unfortunately, max-over-latents is not practical for selecting a player to play in an opening position, since we do not know the outcome of the game in the opening (when we select the player to play). On the other hand, sub-additive planning is practical, and we now discuss how we implemented it. For each opening and seed, we calculated the average score of each player across all other seeds (leaving the current seed out) and selected the player with the highest score. We then reported the score of this player against the current hold-out seed (more details in the Appendix). Table 2 shows the results for the Gap sub-additive planning method (Eq. (9)), where the gap is defined to be $2 / 500$. This value assures that the candidates are all the policies that can become optimal if we add one more game in which they win and the optimal policy loses. As we can see, this improves $\mathrm{AZ}_{\mathrm{db}}$ 's win rate to $57.18 \%$, which translates to a 50.3 ELO improvement over AZ. The results for the other sub-additive rules were 40 for the value and visit counts, and 41 for the LCB, i.e., they all improve by around 10 Elo over player 0 , but the gap method was better than all of them.

In Fig. 6 we further inspect these results. We report the average score (a win is scored as 1, draw is 0 and loss is -1 ) of the players in $\mathrm{AZ}_{\mathrm{db}}$ when playing as white in a subset of openings. The results on all the opening positions can be found in the Appendix (Fig. 22). We can see that the performance of the players in $\mathrm{AZ}_{\mathrm{db}}$ vary across openings. In French Winawer C16, all the players perform roughly the same. However, in other openings, there are specific players that perform significantly better than others. For example, player 0 is strong in Benoni Wall A56, but is weak in comparison to the other players in Blumenfeld E10. While player 0 is the overall best player, they are not the best player in any specific opening. They are also not the best player when playing as white or black. Table 3 in the Appendix shows the average win rate of each player when playing as white and black. Player 0 won $68.27 \%$ as white and $40.21 \%$ as black. However, Player 2 had the highest win rate as white ( $69.86 \%$ ), and player 9 as black ( $40.38 \%$ ). These results suggest that different players specialize in different openings and that sub-additive planning can be used to select the better player in each opening. Further, Fig. 20 in the Appendix shows how sub-additive planning performs as a function of the number of seeds.


Figure 7 | Scaling laws with $\mathrm{AZ}_{\mathrm{db}}$. Top: Max over trials, Bottom: Sub-additive planning. Left to right: (1) Solve rate in $\%$ on Lichess puzzles with a different number of simulations and latents. (2) Relative gains in \% from increasing the number of latents for each simulation budget. (3) scaling with the number of latents for different simulation budgets. (4) Relative gains with a different number of trials - latent in solid lines, seeds in dashed lines - at different simulation budgets.

Analysis of diversity bonuses in $\mathrm{AZ}_{\mathrm{db}}$. In the puzzle evaluation section, we observed that diversity bonuses emerge at the computational boundaries of $\mathrm{AZ}_{\mathrm{db}}$. In this section, we analyse what components of $\mathrm{AZ}_{\mathrm{db}}$ are the most important for diversity bonuses and if diversity bonuses emerge at other compute budgets. We focus our evaluation on the Lichess data set and use the fast configuration for that. In Fig. 7 we study how $\mathrm{AZ}_{\mathrm{db}}$ scales with different simulation budgets and team sizes. The top figure presents results for max-over-latents and the bottom figure shows results for sub-additive planning based on LCB (Eq. (9)). Most importantly, we observe diversity bonuses for all compute budgets and team sizes. In the leftmost table, we present the absolute solve rate in $\%$. We can see that $A Z_{d b}$ 's performance improves monotonically with the number of simulations and the number of trials, implying that larger teams solve more puzzles together. We can also see that on the third sub-figure, which presents the same data in a different manner. For each column in the first table (simulation budget) we draw a line that presents the solve rate in $\%$ as a function of the number of trials ( x -axis). We can see that the diversity bonuses keep increasing as we increase the number of trials for each simulation budget.

The second table from the right shows the relative gains computed in $\%^{1}$ of $A Z_{d b}$ from having more players in the team. Interestingly, the highest relative gains are achieved when the number of simulations is $5^{4}=625$, which is the simulation budget that is closest to the one we use in training (see the discussion section). On the rightmost sub-figure, we compare a diverse team of agents with a more homogeneous team. For the diverse team, we use different latents as before (solid lines) and for the homogeneous group, we use the best latent in the group (latent 0 ) and allow it different trials of search (with different seeds, in dashed lines). We can see that across different group sizes, simulation budgets, and for both max-over-latents and sub-additive planning, a diverse team outperforms the homogeneous one.

We further study diversity bonuses in a few variations of $\mathrm{AZ}_{\mathrm{db}}$ and compare different sub-additive planning methods (counts, value, and LCB) in Eq. (9). We also compare $A Z_{d b}$ with a variation that only uses the extrinsic reward and extrinsic value function at test time (dashed lines). Inspecting Fig. 8, we can see that using the intrinsic reward and value function (solid lines) receives higher diversity bonuses across different action selection rules and simulation budgets. We also see higher

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Figure $8 \mid$ An ablation of action selection rules (color) and search type (solid/dashed) with max-overlatents (top) and sub-additve planning (bottom). Sub figures correspond to the number of trials.
diversity bonuses when selecting actions based on value and LCB rather than counts.
Discussion. $\mathrm{AZ}_{\mathrm{db}}$ benefited from diversity bonuses regardless of the amount of simulations it was given. However, it gained the most from diversity in solving puzzles when it was given 625 simulations (see Fig. 7), and it discovered the most unique openings when it was given 400 simulations. One possible explanation for these findings is the spinning top hypothesis (Czarnecki et al., 2020), which states that the largest diversity of a population of players is observed at a medium level of play, and at the low and high levels of play there is less room for diversity. Indeed, Sanjaya et al. (Sanjaya et al., 2022) observed that in chess, human play exhibits the most diversity in the medium levels of play ( 1600 ELO) compared to the higher and lower levels. A different possible explanation is that $\mathrm{AZ}_{\mathrm{db}}$ 's diversity overfits to the number of simulations it uses for training (400), in the sense that it achieves higher diversity bonuses when it uses the same number of simulations it used for training compared to other simulation budgets. Note that $A Z$ 's and $A Z_{d b}$ 's performance improves monotonically with the number of simulations and we do not suggest that the performance overfits to the number of simulations, only that the diversity does. To better understand this explanation, recall that the expected features $\psi$ in our diversity objective are estimated from the average games played by $\mathrm{AZ}_{\mathrm{db}}$, and since these games are played with 400 simulations, it is possible that the diversity objective itself overfits to the behavior of $\mathrm{AZ}_{\mathrm{db}}$ 's policies with 400 simulations.

## 5. Related work

Chess has been a long-standing subject of AI research, and is often called the "Drosophila of AI" (Kasparov, 2018). The first chess program was written by Alan Turing on slips of paper, before the invention of the computer. Achieving human-level performance in chess was known as the "chess Turing test", and computer scientists made significant progress towards this goal until Deep Blue finally beat the world chess champion in 1996. In his book "Deep Thinking" (Kasparov, 2017) Kasparov tells his side of the story of his loss to Deep Blue. He describes the experience of strategizing
against an opponent that is tireless and never makes mistakes, and the mistakes he made that led to his defeat. While some have expressed concerns that chess will become less popular as machines become stronger than humans, chess is now more popular than ever due to an increase in online play during the COVID-19 pandemic, and the success of the Netflix series "The Queen's Gambit" and streamers in bringing attention to the sport (WUFT).

In 2018, AZ made a significant impact on the world of chess by learning to play chess on its own, without any human knowledge. The games between AZ and SF drew a lot of attention from the chess community, on which Kasparov wrote that "Deep blue was the end, AlphaZero is a beginning". In fact, almost all modern chess engines today have followed AZ's lead and use a neural network score function instead of a human-designed one. Professional chess players also changed their playing style after the AZ vs SF games were introduced (González-Díaz and Palacios-Huerta, 2022), prototyped new variants of chess using AZ (Tomašev et al., 2020), and investigated when and where human chess concepts are represented in AZ (McGrath et al., 2022).

Despite the strength of chess engines, it is uncertain whether we are near optimal play, as evidenced by the results of computer chess competitions like the TCEC, where the strength of the top engines continue to increase with each season. Another piece of evidence is that modern chess engines tend to make blunders when constrained to use a limited amount of search. A famous example is the winning move in game eight of the Classical World Chess Championship 2004 between Peter Leko and Vladimir Kramnik (chessbase, Agadmator's Chess Channel): "Grand Master (GM) Vladimir Kramnik relied a bit too much on the engine in his Marshall Gambit preparation. The engine initially told Kramnik he was winning, but Leko let his engine calculate more deeply and realized that his mating attack would triumph over Kramnik's passed pawn" (Copeland, 2021a). While this example is from 2004 and nowadays chess engines can easily solve it, we can find similar cases on "chess twitter" on a regular basis. For example, GM Anish Giri explains that for similar reasons "top players use cloud engines and not the free stuff available online" (Twitter).

In order to beat superhuman computers, chess players developed anti-computer tactics, that exploit blind spots in how computers reason about chess. Chess players have been using these tactics against chess programs in their early days, but successful examples became fewer as machines became better. One notable exception is the achievements of GM Hikaru Nakamura against modern chess engines. In 2008, Nakamura played against the top engine at the time, Rybka, and managed to close the position, offer sacrifices, and convince the engine to overpress and eventually lose (Copeland, 2021b); more recently Nakamura used similar tactics against Mittens and secured a draw. Another example of the limitations of computer chess programs is that they cannot solve certain positions (Copeland, 2021a; Doggers, 2017; Penrose, 2020). To address this, scientists have developed puzzle-specific chess programs like Crystal and worked on specific methods for specific positions like fortresses (Guid and Bratko, 2012).

In this work, we investigated whether creative problem-solving mechanisms identified in humans can make machines more creative and help them solve such positions. This was inspired by Kasparov's statement that "creativity has a human quality: it accepts the notion of failure" (Kasparov, 2017). We focused on diverse policy discovery, since diverse teams are known to be more creative and robust to failures.

Although diverse policy discovery has not been extensively studied in chess, there are some related mentions. For example, chess engine designers make different choices that can lead to different playing styles. Lc0 and AZ use MCTS, while SF uses alpha-beta pruning. Even the rules of chess have some references to diversity, such as the tension between the bishop and the knight (Shead, 2020). Chess opening theory is also diverse, as many opening positions have multiple possible variations. As an example, different AZ seeds prefer different moves in the Ruy Lopez opening (McGrath et al.,
2022). GM Magnus Carlsen has also commented on the importance of finding ideas that are missed by other players in the Lex Fridman Podcast: "Now it's all about finding ideas that are missed by agents, either that they are missed entirely or missed at low depth. These are used for surprising your opponent with lines in which you have more knowledge".

In AI, the concept of diversity dates back to Turing's cultural search in "Intelligent Machinery" (Turing, 1948): "it is necessary for a man to be immersed in an environment of other men, whose techniques he absorbs, ..., he may then perhaps do little search on his own to make new discoveries which are passed to other men". Turing listed cultural search as one of three types of search in which machines can potentially learn. Since then, diversity had been studied in different sub topics. The Quality-Diversity web page provides an excellent overview of the work done in the evolutionary learning community (Cully and Demiris, 2017; Mouret and Clune, 2015; Pugh et al., 2016). In RL, research had been conducted on intrinsic rewards for diversity (Eysenbach et al., 2019; Gregor et al., 2017), on repulsive and attractive forces (Flet-Berliac et al., 2021; Liu et al., 2017; Vassiliades et al., 2017; Zahavy et al., 2023), and on learning a behavior that maximizes a general utility function (Geist et al., 2022; Hazan et al., 2019; Zahavy et al., 2021b; Zhang et al., 2020). There had also been a significant amount of study on diversity in the multi-agent community (Balduzzi et al., 2019; Czarnecki et al., 2020; Liu et al., 2022b; Perez-Nieves et al., 2021; Vinyals et al., 2019). We refer the reader to the Appendix for further discussion about these works.

Lastly, sub-additive planning had been investigated in AI as well as in other fields. In psychology, heuristics is the process by which humans use mental short cuts to arrive at decisions. Heuristics are simple strategies that humans, animals, organizations, and even machines use to quickly form judgments, make decisions, and find solutions to complex problems. Heuristics are also considered to be an evidence for bounded rationality in human decision making. In RL, a commonly used heuristic is General Policy Improvement (GPI; Barreto et al., 2017b), which is similar to sub-additive planning based on value. However, in special situations GPI is sub optimal, and can be improved (Zahavy et al., 2020b). Similarly, our results suggest that the LCB and Gap methods performed better than value.

## 6. Summary

This paper investigated whether AI can benefit from diversity bonuses, inspired by how teams of diverse thinkers outperform homogenous teams in challenging tasks. We tested this hypothesis in the game of chess, the "drosophila of AI", which poses computational challenges for AI systems due to the large number of possibilities that have to be calculated. We proposed $A Z_{\mathrm{db}}$, a league of AlphaZero (AZ) agents that are modeled via a latent-conditioned architecture, and trained its players to play chess differently via behavioral diversity techniques and observed that they choose different pawn structures, castle at different times, and prefer different moves in the opening. In a chess tournament against $A Z$, we observed that different players in $A Z_{d b}$ specialize in different openings, and, that selecting a player from $\mathrm{AZ}_{\mathrm{db}}$ via sub-additive planning leads to an improvement in Elo points.

We also found that diversity bonuses are present in solving puzzles regardless of the computational budget. In particular, they persisted even when the computational budget of a single search player was pushed to its upper computational rationality limit of 100 M simulations (using more simulations resulted in out-of-memory problems). In this setting, we observed that $\mathrm{AZ}_{\mathrm{db}}$ achieved twice the solve rate of $A Z$ on the hardest of our data sets (the Challenge set), suggesting that diversity bonuses emerge even in this limit. We note that physical limitations bound humans, and some hardware constraints bound most AI agents. While it should be possible to improve these memory constraints, there should always be some limit on which we can achieve with existing hardware, setting a different bounded rationality limit (Lewis et al., 2014; Wolfram, 2023).

Some of the hardest chess puzzles we considered were created by Sir Roger Penrose. Penrose
argued that human creativity is not entirely algorithmic and cannot be replicated by a sufficiently complex computer (Penrose, 1994; Penrose and Mermin, 1990; Wikipedia, 2023). By understanding why humans can solve puzzles that AI cannot, we may be able to uncover the non-algorithmic aspects of human thinking and gain a better understanding of human consciousness (Doggers, 2017). While Fig. 4 does show that AZ does not understand these positions, it also suggests that AZ can solve almost any puzzle using a simple computational process: learning from trial and error via RL by starting chess games from puzzle positions and playing against itself. In other words, Fig. 4 demonstrates that the Penrose positions are computable in the sense presented in (Penrose, 1994) and implied by the finiteness of chess, but also, that there are indeed gaps between human and machine thinking. Through careful analysis, we suggested that the challenge for AZ is that it does not see similar positions when it learns to play chess by playing against itself, and therefore, struggles to generalize to these unseen, OOD positions. In contrast, each policy in $\mathrm{AZ}_{\mathrm{db}}$ is intrinsically motivated to experience different games, making it less likely that a specific position will be OOD for any of its policies. Indeed, in Fig. 5 we observed that some of the players in the $\mathrm{AZ}_{\mathrm{db}}$ team were able to solve the Penrose positions without training on them, while other players, including AZ, were not. This suggests that incorporating human-like creativity and diversity into AZ can improve its ability to generalize. On the other hand, there were still many puzzle positions that $\mathrm{AZ}_{\mathrm{db}}$ failed to generalize to as a team, suggesting that there is still a gap between human and machine thinking. We hope that our paper will inspire future research of these gaps.

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## A. Additional related work on QD

QD optimization is a type of evolutionary algorithm that aims at generating large collections of diverse solutions that are all high-performing (Cully and Demiris, 2017; Pugh et al., 2016, QD). It comprises two main families of approaches: MAP-Elites (Cully et al., 2015; Mouret and Clune, 2015) and novelty search with local competition (Lehman and Stanley, 2011, NSLC), which both distinguish and maintain policies that are different in the behavior space. The main difference is how the policy collection is implemented, either as a structured grid or an unstructured collection, respectively. The behavior space is either handcrafted based on domain knowledge (Cully et al., 2015; Tarapore et al., 2016) or learned from data (Cully, 2019). Some other works combine evolutionary QD with RL (Nilsson and Cully, 2021; Pierrot et al., 2022; Tjanaka et al., 2022). Further references can be found on the QD webpage.

In RL, intrinsic rewards have been used for discovering diverse skills. The most common approach is to define diversity in terms of the discriminability of different trajectory-specific quantities and to use these ideas to maximize the Mutual information between states and skills (Baumli et al., 2021; Eysenbach et al., 2019; Gregor et al., 2017; Sharma et al., 2020) or eigenvectors of the graph Laplacian (Klissarov and Machado, 2023). Other works implicitly induce diversity to learn policies that maximize the set robustness to the worst-possible reward (Kumar et al., 2020; Zahavy et al., 2021a), and some add diversity as a regularizer when maximizing the extrinsic reward (Badia et al., 2020; Hong et al., 2018; Masood and Doshi-Velez, 2019; Pathak et al., 2017; Peng et al., 2020; Sharma et al., 2020; Sun et al., 2021; Zhang et al., 2020).

Parker-Holder et al. (Parker-Holder et al., 2020) measure diversity between behavioral embeddings of policies. The advantage is that the behavioral embeddings can be defined via a differential function directly on the parameters of the policy, which makes the diversity objective differentiable w.r.t to the diversity measure. Other works use successor features to discover and control policies (Alver and Precup, 2022; Barreto et al., 2017a, 2018, 2019; Nangue Tasse et al., 2020; Tasse et al., 2021; Zahavy et al., 2021a). In this line of work, there is a sequence of rounds, and a new policy is discovered in each round by maximizing a stationary reward signal (the objective for each new policy is a standard RL problem). The rewards can be random vectors, one hot vectors, or an output of an algorithm (for example, an algorithm can be designed to increase the diversity of the set). There is also a growing interest in techniques for solving MDPs with general utilities (Abbeel and Ng, 2004; Belogolovsky et al., 2021; Geist et al., 2022; Hazan et al., 2019; Mutti et al., 2022; Shani et al., 2022; Zahavy et al., 2020a, 2021b; Zhang et al., 2020) which can be used for designing diversity objectives.

Repulsive and attractive forces have also been studied in related work. Vassiliades et al. (Vassiliades et al., 2017) suggested to use Voronoi tessellation to partition the feature space of the MAP-Elite algorithm to regions of equal size and Liu et al. (Liu et al., 2017) proposed a Stein Variational Policy Gradient with repulsive and attractive components. Flet-Berliac et al. (Flet-Berliac et al., 2021) introduced an adversary that mimics the actor in an actor-critic agent and then added a repulsive force between the agent and the adversary.

There has also been a significant amount of work in multi-agent learning on discovering diverse policies. A common approach in this literature is to encourage response diversity via matchmaking to increase the space of strategies (Balduzzi et al., 2019; Perez-Nieves et al., 2021), which is particularly useful in non-transitive games. Sanjaya et al. (Sanjaya et al., 2022) quantified the non-transitivity in chess through real-world data from human players over one billion chess games from Lichess and FICS. Their findings suggest that the strategy space occupied by real-world chess strategies demonstrates a spinning top geometry (Czarnecki et al., 2020). These findings are correlated with our observation that there is more diversity in $\mathrm{AZ}_{\mathrm{db}}$ play style when it uses a medium number of simulations (400)
and less when it uses a high or low number of simulations.
Response diversity techniques are usually combined with population-based training (Jaderberg et al., 2017), which represents a collection of players with a separate set of parameters for each player. One important example is the Alpha League, which led to significantly improved AlphaStar's performance in Starcraft 2 (Vinyals et al., 2019). More recently, response diversity has also been used with a latent conditioned architecture (Liu et al., 2022a,b), closer to our setup.

Another important use case for diversity in multi-agent learning is to first discover diverse highquality policies and then train the best response policy that exploits all of the discovered policies (Lupu et al., 2021). In another example, Liu et al. (Liu et al., 2017) considered diversity in Markov games and proposed a state-occupancy-based diversity objective via the shared state-action occupancy of all the players in the game.

## B. Response diversity

## B.1. Technical details

We encourage response diversity in a league of players $\boldsymbol{\Pi}$ by training on matchups sampled from a probability function $\mathbb{P}\left(i, j, t^{i}\right)$. Intuitively, the matchmaking works by first uniformly sampling player $i$ from П. It then uniformly samples an indicator $t^{i}$ to denote whether player $i$ is playing as black or white, and the oponent player $j$ is sampled conditionally as:

$$
\begin{equation*}
\mathbb{P}\left(i, j, t^{i}\right)=\mathbb{P}\left(j \mid i, t^{i}\right) \mathbb{P}_{\text {unif }}(i) \mathbb{P}_{\text {unif }}\left(t^{i}\right) \tag{10}
\end{equation*}
$$

Note that chess is not a symmetric game. There is "a general consensus among players and theorists that the player who makes the first move (white) has an inherent advantage" (Wikipedia). Hence we condition the sampling of $j$ on both $i$ and $t^{i}$.

Several population learning frameworks can be expressed this way. In practice, $\mathbb{P}\left(j \mid i, t^{i}\right)$ is represented as the adjacency matrix of an interaction graph $\Sigma \in \mathbb{R}^{N \times N}=\left\{\sigma^{i}\right\}_{i=1}^{N}$, where each row $\sigma^{i}$ corresponds to a mixture policy over $\Pi$, and the $j^{\text {th }}$ element is the probability of $i$ playing against $j$. For example, in Policy Space Response Oracle (PSRO; Lanctot et al., 2017), each agent is computed as the approximate best response to the Nash equilibrium over players in the current population for some fixed iteration order. Specifically, we consider the following matchmaking algorithms, also illustrated in Fig. 9:

- Selfplay each player only plays against itself, i.e., $j=i$
- Uniform player $j$ is sampled uniformly from $\Pi$, i.e., $\mathbb{P}\left(j \mid i, t^{i}\right)=\mathbb{P}_{\text {unif }}(j)$
- PSRO-NASH player $j$ is sampled from a mixture policy $\sigma_{b}^{i}$ or a mixture policy $\sigma_{w}^{i}$, which are the Nash equilibria over $\left\{\pi_{k}\right\}_{k=0}^{i}$ playing as (b)lack and (w)hite respectively. For a real example of interaction graphs for a PSRO-NASH league, see Fig. 10.
- PSRO-RECTIFIED is the same as PSRO-NASH, except we respond to the "rectified" Nash as per (Balduzzi et al., 2019), i.e., each player is trained against the Nash weighted mixture of players that it beats or ties, in order to discover strategic niches and enlarge the empirical gamescape.
- Fictitious Play or PSRO-UNIFORM or (Brown, 1951; Leslie and Collins, 2006): player $i$ responds to the uniform mixture over the current population of players. This has been shown to perform well empirically.
- PSRO-CYCLE the first $n-1$ players forms a strategic cycle and the last player responds to the Nash equilibrium over the entire league.

$$
\begin{aligned}
& {\left[\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right]} \\
& \text { (a) Selfplay } \\
& \text { (b) Uniform } \\
& \text { (e) Fictitious Play } \\
& \text { (c) PSRO-NASH } \\
& \text { (f) PSRO-CYCLE }
\end{aligned}
$$

Figure 9 | Matchmaking Algorithms: (a) Selfplay: Each player only plays against itself. (b) Uniform: Each player is sampled uniformly at random. (c) PSRO-NASH: Player $j$ is sampled from a Nash mixture policy over the current population (up to $i$ ) that is gradually updated over the course of training. (d) PSRO-RECTIFIED: Similar to PSRO-NASH, except player $j$ is sampled from a "rectified" Nash mixture policy. (e) PSRO-UNIFORM: Player $j$ is sampled from the uniform mixture over the current population of players. (f) PSRO-CYCLE: The first $n-1$ players form a strategic cycle and the last player responds to Nash equilibrium over the entire league.

In contrast to the typical approach where a policy population is grown by iteratively training new policies against snapshots of existing policies, we train all players in the $\mathrm{AZ}_{\mathrm{db}}$ league concurrently.

For PSRO variants, we compute separate interaction graphs $\Sigma_{b}$ and $\Sigma_{w}$ for playing as black and white respectively. During training, we track the outcome of matchups in a payoff matrix and compute $\Sigma_{w}$ and $\Sigma_{b}$ for the row (white) and column (black) players respectively. We also differ slightly from the standard PSRO setup and include the current player in the population it is responding to. This means player 0 is not treated as a fixed policy and essentially engages in standard AZ self-play. This works well empirically.

Practical Considerations. For PSRO variants where each player is potentially responding to a different mixture policy or matched against specific opponents to discover strategic niches, it is necessary to filter the experience generated from each matchup so that only $i$ 's experience (the exploiter) is used to update the agent, and not j's experience (the exploitee). This is because updating from both players' experiences will effectively cancel out the diversity effect we are seeking when players are trained concurrently.

Information Hiding. For standard AZ self-play, MCTS uses the same agent to play both sides of the game during search. This is no longer true for $A Z_{d b}$ as each player in the league is conditioned on a latent variable $l$, and care needs to be taken to restrict the searching player from using privileged information about their opponent's identity. Therefore during training, we ensure that each player can only plan with their own policy and values.

(a) Player One (White)

(b) Player Two (Black)

Figure 10 | Empirical PSRO-NASH Interaction Graphs for a league with 5 players. Each grid represents a matchup between exploiter player $i$ (row) and exploitee player $j$ (column), lighter color implies higher probability (white is probability 1 and black is 0 ). Since we only match an opponent $j$ with player $i$ for $j<=i$, the interaction graph is lower diagonal (but includes the diagonal and therefore allows self-play). We can see that most players get to play self-play games (have probability mass on the diagonal) but also get to play against other players.

## B.2. Matchmaker comparisons

We now compare the six matchmaking mechanisms proposed above in four experiments (Fig. 11-14). In each experiment, we trained six agents using the fast configuration. These experiments differ in two aspects: we trained the agents with and without the diversity intrinsic reward (when there is no intrinsic reward, there is only response diversity), and with and without "information hiding", i.e., hiding the privileged information about the opponent during planning. The columns correspond to different matchmakers, grouped in triplets, where for each matchmaker we present the results for latent 0 , max-over-latents and sub additive planning (left-to-right).

The rows correspond to the data sets in the main paper, where we additionally include a version of STS with a $0 / 1$ loss (the agent gets a score of 1 if it finds any of the propose solutions, regardless of their internal scores). In the Penrose set, we include two thresholds: 0.25 as in the main paper and 0.1.

Inspecting the results, we could not identify a significant advantage to any of the match making mechanisms. The different matchmakers perform roughly the same, in particular, on the larger and more statistically significant data sets (STS, Lichess). Furthermore, different matchmakers were better than others in different configurations. We could not make an informed decision regarding which matchmaker to use given these results. Nevertheless, we believe that presenting these results here may be of benefit for other researchers interested in match making ideas, in particular in chess and other transitive games.


Figure 11 | No diversity, without privileged information.


Figure 12 | With diversity, without privileged information.


Figure 13 | No diversity, with privileged information.


Figure 14 | With diversity, with privileged information.

## C. Diversity bonuses in AZ

It might surprise some readers that RL can benefit from creative-problem solving mechanisms. In principle, RL can solve any problem via trial and error. However, RL methods cannot find truly optimal policies in most problems of practical interest and hence find a particular (hopefully) near-optimal solution whose choice is determined by the nature of the agent's bounds (memory, compute, training experience), as depicted in Fig. 15 (left). This singular sub-optimal choice can potentially generalise poorly when faced with situations it did not encounter during its training. In other words, a single policy will face Out of Distribution (OOD) situations w.r.t to its self-play distribution (the games that the agent plays against itself and gets to train on). Incorporating multiple policies with different self-play distributions (diverse $d_{\pi}$ ) extends the self-play distribution of $A Z_{\mathrm{db}}$ as a team, and we can therefore expect that some players will generalize better than others in some situations.

Another potential issue is that RL is designed to find an optimal policy from an initial state distribution. This is fine if one only cares about playing chess from the initial board, but people are also interested in knowing what the optimal move is from a variety of positions, potentially outside of the path of the optimal policy. Even with advanced exploration techniques, this fundamental problem remains: exploration is designed to explore the state space until the agent is confident enough about the optimal policy, and at this point, it becomes less likely for it to encounter sub-optimal states. Another issue is that the policy is often deterministic, and as such, will play the same move from each position, ignoring other potentially optimal moves. Modern chess engines, however, are required to do much more than play perfect chess from the initial board: they are being asked to recommend moves from sub-optimal positions, analyze games, and more.

In Fig. 15 (right), we depict one hypothetical optimal trajectory (assuming access to an optimal policy) starting from the initial board (state 0 ) and continuing to states 1,4 and 6 with red arrows (self-play). Having a diverse team of agents can help in alleviating this issue and improving our data distribution in the following manner. In green color, we depict a different optimal trajectory in which the opponent selects a different optimal action in state 1 leading the game to states $5 \& 7$. The agent might miss such a trajectory when training with a self-play league and using other matchmakers can help to explore it. Alternatively, an agent may choose to play a different optimal action in state 0 leading it to visit $2,8 \& 9$ by optimizing quality diversity (purple).


Figure 15 | Left: an illustration of the space of chess agents. The optimal policy is not computeable; within the computeable policies there are different $\epsilon$-optimal policies. Right: An illustration of a state space. Blue colors represent optimal states, i.e., states that can be reached with an optimal policy. Red arrows (starting from state 0 ) represent one possible optimal trajectory, whereas green and purple arrows represent alternative optimal trajectories. State 3 is a sub-optimal state that would not be visited by an optimal policy.

## C.1. Evaluation of external chess engines in puzzle

The goal of this work is to study diversity bonuses in AZ. Our focus was not on comparing or making any claims about the strength of a particular chess engine compared to others. Nevertheless we believe it is informative to present the solve rate of reference chess engines, as it provides further evidence of the challenges in solving these puzzles. We evaluated Stockfish $8 \& 15$, and Crystal 4.1 with the following configurations: Level $=20$, Number of threads $=16$, Search time $/$ move $=20$ mins, Hash table size $=1024 \mathrm{MB}$.

We would like to emphasize that our methods are not specific to chess and can be applied to other domains.


Figure 16 | The solve rate of external chess engines across different data sets.

## C.2. Visualizing the piece occupancies



Figure 17 | Piece occupancies of $\mathrm{AZ}_{\mathrm{db}}$. Columns correspond to pieces: leftmost five as white and rightmost as black. Rows correspond to players playing as white (odd rows) and black (even rows). Numbers above sub figures indicate the sum of the occupancy over the board divided by the number of pieces (eg 1 for king, 8 for pawns) and indicate how long does a piece stays on the board on average. Black rectangles highlight the starting position of each piece. Color units (in the colorbars) correspond to occupancy in \% multiplied by the average number of moves in a game (65). For orientation, the chess coordinate system is displayed in Figure 3 in the main paper, top-left.


Figure 18 | Mean-subtracted piece occupancies of $\mathrm{AZ}_{\mathrm{db}}: \tilde{\psi}^{i}=\psi^{i}-\frac{1}{N_{\text {Players }}} \sum \psi^{i}$. Columns correspond to pieces: leftmost five as white and rightmost as black. Rows correspond to players playing as white (odd rows) and black (even rows). Blue color implies that a specific player has higher occupancy than the average, and red color implies lower occupancy. Black rectangles highlight the starting position of each piece. Color units (in the colorbars) correspond to occupancy in \% multiplied by the average number of moves in a game (65). For orientation, the chess coordinate system is displayed in Figure 3 in the main paper, top-left.

## C.3. Details on self-play from puzzle positions.

Table 1 in the main paper presents the performance of AZ on the challenging puzzles sets (Challenge and Penrose) when we allow AZ to begin self-play games from puzzle positions. Here we further explain the details for each one of the variations in the table.

Self-play from puzzle positions: This agent uses a start-position sampler that samples an initial board position from the following distribution: with $\mathbb{P}=0.5$ it uses the standard initial chess board and with $\mathbb{P}=0.5$ it uniformly samples a position from the Challenge and Penrose Sets. Note that we do not give the solutions to the puzzles to the agent in any form. AZ is allowed to train on self-play games that it plays from these positions.

+ intermediate positions: While the previous agent used the first position from each puzzle in the start-position sampler, this agent also samples intermediate positions from each puzzle in the Challenge set. Since those puzzles have a unique multi-step solution, adding intermediate positions allows the agent to play on more advanced steps of a puzzle and can help the agent with exploration.
+ exploration: This agent additionally uses an exploration mechanism to sample actions during training. The agent samples actions from a softmax distribution ( $\tau=10$; identical setup for exploration is used in AZ (Silver et al., 2018b)) constructed over the MCTS visit-counts $N^{0}(s, a)$ for the first 15 steps of an episode. After the first 15 steps, the agent continues to sample actions greedily from its visit-counts.
+ half-move clock: The half-move clock in chess counts how many moves have been played since the last move where a pawn advanced or a piece was captured. When this counter reaches 100 the game ends in a draw, which is known as the 50 -move draw rule. The closer this counter is to 100 , the more likely it is that a position will end up in a draw. Whenever we introduce positions in the start position matchmaker, we introduce them with the half-move clock set to 0 . However, in this experiment, we also included puzzle positions with half-move clocks set from 0 to 80, in increments of 20. This data augmentation should make it easier for the agent to learn that some positions are leading to a draw.

Train/test splits. In the middle panel of Table 1, we conducted two more experiments to understand the generalization ability of AZ. The first experiment focused on in distribution generalization, i.e., AZ used a start-position sampler that consisted of 36 positions from the Penrose set and was evaluated on the remaining 17 held-out positions. This split implies that AZ had access to some of the variations of each Penrose position in its training set and the others in its test set (see Tables 4-11). Inspecting the results, we can see that the agent achieves $88.24 \%$ (see (3) in Table 1 in the main paper) suggesting that it generalizes well in distribution (across variations of the same position). The second experiment focused on OOD generalization, where AZ used all the puzzles from the Penrose set except the original (position 2) Penrose puzzle position and its variations (training set = 36 puzzles; test set $=17$ puzzles). This agent achieved a performance of $11.76 \%$ on the test set (see (4) in Table 1 in the main paper).

## C.4. Additional results on AZ's understanding of puzzles

In the main paper, we inspected AZ's understanding of the Penrose positions. We now complement this analysis with a position from the Challenge set in Fig. 19.

The first and second rows in Fig. 19 shows the first and third steps respectively of the Challenge set puzzle. Inspecting the first step we can see that AZ has a higher probability for selecting the correct action Nxa2 and also an accurate raw value estimate for this move (draw). However, the raw value estimates for the other actions (which are not part of the solution) suggest that the agent can win if it played any of them, and after MCTS, AZ predicts that all actions are equally likely to lose the game.

In the third step of this puzzle (second row), it is white's turn to play, black has the possibility of promoting its a2 pawn in the next move, and thus, it is important to pick the correct move here. We indicate some of the legal moves with arrows, where red arrows indicate wrong moves that lead to a loss and the blue arrow shows the unique, correct move (Kc1) that leads to a draw (if black promotes the a2 pawn to a queen, white responds with Bishop b1 that locks the position).

AZ again selects the wrong move, it has low prior probability for all the legal actions available from this position, and more importantly, its raw value estimates predict that it is a win for all of those legal moves! When AZ trained on puzzles with self-play, it correctly predicts the action (in terms of prior probability) and also understands the position correctly (measured in terms of raw and MCTS values).


Figure 19 |Left: Two puzzle positions from the Challenge set. Right: Visualizations of prior probability from a subset of legal actions, and its corresponding raw value and MCTS value estimates for AZ and AZ trained on puzzle sets. Correct and Incorrect moves are colored in Blue and Red respectively.

## C.5. Sub-additive planning in chess matchups

In this ablation experiment, we looked at the performance of sub-additivity as a function of the number of seeds in matchups. We looked at the averaged scores from matchups across opening positions generated using a certain number of random seeds and, from those matchups, defined a look-up table that mapped from an opening position and $A Z_{d b}$ 's player color to the player from the team with the highest score against AZ. This look-up table was used to select a player on hold-out matchups from a distinct set of 30 seeds. This answers the question of whether such a sub-additive approach can generalize to a hold-out set of matchups and more broadly answers the question of whether different players specialize to specific opening positions. The results from this study are presented in Fig. 20, where the average win rate (scores in [ $-1,1$ ] are transformed to $[0,1]$ ) against AZ as a function of training seeds, i.e., the number of matchups that were used to define the look-up table for sub-additive player selection. The figure also shows in dashed horizontal lines the average win rate of the best latent (black) and max-over-latents (red). From the plot, we see that when players are selected sub-additively using the look-up table (constructed from 90 seeds), the win rate of $A Z_{d b}$ improves to 0.598 on the hold-out set of matchups (from 30 random seeds). This finding is similar to the one that was previously described in Figure 1 in the main paper (Right): sub-additive planning with players in $\mathrm{AZ}_{\mathrm{db}}$ improves performance also in matches, while the previous experiments demonstrated this only in puzzles. The figure also shows that sub-additive planning in matchups improves as a function of training seeds (that are used to construct the look-up table).

For each opening and seed, we calculated the average score of each player across all other seeds (leaving one seed out) and defined a mapping from an opening to a player with the highest score. We then evaluated this mapping on the held-out seed of matchup. This process is repeated for each seed that is held-out for evaluation and the scores obtained from the evaluation are averaged and reported as the sub-additive planning scores in Fig. 21.


Figure 20 | Sub-additive planning in chess matchups against AZ. Reports the average winrate of $\mathrm{AZ}_{\mathrm{db}}$ against AZ, generated from 500 random seeds. Also shows the winrate of the best latent (in Black) and max-over-latents (in Red) across those matchups.


Figure 21 | Summary of chess matchups between $A Z_{d b}$ and $A Z$. The first ten rows reports the average of the match outcomes (i.e., wins, draws and loses) for each player in the team. The last two rows reports the same for sub-additive planning and max-over-latents. In addition to game outcomes, we also report the average winrate and relative Elo improvement over AZ.


Figure 22 | Results from different chess openings between $\mathrm{AZ}_{\mathrm{db}}$ and AZ (scores averaged from 30 random seeds). In the figure on the left, $\mathrm{AZ}_{\mathrm{db}}$ played as White and AZ as Black; the colors were flipped for the figure in right.

Table $3 \mid$ Average winrates of each player in $A Z_{d b}$ when playing as White and as Black against $A Z$.

| $\mathrm{AZ}_{\mathrm{db}}$ team | as White | as Black |
| :--- | :--- | :--- |
| Player 0 | $68.27 \%$ | $40.21 \%$ |
| Player 1 | $67.39 \%$ | $39.63 \%$ |
| Player 2 | $\mathbf{6 9 . 8 6 \%}$ | $38.57 \%$ |
| Player 3 | $68.31 \%$ | $37.83 \%$ |
| Player 4 | $69.26 \%$ | $37.79 \%$ |
| Player 5 | $68.32 \%$ | $38.19 \%$ |
| Player 6 | $69.23 \%$ | $38.98 \%$ |
| Player 7 | $69.36 \%$ | $38.38 \%$ |
| Player 8 | $69.24 \%$ | $38.26 \%$ |
| Player 9 | $67.30 \%$ | $\mathbf{4 0 . 3 8 \%}$ |

## D. Puzzle sets

The Lichess data set is composed of 560 puzzles that we selected from a larger data set provided by lichess.org. The complete data set includes $3 M$ puzzles collected from 300 M analysed games from the Lichess database and re-analyzed with SF. We selected 560 puzzles from them by creating a subset of the 20 K hardest puzzles (rated by "ELO" score) and then further selecting from them the positions that were unsolved by SF15 with a low number of simulations (10k). Each puzzle in the set requires multiple steps; the agent receives a score of 1 if it predicts the correct unique action in all the steps and 0 otherwise.

The Strategic Test Suite (STS) is a data set of 1088 single-step, multi-choice chess puzzles, designed to evaluate chess engine's long term understanding of strategical and positional concepts. The suite was created by Dann Corbit and Swaminathan Natarajan, but we adapt the more recent STS-Rating (v6) by Ferdinand Mosca. Actions receive scores $\in[0,1000]$, we normalize the score for each action by the score of the best action (1000), so the score in each puzzle is $\in[0,1]$.

The next two data sets were collected and created by our team. They include puzzles from different sources and we refer the reader to the tables in the end of the Appendix for more details.

The Challenge set includes 15 multi-choice \& step puzzles that are designed to be challenging to modern chess engines. A score of one is given if the agent predicts the correct unique action in each step of the puzzle and 0 otherwise. We deal with a few cases of ambiguous solutions via a simple concept of "or lists", if the agent finds one of the possible unique multi-step solutions to the puzzle it gets a score of 1 in this puzzle. Sometimes the opponent has different ways to respond to the agent's moves, in this case, we apply an "and list" and require the agent to find the unique multi-step solution on all the variations.

The Penrose set includes 53 challenging single-step puzzles, where the goal is to predict the value of the position (in $[0,0.5,1]$ ). A score of one is given if the value prediction (after a search) is within a threshold (of 0.25 or 0.1 ) from the correct value and 0 otherwise. The set includes three sources of puzzles: (1) The Penrose position(s): a chess puzzle proposed by Sir Roger Penrose to "learn more about the uniqueness of the human brain" (Doggers, 2017), can be seen in Table 7, top. We also include a second position by Penrose with a similar idea that we found here (Table 4, top). (2) A set of variations of the two Penrose positions as well as other puzzles created by our team (Tables 4-11). (3) Fortress positions from (Guid and Bratko, 2012), selected from (Dvoretsky, 2010) (Tables 19-20) and blocked positions composed by us (Tables 12-18). Together with the Lichess data set, these puzzle sets present a diverse set of challenges for chess engines.

The following tables present positions from the Penrose and Challenge sets respectively. The tables include the starting position of each puzzle, the FEN, the solution, the player to play and comments on each position. The comment provides context on the position and sometimes explain why it may be hard for engines to correctly evaluate. This analysis was performed using a web version of SF, and we emphasize that it is not using SF at its full strength. The goal of these comments is to provide context on why the position is hard to chess programs and we use SF due to its popularity.

| Board | Solution | To Play | Comment |
| :---: | :---: | :---: | :---: |
| knb5/1b1p4/p1pPb3/P1P5/6p1/6Pp/7P/K7 w -- <br> 6) | Draw | White | White can draw in several ways, for example, by repeating Kb2-a1 to draw via the three-fold repetition rule or the 50 move rule. There is no way for white or black to make progress. This position would be even be drawn is white picks up the pawns on g 4 and h3. The reason is that black can sacrifice the bishop for one of the pawns. The resulting position is a draw because it's a fortress. |
| knb4Q/1b1p4/p1pP2K1/P1P5/8/8/8/8 b - . | Draw | Black | A position that arises from a calculation sequence in the baseline puzzle. This position is a fortress, and white cannot make further progress. |
| knb5/1b1p1b2/p1pPb3/P1P5/6p1/6Pp/7P/K7 w ゅ <br> B | Draw | White | This puzzle is even more difficult for SF , as there is an additional piece meaning more possible moves. However, for humans, it's clear that the fundamental aspects are the same. |
| knb5/pb1p4/p1pPb3/P1P5/6p1/6Pp/7P/K7 w - - $2$ $8 \text { i }$ $\varepsilon$ | Draw | White | Interestingly enough, this position is easier for Stockfish to evaluate. This is likely because the pieces in the left top of the board have no moves, and SF recognizes that stalemate (no moves left, resulting in a draw) is a likely outcome. |

Table 4 | Penrose set positions, Penrose variation 1, positions 1-4


Table 5 | Penrose set positions, Penrose variation 1, positions 5-8


Table 6 | Penrose set positions, Penrose variation 1, positions 9-12


Table 7 | Penrose set positions, Penrose variation 2, positions 1-4


Table 8 | Penrose set positions, Penrose variation 2, positions 5-8


Table 9 | Penrose set positions, Penrose variation 2, positions 9-12


Table 10 | Penrose set positions, Penrose variation 2, positions 13-16


Table 11 | Penrose set positions, Penrose variation 2, position 17

| Board | Solution | To Play | Comment |
| :---: | :---: | :---: | :---: |
| n1B4r／r1p2k2／＿Bppp3p／pp1ppBpp／／P2bpppb 1R1RbPb1／R1K1R1R1／R3R2 w－ | Draw | White | As the pawn structure is locked，and White is unable to remove any of the Black pawns by force，this is a trivial draw．Should White capture one of Black＇s dark－squared bishops，Black should avoid recapturing，and keep the blockade． |
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| n1B4r／r1p2k2／BpPp3p／pP1PpBpP／P2bPpPb／ 1R1RbPb1／R1K1B1R1／1R3R2 w－ |  |  |  |
| 2 |  |  | As the pawn structure is locked，and |
| 当 |  |  | White is unable to remove any of the |
|  | Draw | White | Black pawns by force，this is a trivial |
|  | Draw |  |  |
|  |  |  | should avoid recapturing，and keep |
| 品 \％\＆\％ |  |  | the blockade． |
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| 23 |  |  | As the pawn structure is locked，and |
| $\pm$ |  |  | White is unable to remove any of the |
| 瓦 $\hat{\sim}$ |  |  | Black pawns by force，this is a trivial |
|  | Draw | White | draw．Should White capture one of |
|  |  |  | should avoid recapturing，and keep |
| \％\％\＆\％붕 |  |  | the blockade． |
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Table 12 ｜Penrose set positions，Blocked set variation 1，positions 1－3．These represent the same theme（blockade），albeit with a slight variation in the total amount of material on each side，and therefore－the branching factor in search．


Table 13 | Penrose set positions, Blocked set variation 2, positions 1-3

| Board | Solution | To Play | Comment |
| :---: | :---: | :---: | :---: |
| 5k2/5Bp1/5pP1/1K2pP2/4P3/1B3B2/8/5B2 w -- | Draw | White | White has no way of challenging the dark squares and the pawn on g7. Black should just move the king Kf8-e7-f8, and the game would end in a draw. If White vacates the a2-g8 diagonal, the Black king could be forced to g 8 or h8, but that wouldn't change the outcome. Different amounts of extra material test for whether having extra light-squared bishops affects the engine's judgement. |
| 5k2/5Bp1/5pP1/1K2pP2/4P3/8/8/8 w - - | Draw | White | White has no way of challenging the dark squares and the pawn on g7. Black should just move the king Kf8-e7-f8, and the game would end in a draw. If White vacates the a2-g8 diagonal, the Black king could be forced to g 8 or h8, but that wouldn't change the outcome. Different amounts of extra material test for whether having extra light-squared bishops affects the engine's judgement. |
| B4k2/5BpB/2B2pP1/1K2pP1B/4P3/3B1B1B/B7/8 w | Draw | White | White has no way of challenging the dark squares and the pawn on g7. Black should just move the king Kf8-e7-f8, and the game would end in a draw. If White vacates the a2-g8 diagonal, the Black king could be forced to $g 8$ or h 8 , but that wouldn't change the outcome. Different amounts of extra material test for whether having extra light-squared bishops affects the engine's judgement. |

Table 14 | Penrose set positions, Blocked set variation 3, positions 1-3

| Board | Solution | To Play | Comment |
| :---: | :---: | :---: | :---: |
| rb1b3k/2b1p3/1p1pP3/pPpP1B2/P1P5/4K3/8/8 w - | Draw | White | By getting the king to g5, White blocks the activation of the Black king, which cannot make further progress. Thanks to the lightsquared bishop, which will penetrate the light squares on the kingside, Black will not be able to safely get the rook out, and the dark-squared bishops cannot escape. Sample line to illustrate the point: 1. Kf4 Ba7 2. Bg6 Rb8 3. Be8 Rb7 4. Bc6 |

Table 15 | Penrose set positions, Blocked set variation 4, position 1


Table 16 | Penrose set positions, Blocked set variation 5, positions 1-3


Table 17 | Penrose set positions, Blocked set variation 5, positions 4-5


Table 18 | Penrose set positions, Blocked set variation 6, positions 1-3


Table 19 | Penrose set positions, Detecting Fortresses in Chess, Dvoretsky, positions 1-3


Table 20 | Value set positions, Detecting Fortresses in Chess, Dvoretsky, positions 4-6

| Board | Solution | Comment |  |
| :---: | :---: | :---: | :---: |
| 3B4／1r2p3／r2p1p2／bkp1P1p1／1p1P1PPp／ p1P4P／PPB1K3／8 w－ | Draw | White | William Rudolph vs．Unknown player．White sacrifices the bishop， marches its pawns while delivering checks，and closes the position． |
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| 党 | Draw | White | Hasek vs．Unknown player．White sacrifices its rook and builds a fortress． |
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| 8／1p1q1k2／1Pp5／p1Pp4／P2Pp1p1／ <br> 4PpPp／1N3P1P／3B2K1 w－－ | Draw | White | One of those puzzles where the so－ lution is still difficult to reconstruct even if you＇ve solved it before！White has a choice of pieces to sacrifices and where to sacrifice them to create a fortress and the solution is the least obvious of all！ |
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Table 21 ｜Challenge set positions，positions 1－3


Table 22 | Challenge set positions, positions 4-6

\left.| Board | Solution | Comment |  |
| :--- | :--- | :--- | :--- |
| Troitsky, 1916. To win, white must |  |  |  |
| force the black king to the a1 square, |  |  |  |
| the black pawn to a2, the white king |  |  |  |
| has to control the b1 square (via c1 or |  |  |  |
| c2), and have a bishop checking the |  |  |  |
| king on the long diagonal. This can |  |  |  |
| be achieved via a sequence of manea- |  |  |  |
| vers, zugzwangs that force the black |  |  |  |
| pawn to march to a2) and a discov- |  |  |  |
| ered check. Otherwise, white cannot |  |  |  |
| mate black with the same color bish- |  |  |  |
| ops. Engines miss this long mating |  |  |  |
| sequence. |  |  |  |$\right\}$

Table 23 | Challenge set positions, positions 7-9


Table 24 | Challenge set positions, positions 10-12


Table 25 | Challenge set positions, positions 13-15

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[^0]:    ${ }^{1}$ we divide each row by the first row (player 0 ), subtract 1 and multiply by 100

