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Accelerating Self-Play Learning in Go

KataGo是David J. Wu依照DeepMind的AlphaGo Zero与AlphaZero论文为基础,以及许多在 DeepMind论文之后的相关研究及原创的研究,大幅改善了训练速度(超过50倍:1),也因 此搭配所发布训练网络资料,成为目前世界上最强的电脑围棋软件之

David J. Wu* KataGo所实做的电脑围棋程序包括了

|我对弈训练的程序(使用C++、Python 3与TensorFlow实做) Jane Street Group, 透过软体操作的GTP引擎(使用C++实做)

另外由Jane Street Capital (英语: Jane Street Capital) (作者所在的公司)提供运算所需 资源外,也公开发布训练的成果(训练网络资料)

March 4, 2019 KataGo因丰富的分析能力,被用在围棋在线分析网站Al Sensei作为默认的分析引擎。 KataGo " 这个名字来源于日语单词 " かた (kata) " (类型) 。目前,即使在英语中,武道 的形式也被称为 " kata " 。作者 lightvector (David J. Wu) 表示,它作为一个通过强化学习永

久训练自己并旨在完成自己的形式的人工智能的名称似乎是合理的。

https://www.wanweibaike.net/wiki-KataGo

Abstract

围棋专用 By introducing several new Go-specific and non-Go-specific techniques along with other tuning, we accelerate self-play learning in Go. Like AlphaZero and Leela Zero, a popular opensource distributed project based on AlphaZero, our bot KataGo only learns from neural net Monte-Carlo tree-search self-play. With our techniques, in only a week with several dozen GPUs it achieves a likely strong pro or perhaps just-super-human level of strength. Compared to Leela Zero, we estimate a roughly 5x reduction in self-play computation required to achieve that level of strength, as well as a 30x to 100x reduction for reaching moderate to strong amateur levels. Although we so far have not tested in longer runs, we believe that our techniques hold promise for future research.

Introduction 1

In 2017, DeepMind's AlphaGoZero demonstrated in a landmark result that it was possible to achieve superhuman performance in the game of Go starting from random play and learning only via reinforcement learning of a neural network using self-play bootstrapping from Monte-Carlo tree search[9]. Moreover, AlphaGoZero used only fairly minimal game-specific tuning. Subsequently, DeepMind's AlphaZero demonstrated that the same methods could also be used to train extremely strong agents in Chess and Shogi. However, the amount of computation required was large, with DeepMind's main reported run taking about 41 TPU-years in total parallelized over 5000 TPUs [8]. The significant cost of reproducing this work has slowed research, putting it out of reach for all but major companies such as Facebook[11], as well as a few online massively distributed computation projects, notably Leela Zero for Go[14], and Leela Chess Zero for Chess[17].

In this paper, we introduce several new techniques, while also reviving some ideas from pre-AlphaZero research in computer Go and newly applying them to the AlphaZero process. Combined with minor domain-specific heuristic optimizations and overall tuning, these ideas greatly improve the efficiency of self-play learning. Still starting only from random play, training on merely about 30 GPUs for a week our bot KataGo reaches just below the strength of Leela Zero as of Leela Zero's 15-block neural net "LZ130", a likely professional or possibly just-superhuman level when run on strong consumer hardware. Based on estimates of the number of neural net queries involved,

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we achieve approximately a 5x reduction in the self-play computation required to reach this level compared to Leela Zero, and earlier in training a 30x to 100x reduction for reaching moderate to strong amateur levels of strength.

In doing so, we make several contributions:

Firstly, from a broader machine-learning perspective: our results give evidence that there is a significant efficiency gap between the somewhat more general methods of AlphaZero and what is theoretically possible from self-play learning in Go. This suggests that there may still be significant room for improvement in those general methods. KataGo, while leveraging details of the domain, still learns entirely from MCTS-bootstrapped self-play without using any pre-existing human-generated data or expert strategic knowledge.

Additionally, many of the ideas we present are non-Go-specific and might be applied to AlphaZero-like learning in other games, or perhaps to other tasks entirely. These include our technique of playout or visit cap oscillation to improve the quantity of data generated by MCTS, an idea from older computer Go literature to add auxiliary policy targets from future actions for additional regularization, which might be applicable to other sequential action environments, or our observation that a global-pooling mechanism can add new representational power to a convolutional net, in agreement with other research on global context in image-related tasks. We also present a very simple trick for sharing learned weights across multiple board sizes which might be useful for convolutional networks with inputs of variable size in other contexts.

We also hope this work serves as a case study on how when learning is highly data-constrained, one might enrich the data. Something as simple as *adding new auxiliary outputs and training targets* to a neural net can improve the quality of predictions, even if those outputs are completely unused outside of training. And we find there are often many tradeoffs between data quantity and quality in different dimensions in reinforcement learning that can be tuned.

Lastly, for the computer-Go community: we hope that KataGo is of interest in that it shows how one might train a neural net to directly predict the final score difference of a Go game rather than merely the winner, to play well under a wide variety of komi rather than only a single fixed value¹, and to handle multiple rulesets and board sizes simultaneously. To our knowledge, most of these features are not yet present in most strong modern open-source Go programs. KataGo is open-source on GitHub and along with this paper demonstrates how they can be implemented².

A note of caution is warranted, however. KataGo has *not* yet had the resources to test with training runs nearly as long and large as those of larger research efforts. While KataGo learns much faster up to just-super-human levels, further beyond that it is possible that some of the techniques presented here could need to be modified or annealed away in the late stages of a longer run when fine-tuning for final strength. Nonetheless, we believe these techniques hold promise, and it is our hope that these ideas can serve as the seed for future research and more rigorous testing and experimentation.

不过,需要注意的是。KataGo还没有足够的资源来测试像大型研究项目那样长和大的训练运行。虽然KataGo的学习速度快得多,达到了超人类的水平,但再往后,这里介绍的一些技术有可能需要修改,或者在长期运行的后期为最终实力进行退火处理。尽管如此,我们相信这些技术是有希望的,而且我们希望这些想法可以作为未来研究和更严格的测试和实验的种子。

¹In Go, *komi* is the number of points given to the second player as compensation. It can also be varied to equalize winning chances between players of different skill levels.

²The code and links to download the neural nets and training data from KataGo's main run can be found at: https://github.com/lightvector/KataGo. For any interested enthusiasts, with our code just three or four strong GPUs is sufficient for anyone to train a bot from random all the way to amateur-dan-strength on the full 19x19 board in only a few days!

2 Related Work

Aside from AlphaZero, in recent years a few other notable projects have emerged in its footsteps. These initially included the open-source Leela Zero and Leela Chess Zero distributed projects, producing very strong programs in Go and Chess[14, 17]. Others include the MiniGo project, establishing basic technical details of the AlphaZero process not obvious from high-level descriptions in the original AlphaZero papers[21], as well as the SAI project, which has explored self-play learning on smaller boards as well as new architectures for handling komi and multi-valued predictions[6]. And most recently, a paper and new release by Facebook AI Research of ELF OpenGo has also contributed to basic understanding of AlphaZero in Go[10].

Our work in KataGo borrows a number of minor techniques and ideas from these other projects, particularly Leela Zero, and where appropriate we mention this and/or contrast the differences.

KataGo also draws from work prior to AlphaZero on the value of game-specific features[2] and of auxiliary prediction targets in the context of supervised learning[12, 13], and extends these ideas to self-play reinforcement learning. While AlphaZero and reproductions like ELF OpenGo and others we shown that such ideas are not strictly necessary to achieve superhuman strength given enough sheer computing resources, we provide evidence that many of these earlier ideas still provide benefits and should not be lightly discarded. In combination with future improvements and discoveries, they could potentially bring the otherwise prohibitively-expensive AlphaZero process in games as massive as Go down to a cost accessible to smaller research groups and institutions.

3 Overview

在高层次上,KataGo的整体架构类似于AlphaZero的架构。它的基础是反复改进一个神经网络,该网络可以输出合法棋步的策略分布和 对游戏结果的预测。神经网络被用于蒙特卡洛树搜索,通过自我游戏产生数据,用于进一步训练神经网络。训练中的神经网络的周期 性快照,并通过一个门控机制以确保新网络的质量,它取代了用于后续自我游戏的网络。在KataGo中,所有这些步骤都是连续和异步

At a high level, KataGo's overall architecture resembles the AlphaZero architecture. It is based around iteratively improving a neural net that outputs both a policy distribution over legal moves and a prediction of the game outcome. The neural net is used in a Monte-Carlo tree search which generates data via self-play that is used to further train the neural net. Periodic snapshots of the neural net in training are taken, and subject to passing a gating mechanism to ensure the quality of the new net, it replaces the net to be used for subsequent self-play. In KataGo, all these steps 也就是还是基于蒙特卡洛树搜索,只是用神经网络进行

We give an overview of the components of the architecture in three major sections:

- Neural Net Training: its architecture, inputs, outputs, loss function, and hyperparameters.
- Search and Target Generation: the tree search, exploration formula, utility function, and generation of the policy target for training from the search result.
- Self-play: the initialization of games, variation of search parameters, branching of game positions, and optimizations to playing and terminating those games.

In each, we will highlight the major and minor innovations and/or differences from AlphaZero, as well as the differences from other prior work, most notably that of Leela Zero, the most popular open-source Go project modeled on AlphaZero. After that, we will present data from KataGo's main run and other experimental results from a variety of ablation studies.

run continuously and asynchronously.

主要面向用户的功能:
1预测分析分数和地空,

2处理多个规则和贴目值,包括古老的"还棋头"规则, 3同一网络能够在从7x7到19x19的所有棋盘里下棋*,* 4特殊的不对称训练以提高让子游戏发挥。

4 Neural Net Training

KataGo的神经网是一个卷积残差神经网,它采用了预激活架构[3]。 与AlphaZero的一样,它是由残留块的主干和几个输出头组成的,这 些输出头平行地转换主干的第1层以产生各种输出。这些包括一个政 策和一个游戏结果值预测,这些都是针对自我游戏产生的目标而训练 的。在这里,我们将只关注我们认为有助于提高KataGo学习效率的主 要差异。关于我们的神经网络结构的完整描述,见附录A。

预激活架

KataGo's neural net is a convolutional residual neural net that uses a *preactivation* architecture[3]. Like AlphaZero's, it is composed of a trunk of residual blocks, along with several output heads that in parallel transform the final layer of the trunk to produce <u>various outputs</u>. These include a *policy* and a *game outcome value* prediction that are trained towards targets generated from self-play.

We will focus here only on the major differences that we believe contribute to KataGo's improved learning efficiency. For a full description of our neural net architecture see Appendix A.

辅助

训练目标的得分

4.1 Auxiliary Ownership and Score Targets

One of the improvements in KataGo's neural net training over AlphaZero and Leela Zero in Go is from the use of auxiliary ownership and score prediction targets. The use of such targets was earlier explored in work by Ti-Rong Wu et al. in the context of supervised learning, and there they found that including these extra targets reduced the mean squared error on game result prediction by a neural net and mildly improved the strength of their overall bot, CGI[13].

We find in KataGo that such targets also greatly improve the neural net's ability to learn from limited data in the reinforcement learning context of self-play training as well. The resulting improvement demonstrates the heuristic that when data is noisy or scarce, it can be beneficial to add more data-rich auxiliary targets.

Boundary | Boundary** | Boundary**

数据匮乏

In the AlphaZero process, noise and data-scarcity are particularly severe for the game outcome prediction, as compared to the other important prediction by the neural net, the policy. Whereas the policy target receives one sample per move of a game, each of which is a rich distribution over legal moves³, the game outcome target receives only one independent sample per entire game and that sample is merely a single noisy binary win or loss.

This makes the game outcome prediction particularly prone to fitting poorly, greatly benefiting from regularization from additional targets. In fact, Silver et al. found in AlphaGoZero that forcing the same neural net to predict both the policy and the game outcome value greatly improved the quality of the value prediction over training on value alone[9]. So, even if one cared only about the value prediction and not at all about the policy, one would still want to predict the policy purely to regularize the value head!

Since the final winner in Go is the player who owns more of the board (plus komi) and the game terminates not just with a win/loss outcome but a numerical score difference⁴, predicting these as well should provide far better regularization than the policy alone. So following the same motivation as CGI, we introduce into KataGo the auxiliary targets of:

• Ownership - For each point on the board, predict the expectation of the final owner of that board point, equal to 1 if the final owner is the current player and -1 if it is the opponent (and 0 in the rare case of neither). 预测已方占领为1,对手占领为-1,双方都能占领为0,领地占领

得分信度

衡量ML值网络对最终分数的预测

Score Belief - For each possible final score difference, predict the probability that the game ends with exactly that score difference. 对于每个可能的最终比分差距,预测比赛结束时正好是这个分数差距的概率。 就是说给出一个预测比赛结束时的分差,和真正比赛结束时的分差,预测和实际之间的准确率

在AlphaZero过程中,政策目标是完整的MCTS出牌分布,而不仅仅是对实际出了什么棋的一次性编码。

1

³In the AlphaZero process, the **policy target** is the full MCTS playout distribution, rather than merely a one-hot encoding of what move was actually played.

We then augment the loss function as follows. We begin first with the basic loss function: 然后我们如下增加损失函数。 我们首先从基本的损失函数开始:

$$L = c_{\text{value}} \sum_{r \in \{\text{win,loss}\}} \underbrace{z(r) \log(\hat{\underline{z}(r)})} - \sum_{m \in \text{moves}} \pi(m) \log(\hat{\pi}(m)) + \underbrace{c_{L2} |\theta||^2}_{\text{L2正则项,对参数 正则化操作}}$$

其中z是当前玩家赢得或输掉游戏的单次编码。

where z is a one-hot encoding of whether the game was won or lost by the current player⁵, \hat{z} is the neural net's prediction of z, π is the target policy distribution, $\hat{\pi}$ is the predicted policy distribution, c_{L2} is a standard L2 penalty coefficient on the model parameters θ , and $c_{\text{value}} = 1.5$ is a scaling constant for the game outcome value target relative to the policy target⁶.

We then add three additional terms: ownership_output.shape = (b,19,19)

每个样本对对应有一个 19x19的ownership信息, 取值为(-1,0,1)取-1代表属于对手的领地, 1表示属于自己的领地,0代表双方共享

• Ownership loss:

$$-w_o \sum_{l \in \text{board}} \frac{1 + o(l)}{2} \log \left(\frac{1 + \hat{o}(l)}{2} \right) + \frac{1 - o(l)}{2} \log \left(\frac{1 + \hat{o}(l)}{2} \right)$$

where $o(l) \in \{-1, 0, 1\}$ is the actual final owner of board location $l, \hat{o}(l) \in [-1, 1]$ is the neural net's prediction, and $\underline{w_o}$ is a coefficient weighting this objective. import tensorflow as tf

• Score belief loss ("pdf"):

用得分的预测的准确程度概率密度函数来作为分数预测的奖励

data3 = np.load('t3.npz')print(data3["scoreDistrN"].shape) sdn0 = data3["scoreDistrN"] sdn0= tf.cast(sdn0.tf.float32) sdn0= sdn0/100.0 print(sdn0[100])

网络预测输出

标签的独热码向量长度为842 信度,可信度 同样的在value价值评估子网络中的score belief 预测输出 标签的独热码向量长度为842 也是要842,每一手落子都要输出一个842长度的预测独热码

络中的score belief 预测输出
$$-w_{\mathrm{spdf}}$$
 \bullet $\left(\sum_{x \in \mathrm{possible\ scores}} p_s(x) \log(\hat{p}_s(x))\right)$ $p_s(x)$ 是一个独热码,表示最后的分数差是否正好是 \mathbf{x} 。 $\mathbf{x} \in \mathrm{possible\ scores}$

验证 ps(x)是个独热码 where $p_s(x)$ is a one-hot encoding of whether the final score difference is exactly x, and $\hat{p}_s(x)$ is the neural net's predicted probability that the final score difference is exactly x, and w_{spdf} is a coefficient weighting this objective.

ps(x) 是神经网络预测的最终得分差正好是 x 的概率, wspdf 是加权这个目标的系数。

• Score belief loss ("cdf"):

按照正常的CDF函数应该是PDF的积分, 但这个换了种方式用PDF计算CDF

$$w_{
m scdf}$$
 • $\sum_{x\in {
m possible \ scores}} \left(\sum_{y< x} p_s(y) - \hat{p}_s(y)\right)^{\frac{1}{2}}$ 用来推动,引导预测分布向目标接近

where w_{scdf} is a coefficient weighting this objective. Whereas the "pdf" loss rewards guessing the score exactly, this "cdf" loss is smoother, encouraging the bulk mass of the predicted distribution to be near the final score. 而 "pdf" 损失是对准确猜测分数的奖励。

这个 "cdf "损失更平滑,鼓励预测分布的主体部分接近最终得分。

Additionally as a technical detail, the architecture of KataGo's score belief distribution head internally contains a scaling component that unchecked can sometimes result in training instability, so we add an additional regularization penalty $w_{\text{scale}}\gamma^2$ where γ is the internal activation value of the scaling component.

⁴In Go, every point occupied or surrounded by a player at the end of the game scores 1 point. The second player also receives a komi of typically 7.5 points for going second, and then the player who has more points is the winner.

⁵As a minor difference from AlphaZero, KataGo uses a cross-entropy loss for the game outcome instead of squared error, treating it as a two-category classification. This allows extension to Japanese Go rules, under which a game can end in a third category no-result since the Japanese rules do not prohibit long cycles.

 $^{^6}c_{\text{value}} = 1.5$ was chosen so that that typical gradients from the cross-entropy value loss would be roughly comparable to those of a squared error.

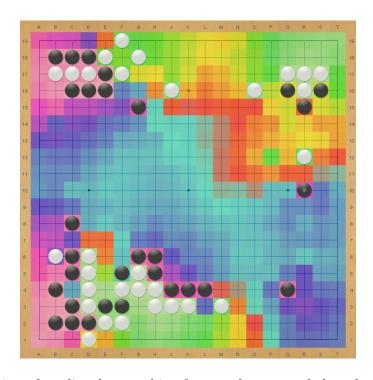


Figure 1: Visualization of predicted ownership of areas of an example board position by KataGo's neural net. Red through green increasingly indicate white ownership. Cyan through magenta increasingly indicate black ownership.用颜色分布来表示ownership分布,白子的领域用绿色到红色的深浅来表示归属占 领程度,青色到紫红色表示黑子的领域强度

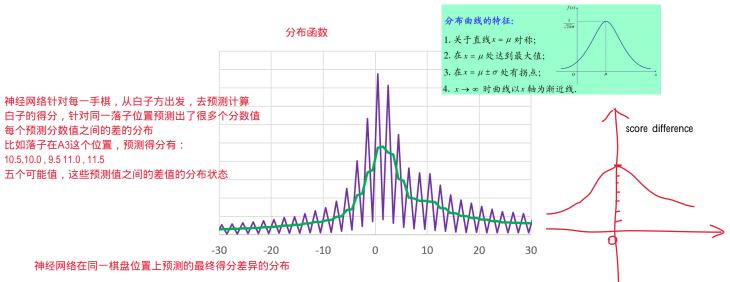


Figure 2: Distribution of predicted final score difference in points by the neural net in the same board position as in Figure 1 (purple), along with a smoothed version (green). White is predicted to win about 65% of the time, the mean score difference is about +6.

神经网络在相同的棋盘位置上预测的最终得分差异的分布(紫色)以及平滑的版本(绿色) 白方被预测为 65%的情况下获胜,平均分差约为+6。 We show in our experimental results in section 7.2 that these auxiliary targets greatly improve the efficiency of learning, even up through strong amateur strength. This might be surprising in some ways. Presumably past beginner-level strength the neural net must have already "discovered" that the game outcome is highly correlated with the sum of control of regions of the board, so why would predicting ownership continue to provide a benefit beyond the very early stages of training?

Although with no formal evidence, we offer one intuition: consider the task of learning from a game lost due to evaluating a certain pattern of stones as safe when in fact the opponent managed to capture them. Even at very strong levels, games can hinge on the uncertain life or death of groups of stones. With only the final binary win/loss result, the neural net must "guess" at what aspect of the board position caused the loss, and may require more examples to infer the correct credit assignment. By contrast, with an ownership target the neural net receives direct feedback on exactly which stones it would have predicted as safe instead were captured, and therefore should require fewer samples to generalize.

See Appendix A for the architecture of the output heads for these targets, as well as Appendix B for the values of the various weighting constants.

4.2 Auxiliary Policy Targets

辅助策略目标

增加一个与政策相关的辅助目标,预测对手在下一回合的回复动作。

As another difference from AlphaZero and other bots, in KataGo we also add an auxiliary policy-related target predicting the opponent's reply on the following turn. This idea is not entirely new either, having been found by Tian and Zhu in Facebook AI Research's bot Darkforest to provide benefits in the context of supervised move prediction [12], but as far as we know, KataGo is the first to apply it to the AlphaZero process.

In KataGo, this is done simply with another output and new term in the loss function:

$$-w_{\text{opp}} = \sum_{m \in \text{moves}} \pi_{\text{opp}}(m) \log(\hat{\pi}_{\text{opp}}(m))$$

Where π_{opp} is the policy training distribution that will be recorded for the turn *after* the current turn, $\hat{\pi}_{\text{opp}}$ is the neural net's prediction of that target, and $w_{\text{opp}} = 0.15$ weights this target only a fraction as much as the actual policy.

The neural net prediction $\hat{\pi}_{opp}$ is completely unused thereafter, but in informal early testing, we found that although the benefit was very small, adding a reasonable small weight on this target slightly improved the speed of learning. Unlike Tian and Zhu in Darkforest, we did not investigate predicting further additional moves. This might be a direction for future improvements, although there will likely be diminishing returns.

Notably, this additional policy target relies on none of the properties of Go and *potentially could apply to any sequential action environment*. In any specific environment, it is of course not guaranteed to provide a benefit, but wherever generation of data is the bottleneck, as in the AlphaZero process, this target could potentially be an easy and cheap way to achieve slightly better regularization.



Figure 3: Visualization of auxiliary policy target prediction by the neural net. Red to yellow indicates increasingly probable moves. Left: prediction of opponent's replies to our likely moves. Right: actual policy prediction on the opponent's turn if our most likely move occurs. 神经网络对辅助政策目标预测的可视化。红色到黄色表示越来越可能的棋步。左图:预测对手(白子)对我们的可能棋步的回合。右图:如果我们(黑子)最可能的棋步发生,对手回合的实际政策预测。

4.3 Sharing Weights Across Board Sizes 在不同大小的棋盘上分享权重

KataGo also uses a simple new method of sharing the same neural network weights across multiple board sizes, training jointly on all sizes. We see no reason why this method cannot also be applied to other games with variable board sizes, or perhaps even more broadly to some image processing tasks for training on multiple image sizes without cropping!

KataGo trains on a mixture of games with random board sizes ranging from 9x9 to 19x19. Positions from all sizes are shuffled together into the same training batches, training on all sizes jointly.

Mechanically, the obvious way to do this would be to embed the representation for smaller boards into larger tensors, padding the remainder with zeros. For example, embedding a 9x9 board into the upper-left 9x9 square of a 19x19 tensor. However, during convolution, non-zero values will be computed in the region within the 19x19 tensor but outside the 9x9 board. Then, subsequent convolutions near the lower-right of the 9x9 board will observe those non-zero values rather than the zero-padding they would observe for a properly-sized tensor.

We solve this by including with each training sample a *binary mask channel* indicating all on-board locations. Then:

_进制掩码通道

• Between every pair of convolutions and/or other affected operations, we apply this mask, ensuring that the next convolution receives only zeros for off-board locations. This is a cheap pointwise multiplication, which can easily be fused with adjacent GPU kernels.

 $^{^{7}}$ Since smaller boards require less training data, KataGo uses an asymmetric weighting, randomly choosing between sizes $\{9, 10, 11, \ldots, 18, 19\}$ with probabilities proportional to $\{1, 2, 3, \ldots, 10, 11\}$. But since 19 is by far the most important size for human play, we then triple the weight on size 19 up to 33, annealing further to 55 and 110 when we anneal upward the number of playouts in self-play, as described in section 6.1.

KataGo还使用了一种简单的新方法,即在多个棋盘尺寸上共享相同的神经网络权重,在所有尺寸上共同训练。我们认为这种方法没有理由不能应用于其他具有可变棋盘尺寸的游戏,或者甚至更广泛地应用于一些图像处理任务,以便在没有裁剪的情况下对多种图像尺寸进行训练! KataGo在随机棋盘尺寸从9x9到19x19的混合游戏上进行训练。所有尺寸的棋子都被洗成相同的训练批次,在所有尺寸上共同训练。从机制上讲,这样做的明显方法是将较小棋盘的表示嵌入到较大的张量中,用零填充剩余部分。例如,将一个9x9的棋盘嵌入到19x19张量的左上角9x9的方块中。然而,在卷积过程中,非零值将在19x19张量内但在9x9板外的区域被计算出来。然后,在9x9板的右下角附近的后续卷积将观察到这些非零值,而不是对一个适当大小的张量观察到的零填充。我们通过在每个训练样本中加入一个二进制掩码通道来解决这个问题,该通道表示所有板上的位置。然后:

- ·在每一对卷积和/或其他受影响的操作之间,我们应用这个掩码,确保下一个卷积只收到板外位置的零。这是一个廉价的点式乘法,可以很容易地与相邻的GPU内核融合。
- 类似的屏蔽也适用于空间输出--例如,所有权预测。
- 在任何空间均值池操作中,我们不是将张量条目相加并除以张量的维度,而是将屏蔽的条目相加并除以上位数,即屏蔽中存在的1的数量。

图4:卷积产生超大张量区域内的数值。顶部:下一次卷积 破坏了最后的蓝色方块。底部。屏蔽确保最终结果与张量大小无关。

其结果是一组神经网络权重,在推理时可用于不同的棋盘尺寸。此外,在推理时,如果神经网络每次只在单一的棋盘尺寸上玩,而不是在多个尺寸上并行玩,那么批次将只由单一的棋盘尺寸组成。那么,我们就可以根据棋盘的大小来确定张量的大小,不留任何棋盘外的空间,然后就可以省略所有的遮蔽步骤,使这一技巧在推理时成为零成本!"。鉴于该方法的简单性,如果它已经被用于其他地方,我们不会感到惊讶。但据我们所知,之前的围棋神经网络研究只使用了固定的硬编码棋盘尺寸,为每个棋盘尺寸训练独立的神经网络8。更广泛地看一下图像深度学习的文献,我们也没有发现像这样的基于遮蔽的技术作为处理可变图像尺寸的选项,尽管考虑到文献的浩瀚性,这很容易被忽略。我们在第7.2节中的实验表明,在训练的后期,尽管早期的学习速度略微加快,但在多种棋盘尺寸上的训练确实对机器人的最终19x19的强度产生了代价。早期较快的学习可能是由于对小棋盘的模式和战术的概括。正如Morandin等人在SAI项目中所讨论的,在小棋盘上的学习要快得多[6],快速的小棋盘学习可能会泛化到足以推动早期大棋盘学习的速度,这并不令人惊讶。但后来,在小棋盘上下得好可能会影响到大棋盘的发挥,这一点也不奇怪,这可能是由于神经网络能力有限。虽然KataGo显示,这并不妨碍只用一组权重就能达到职业水平甚至更高的水平,但如果严格地优化最大强度,人们可能会设想为特定的重要尺寸(如19x19、13x13)单独进行训练,同时使用我们的共享权重和屏蔽技巧来处理所有其他尺寸(15x15、17x17,甚至非方形棋盘等),进行更广泛的运行。

- Similar masking is applied to spatial outputs for example, the ownership prediction.
- In any spatial mean pooling operations, rather than summing tensor entries and dividing by the dimensions of the tensor, we sum masked entries and divide by the number of on-board locations, i.e. the number of ones present in the mask.

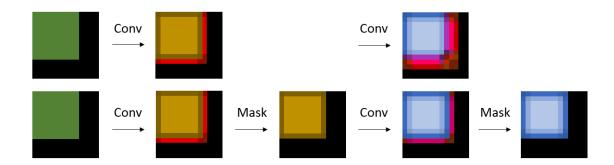


Figure 4: Convolution produces values within oversized tensor area. Top: The next convolution corrupts the final blue square. Bottom: Masking ensures a final result independent of tensor size.

The result is a single set of neural net weights that at inference time can be used with varying board sizes. Moreover, at inference time, if the neural net is playing on only a single board size at a time rather than multiple sizes in parallel, batches will consist of only a single board size. Then, one can just size the tensors to match the board size and leave no off-board space, and then all masking steps can be omitted, making this trick *zero-cost* at inference time!

Given the simplicity of the method, it would not surprise us if it were already used elsewhere. But to our knowledge, prior work neural net research in Go has only used fixed hardcoded board sizes, training separate neural nets per board size⁸. Looking more broadly at the image deep-learning literature, we have also not found mention of masking-based techniques like this as an option for handling variable image sizes, although given the vastness of the literature it would have been very easy to miss.

Our experiments in section 7.2 suggest that later in training, training on multiple board sizes does have a cost in the final 19x19 strength of the bot despite slightly accelerating learning early on. The early faster learning is presumably due to generalization of patterns and tactics from the smaller boards. As discussed by Morandin et al. in the SAI project, learning is much faster on small boards[6], and it is not surprising that fast small-board learning might generalize enough to drive faster early large-board learning.

But later, it is not surprising that playing well on small boards might detract from large-board play, likely due to limited neural net capacity. Although KataGo shows that this is no impediment to reaching pro-level and beyond with just a single set of weights, if strictly optimizing for maximal strength one might imagine separate training runs for specific important sizes (e.g. 19x19, 13x13), along with a more general run using our trick with shared weights and masking to simultaneously handle all other sizes (15x15, 17x17, even non-square boards, etc).

⁸A bot "Golaxy" developed by a Chinese research group has been seen to run on multiple board sizes, but we are not aware of anywhere they have published their methods.

4.4 Global Pooling

Another innovation in KataGo's neural net over AlphaZero and Leela Zero is the use of global pooling between convolutional layers, where at certain points a special layer aggregates per-channel information to be rebroadcast across the entire spatial extent of the board. Global pooling gives a way for the convolutional layers of the neural net to condition on global context, something that would otherwise be hard or impossible with the limited perceptual window of convolution alone.



In KataGo, given a set of C channels, a global pooling layer computes:

- The mean of each channel.

 1--对每个通道计算均值
- The mean of each channel multiplied by $\frac{1}{10}(B-B_{
 m mid})$ 2--每个通道的均值乘以1/10(B-B_mid)
- The maximum of each channel.

 3--取每个通道计算后的最大值

where $B \in [B_{\min}, B_{\max}] = [9, 19]$ is the length of the board and $B_{\min} = \frac{1}{2}(B_{\min} + B_{\max})$.

This produces a total of 3C pooled values. The reason for having both mean values and mean values scaled with board length is to allow the neural net flexibility to choose how the pooling for each channel should vary as a function of the size of the board. Subtracting $B_{\rm mid}$ improves orthogonality, and $\frac{1}{10}$ is an arbitrary reasonable scaling constant so that resulting values remain near unit scale.

然后将全局池化层用于由全局池化偏置结构中。

Global pooling layers are then used in a global pooling bias structure consisting of:

- Input tensors X (shape $B \times B \times C_X$) and G (shape $B \times B \times C_G$), followed by:
- A batch normalization layer and ReLu activation applied to G (output shape $B \times B \times C_G$).
- A global pooling layer on the result (output shape $3C_G$).
- Multiplication by a matrix of size $3C_G \times C_X$ (output shape C_X).
- Channelwise addition with X, treating the C_X different values as per-channel bias terms (output shape $B \times B \times C_X$).

这种结构被用于KataGo神经网络中两个残余块的第一个卷积层,以及策略头的第一个卷积层。它也被用于价值头,并稍作修改,以使平均集合值也能随着棋盘长度的增加而呈四边形,用于与分数有关的价值输出。

This structure is used for the first convolutional layer of two of the residual blocks in KataGo's neural net, and for the first convolution layer in the policy head. It is also used in the value head with a slight modification to allow mean pooled values to also scale quadratically with board length, for the score-related value outputs.

In section 7.2 our experiments show that global pooling provides an improvement in the later stages of training. This accords with our prior research in supervised move prediction showing neural nets with global pooling can handle global tactics like "ko" even when their convolutional receptive field alone is too small[19]. They also automatically discover other global notions such as game phase (e.g. opening vs midgame vs endgame).

More broadly, global context can be valuable for games even without explicit global interactions. For example, in a wide variety of strategy games, expert human players alter their local move preferences when winning to favor options that "simplify" the position, whereas when losing they

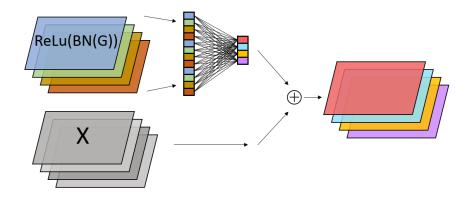


Figure 5: Global pooling bias structure, globally aggregating values of one set of channels to bias another set of channels. 全局汇集偏向结构,全局汇集一组通道的数值,以偏向另一组通道。

seek "complication". Similar emergent behavior can be observed in computer players as well. Global pooling adds representational power to convolutional nets to express these ideas.

The idea of leveraging global context is by no means novel to KataGo, or even to game-playing. In image processing for example, within the last year and a half, Hu et al. have introduced a "Squeeze-and-Excitation" architecture to achieve new results in image classification[4]. Although the details are different, the fundamental concept is the same - giving the power to convolutional layers to condition on global context. This is a capacity missing from the AlphaZero architecture.

The Squeeze-Excite architecture is in fact now being tested by other AlphaZero-related projects[18, 22, and we look forward to trying it ourselves in future research. It is possible that somewhat moreflexible Squeeze-Excite concept may make our method of global pooling redundant, or may lead to even larger and more robust improvements than the one we observed.

4.5 Other Neural Net Training Differences

In addition to the major areas above, KataGo's neural net architecture and training also differ from AlphaZero's in a number of other minor ways.

KataGo的神经网络架构和训练也不同于 AlphaZero的一些其他小方面

4.5.1 Input Features

有14个全局浮点值,表示游戏状态的属性,不与任何具体的棋盘位置相联系。

Rather than only using a raw representation of the Go board as AlphaZero does, KataGo includes a few higher-level features. The input to the neural net (consists of two tensors,) one of them a $19 \times 19 \times 22$ tensor of 22 binary spatial features, and the other a one-dimensional tensor with 14 global floating point values indicating properties of the game state not tied to any specific board location. See Tables 1 and 2 for the input features used. 由于输入特征包括游戏规则的参数,神经网络可以同时学习处理多个不同的规则集。

Since the input features include parameters for the game rules, the neural net can simultaneously learn to handle multiple different rulesets. During self-play, as explained in Appendix C, these rules and komi are randomized. The result is that unlike AlphaZero or Leela Zero. KataGo can play well

⁹In Go, usually every board point is owned by one player or the other in a finished game, so the final score difference varies in increments of 2. Therefore usually only every second point of komi "matters" depending on whether the board size is even or odd. Such a parity component is extremely hard for a neural net to learn on its own.

# Channels	Binary Spatial Feature
1	Location is on board
2	Location has {own,opponent} stone
3	Location has chain with {1,2,3} liberties
1	Illegal move due to ko/superko
5	Previous move $\{1,2,3,4,5\}$ location
3	Stone in or one move from inescapable atari $\{0,1,2\}$ turns ago ("ladder")
1	Move puts opponent in inescapable atari ("ladder")
2	Pass-alive {own,opponent}, or area surrounded by pass-alive {own,opponent} stones
4	Features used for Japanese rules only (unused in this paper)

Table 1: KataGo binary spatial input features. A *pass-alive* stone is one that cannot be captured by the opponent even if the opponent were to get unboundedly many consecutive turns.

# Channels	Global Feature
5	Previous move $\{1,2,3,4,5\}$ was a pass
1	Komi / 15.0 (from current player's perspective)
1	Simple ko rules (1.0) vs superko rules (0.0)
1	Simple ko (0.0) vs positional superko (0.5) vs situational superko (-0.5)
1	Suicide allowed (1.0) vs not allowed (0.0)
1	Komi + board size parity ⁹
4	Features used for Japanese rules only (unused in this paper)

Table 2: KataGo global input features.

under multiple possible rulesets for Go, including nonstandard values of komi. Additionally, for each $i \in \{0, 1, 2, 3, 4\}$ on each training sample independently with a probability of 2% we truncate the history at i moves. This ensures that the neural net will behave reasonably in mid-game positions where history is not known or not available, such as when the position was human-constructed for study rather than the result of earlier play.

4.6 Progressive Neural Net Sizing 新进式神经网状结构

KataGo also employs the technique of *progressive neural net sizing* used by Leela Zero to speed up the early stages of learning, when large and expensive neural nets are not necessary for improvement. Training begins with a 6-block 96-channel net, then progresses to a 10-block 128-channel net, then progresses to a 15-block 192-channel net. The last matches the size of one of Leela Zero's still most-popular neural net sizes, a size capable of reaching super-human playing strength¹⁰.

We make no attempt to transfer learned parameters between neural nets during size increases. Since training is very cheap compared to self-play, we simply choose a point to begin training the next larger neural net in parallel on the same data and then switch to the larger net once it begins to overtake the smaller net in predictive accuracy. See Table 3 for the schedule for switching.

¹⁰The next reasonable step would be 20 blocks and 256 channels, matching a basic neural net size for AlphaGoZero and/or AlphaZero, but we have not yet been able to test a run that progresses that far.

4.7 Other Training Details

与AlphaZero和Leela Zero一样,KataGo通过分批随机梯度下降的势头来训练其神经网络

Like AlphaZero and Leela Zero, KataGo trains its neural net via batched stochastic gradient descent with momentum. Momentum decay is set to 0.9, and for the runs in this paper, each size of neural net was trained with a batch size of 256 samples using a *per-sample* learning rate that varied according to the schedule:

$$\alpha_0(\lambda T+1)^{-4/3}$$

where α_0 is the initial learning rate, λ controls the time-scale on which the learning rate decays, and T is the number of training steps performed with that particular neural net, measured in training samples (i.e. batches \times 256). For all experiments in this paper, $\alpha_0 = 6\text{e-}5$, and λ was set to $10^{-6} \times \{0.1, 0.075, 0.05\}$ respectively for the three neural net sizes used.

Neural Net	Began when $T_{\text{prev}} \approx$	Overtook when $T_{\text{prev}} \approx$	Overtook when new $T \approx$
$6b\times96c$	-	-	0
10b×128c	70M	100M	20M
15b×192c	25M	100M	40M

Tprev是这个网开始训练或超越它时前一个网的训练步数

Table 3: Approximate schedule for each neural net size during KataGo's main run. \underline{T}_{prev} is the training steps for the previous net when this net began training or overtook it.

随机权重平均

KataGo also uses a form of *stochastic weight averaging*[5]. Every approximately 250,000 training samples, a snapshot of the trained weights is taken, and every approximately 1 million training samples, a new candidate neural net is produced whose weights are an exponential moving average of snapshots with decay = 0.75 (i.e. averaging 4 snapshots of lookback). Based on a gating process similar to that of AlphaZero's, described in section 6.2.4, the candidate may become the new net used for self-play.

每隔大约250,000个训练样本,就会对训练后的权重进行一次快照,而每隔大约100万个训练样本,产生一个新的候选神经网,其权重是快照的指数移动平均值,衰减=0.75(即平均4个快照的回溯)。

The data for training consists of batches drawn from a uniformly random permutation from a moving window of the last $N_{\rm window}$ samples of data. Unlike in AlphaZero or Leela Zero, $N_{\rm window}$ is not constant, but rather grows as more training samples are generated. The window initially consists of c=250,000 samples of data resulting from self-play where a random number generator is used in place of a neural net, and then grows as:

$$N_{\text{window}} = c \left(1 + \beta \frac{(N_{\text{total}}/c)^{\alpha} - 1}{\alpha} \right)$$

where N_{total} is the total number of training samples¹¹. Although appearing complicated, this is simply the polynomial curve:

$$f(n) = n^{\alpha}$$

except scaled by c and stretched so that the initial growth rate of the window is β increase in window size per sample generated. For KataGo, following some informal experimentation, we chose $\alpha = 0.75$ for slightly sublinear long-term growth and $\beta = 0.4$ for early quick turnover of data.

 $^{^{-11}}$ For the purpose of computing N_{total} , we also cap the number of initial random game samples at 250,000 even if more are generated. This makes runs slightly more consistent since it reduces dependence on timing of when the training and self-play machines are first started.

5 Search and Target Generation

Like AlphaZero and Leela Zero, KataGo uses a form of Monte-Carlo tree search (MCTS)¹²heavily biased by its neural net to generate self-play data for use in training, although a variety of the technical details differ. The result of a search in a self-play game is used to produce a training sample for the neural net.

(**MalphaZero*** The result of a search in a self-play game is used to produce a training **(**MCTS**)* *(**MCTS***)* *(**MCTS**

KataGo's search is very similar to that of AlphaZero and Leela Zero. However, there are a number of differences and minor innovations worth highlighting in how KataGo performs search and produces a training sample from the search. We will give an overview of these details and differences.

5.1 PUCT, First-play urgency

KataGo currently shares the same basic exploration formula as in the original publication of AlphaGoZero[9]. Search consists of updating a gradually-growing game tree in memory by repeated playouts. Playouts start from the root and descend down the tree at each node n choosing the child c that maximizes:

where V(c) is an estimate of the utility of c based on the average neural net evaluation of all nodes in c's subtree, P(c) is the policy prior of c from the neural net, and N(c) is the number of playouts of previously sent through child c. Upon reaching falling off the end of the tree in memory, a single new child is allocated and added to the tree, and the playout is terminated.

In the case where N(c) = 0 so that there is nothing with which to directly estimate V(c), unlike AlphaZero but modeling closely after Leela Zero, KataGo uses the value estimate of the parent node n with a reduction:

$$V(c) \approx V(n) - c_{\text{FPU}} \sqrt{\sum_{c'} I(N(c') > 0) P(c')}$$

where I(N(c') > 0) is the indicator function of whether a child c' has at least one playout and c_{FPU} is a "first-play-urgency" reduction coefficient where larger values discourage exploration.

For self-play, KataGo uses $c_{PUCT} = 1.1$ and $c_{FPU} = 0.2$ within the tree but $c_{FPU} = 0.0$ at the root. Additionally in KataGo, V(c), rather than being a direct average of neural net evaluations under child c, is instead a weighted average that slightly downweights subchildren highly unlikely to be part of the principal variation. However, the behavior difference is very small[20].

One interesting detail in AlphaZero, is that unlike KataGo, the value estimate when N(c) = 0 is set to that of a complete loss¹³. Experiments by the MiniGo project confirm that the net effect of this relative to other first-play-urgency methods was to result in deeper searches[23] with seemingly positive results on learning efficiency, agreeing with similar informal experiments by Leela Chess

¹²As a reminder, the form of MCTS used by these programs and KataGo is actually *deterministic*, except for multithreading or randomness explicitly injected via board symmetries. The search algorithm was originally developed for use with Monte-Carlo rollouts, but unlike the original AlphaGo or earlier programs, AlphaZero uses only a neural net for evaluation without random rollouts, leaving "Monte-Carlo" a misnomer that has unfortunately stuck.

Zero. Although we are eager to try it, KataGo has not had the chance to test it since the time it was clarified that this was the original method of AlphaZero.

5.2 Root Noise and Scaling

Sensible Artificial Intelligence : SAI 理性的人工智能

Like AlphaZero, to promote discovery of unexpected new moves, KataGo adds noise according to a Dirichlet distribution[8]. Additionally, KataGo makes use of an idea from the SAI project and at the root applies a small temperature to the raw policy distribution to discourage the policy from too-rapidly converging to a single possible move when the estimated difference with alternative moves is small[24]. Both the noise and temperature are both only applied at the root.

The formula used is:

$$P(c) = w_{\text{noise}} \text{ Dirichlet} \left(\alpha = \frac{A}{\# \text{ Legal Moves}(c)} \right) + (1 - w_{\text{noise}}) \frac{P_{\text{raw}}(c)^{1/T_{\text{policy}}}}{\sum_{c'} P_{\text{raw}}(c')^{1/T_{\text{policy}}}}$$

where $w_{\rm noise}=0.25,\,A=10.83=0.03*19^2$ is a constant chosen to match the AlphaZero Dirichlet noise of parameter $\alpha=0.03$ on the empty 19×19 Go board but scale smoothly with the number of moves on the board so as to generalize to smaller board sizes, and $T_{\rm policy}=1.03$ is the temperature for the policy.

温度系数T与最终模型准确率没有直接关系,

但是可以用来调节预测概率分布

什么是深度学习意义上的温度系数 https://www.quora.com/What-isthe-temperature-parameter-indeep-learning

5.3 Forced Playouts and Target Pruning 强制推演模拟和目标修剪

Like AlphaZero and Leela Zero, as KataGo uses the final root playout distribution of each search to produce the training target for the neural net's policy prediction. However, KataGo does not use the raw root playout distribution. Instead, we introduce a new method of policy target pruning to transform the playout distribution first. Additionally, we introduce a new mechanism of forced playouts in the search that combines with the Dirichlet noise to improve the quality of exploration.

In KataGo, we observed in informal tests that even if a noise move could be good, the neural net's evaluation of it might initially be negative, necessitating several additional ply to actually reveal it as good, and the Dirichlet noise alone might only ensure a very shallow search¹⁴. Therefore, for each child c of the root that has received any playouts at all, we ensure it receives a minimum number of *forced playouts* based on the noised policy and the number of playouts in all children so far:

$$n_{\text{forced}}(c) = \left(2P(c)\sum_{c'}N(c')\right)^{1/2}$$

We do this by simply setting the MCTS selection urgency PUCT(c) to infinity whenever a child of the root has fewer than this many playouts. This ensures that random moves selected by Dirichlet noise receive a minimum amount of exploration, yet in practice does not use more than a few percent of additional playouts on average.

¹³This fact is ambiguous in DeepMind's published papers due to ambiguity about whether a [-1,1] or [0,1] scale was used, and was only clarified much later by an individual researcher in a forum post here: http://talkchess.com/forum3/viewtopic.php?f=2&t=69175&start=70#p781765

¹⁴In AlphaZero, this issue might be partly mitigated due to the deeper searches resulting from the "first-play-urgency = loss" detail discussed earlier.



Figure 6: Left: policy prediction. Right: log of policy prediction. Ranking among even very-low-probability moves shows a clear gradient of likely move value, possibly a result of target pruning, although we have not compared to training without target pruning. Probability difference between center (orange, 2e-4) and upper right (faint red, 1e-5) is roughly a factor of 20.

However, the vast majority of the time, noise moves will be very bad moves 15 . To avoid contaminating the policy training target with the extra playouts on these bad moves, we perform a target pruning step that subtracts playouts that the search would not have chosen on its own given the final utility estimate for all children. In particular, we identify the child c^* with the most playouts, and then for each other child, we subtract up to n_{forced} many playouts from it so long as subtracting a playout does not cause $\text{PUCT}(c) >= \text{PUCT}(c^*)$ holding constant the final utility estimate for both. Additionally, we outright prune children that are reduced to only a single playout.

Target pruning can also prune some playouts that are chosen by the search naturally! This can happen when playouts discover a child is worse than expected and a different child is proven to be much better, such that if the search had known the *final* estimated values of all children to begin with, the PUCT formula would never have originally invested playouts in the worse child. By forcing playouts and target pruning, we increase exploration in KataGo while keeping the policy training clean.

5.4 Score Maximization

Another feature of KataGo is that unlike AlphaZero or Leela Zero, KataGo puts nonzero utility on maximizing (a dynamically-determined monotone function of) the score difference.

Letting x be the final score difference of a game, in addition to the utility for losing versus winning:

$$u_{\rm win}(x) = {\rm sign}(x) \in \{-1, 1\}$$

¹⁵Even if a low percent of the policy target mass, this can disrupt the *relative* ordering of low-prior moves, which can be relevant when a search "goes wide" due to promising moves turning out poorly or due to long search times.

We also define the score utility:

$$u_{\text{score}}(x) = c_{\text{score}} f\left(\frac{x - x_0}{B}\right)$$

where c_{score} is a parameter controlling the relative importance of maximizing score, x_0 is a parameter for centering the utility curve, $B \in [9, 19]$ is the length of the board and $f : \mathbb{R} \to (-1, 1)$ is the function:

 $f(x) = \frac{2}{\pi}\arctan(x)$

At the start of each search, the utility is re-centered by setting x_0 to the mean $\hat{\mu}_s$ of the neural net's predicted score distribution at the root node. The search proceeds with the aim to maximize the sum of u_{win} and u_{score} instead of only u_{win} . Estimates of u_{win} are obtained using the game outcome value prediction of the net as usual, and estimates of u_{score} are obtained by querying the neural net for the mean and variance $\hat{\mu}_s$ and $\hat{\sigma}_s^2$ of its predicted score distribution, and computing:

$$E(u_{\text{score}}) \approx \int_{-\infty}^{\infty} u_{\text{score}}(x) N(x, \hat{\mu}_s, \hat{\sigma}_s^2) dx$$

where the integral on the right is estimated quickly by interpolation in a precomputed lookup table. The sum of estimated utilities, averaged across nodes by MCTS, forms the signed value V(c) for the PUCT formula in section 5.1.

Since similar to a sigmoid f saturates far from 0, this provides an incentive for improving the score in simple and likely ways near x_0 without awarding overly large amounts of expected utility for pursuing unlikely but large gains in score or shying away from unlikely but large losses in score. For the experiments in this paper, we set c_{score} initially to 0.5, then anneal it to 0.4 and then 0.3 at the same times as we also anneal the number of playouts upward (see section 6.1 below).

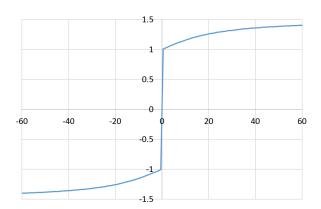


Figure 7: Total utility as a function of score difference, when $x_0 = 0$ and B = 19 and $c_{\text{score}} = 0.5$.

There are several motivations for maximizing score:

• Putting some utility on score should reduce variance in the ownership target for training. Without it for example, sometimes the bot will be indifferent to losing a territory that would not affect the game result, even if preventing the loss would be trivial and those points "should" be safe.

- Maximizing score might ensure a sharper and more consistent policy training target. If a player is strongly winning or losing, u_{win} may no longer meaningfully distinguish between different moves. However, moves that maximize score are highly likely to still be good moves if the game were closer. Score maximization ensures that the policy target remains sharp and continues to give useful data.
- Maximizing score is more useful for human study and play. Humans often find it valuable
 to study and learn the sharpest lines of play even when from a bot's perspective the game's
 outcome is no longer in doubt.

In our experiments in section 7.2, we find evidence that score maximization during self-play does provide a sharpening of the policy target, although its effect on ownership was less clear. Overall, it clearly improves the efficiency of learning.

5.5 Tree Reuse ^{重复使用搜索树}

Unlike AlphaZero or Leela Zero, KataGo deliberately does *not* preserve the search tree between turns during self-play, instead rebuilding it from scratch every turn.

We know of three common approaches for self-play data generation:

- Reuse the search tree between turns, always adding a fixed number of additional playouts to the tree, referred to as a *playout cap* (used by AlphaZero¹⁶).
- Reuse the search tree between turns, always searching until the tree reaches a certain total size, referred to as a *visit cap* (used by Leela Zero, at least for most of its computational lifetime¹⁷).
- Discard the search tree before each turn, searching until the tree reaches a certain total size (KataGo's and possibly some other projects' approach).

Holding computational cost per game constant, the first approach tends to spend more time adding playouts during game sequences that are highly forced or predictable. This results in larger searches on average, since more playouts are spent precisely sequences in which tree reuse is higher. However, compared to the second approach, it results in significantly smaller searches when moves have been less predictable or well-understood by the neural net, where the marginal playout might be more beneficial for improving the policy.

Unfortunately, the second approach has the possible disadvantage that on turns where almost all the tree is reused, there will be too few playouts remaining to properly explore moves upweighted by the Dirichlet noise, since the noise is only applied once a node becomes the root node.

The third approach, taken by KataGo, avoids this disadvantage, ensuring that the full number of playouts is always available to spend exploring noised moves. All neural net evaluations are cached in a large hash table, so rebuilding parts of the game tree that were explored on previous turns only costs some CPU time, which is quite minor given that the search is generally GPU-bound.

¹⁶To our knowledge, this detail of AlphaZero is not explicitly clarified in any of DeepMind's official publications, but was explained by an individual engineer here: http://talkchess.com/forum3/viewtopic.php?p=782297#p782297

¹⁷See discussion at: https://github.com/leela-zero/leela-zero/issues/1416

6 Self-play

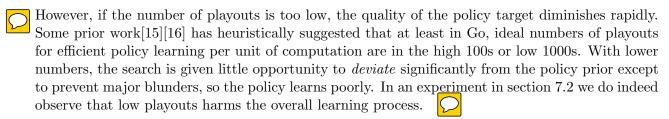
In this section, we describe the high-level process of self-play, including the initialization, randomization, and termination of individual games. KataGo introduces the major innovation of *playout* or visit cap oscillation, as well as differing in several minor ways as well.

6.1 Playout Cap Oscillation 模拟游戏轮数上限波动 (也就是上限值是个变化值)

卡塔围棋的主要创新之一是随机减少下棋次数或花在不同回合的访问次数,以扩大价值头的训练数据量。

One of the major innovations in KataGo is to randomly reduce the number of playouts or visits spent on different turns to expand the amount of training data for the value head.

The game outcome value target is relatively data-starved even with the regularization of the owner-ship and score targets, since all of these targets receive only one new unique sample per entire game. For improving the value prediction of the net, it would be likely beneficial to reduce the number of playouts used per turn to generate more independent data samples per amount of computation, even if the quality of those samples would be slightly worse¹⁸.



As a result, there is significant tension between the ideal number of playouts for policy training and for value training. In KataGo, we mitigate this tension through the technique of *visit cap* oscillation or playout cap oscillation, where the full number of playouts N is only used for a small proportion p of turns, and for all other turns a much smaller number of playouts n < N is used. Only turns that use N playouts are recorded for training. On turns with only n, we also do not clear the search tree and we treat n as a visit cap, moving immediately if the tree already has size >= n. Since these turns are not used for training, we also disable Dirichlet noise and forced playouts and use $c_{\text{FPU}} = 0.2$, maximizing playing strength.

For the runs in this paper, we choose p = 0.25 and (N, n) = (600, 100) early in training, annealing up to (900, 150) and then (1200, 200) later in training at about 90 million and 130 million self-play data samples generated, respectively, corresponding to about 1.4 million and 2.1 million games.

Holding computation fixed, this helps because most moves are played spending only n or fewer new playouts, so many more games are played, obtaining many more independent value training samples. However, since n is small, the majority of the computation is still on turns using N playouts, so the drop in the number of good policy training targets is not large.

The ablation studies presented in section 7.2 indicate that the net benefit of playout oscillation is large. Holding computational cost constant, in our runs it noticeably improves the efficiency of the overall self-play process.

¹⁸For a point of intuition about how high playouts might be less important for the value head, the first AlphaGo paper[7] showed that even a *single* playout per turn (i.e. directly using a policy net), was still sufficient to create data of enough quality to train a value net strong enough to defeat professional human players with the aid of search!

6.2 Other Self-play Differences

In addition to the major difference above, KataGo's self-play parameters also differ from AlphaZero in a number of other minor ways.

6.2.1 Reducing Playouts Instead of Resignation

Unlike AlphaZero or Leela Zero, KataGo does not terminate games early via resignation during self-play.

Instead, in the case of extreme winning chances, KataGo reduces the number of visits used in the search. During self-play, if both sides agree that for the last 5 turns, the worst MCTS winrate estimate p for the losing side has been less than 5%, then the number of visits is capped to $\lambda n + (1 - \lambda)N$ where n and N are the small and large limits used in visit cap oscillation and $\lambda = p/0.05$ is the proportion of the way that p is from 5% to 0%. Additionally, the training positions are recorded with only $0.1 + 0.9 * \lambda$ weight, downweighting training samples where the original AlphaZero process would have already resigned.

Playing out the full game allows the final determination of the ownership of all areas and the final score difference for training the auxiliary targets. Additionally, avoiding resignation also reduces the number of positions that are incorrectly recorded, improving the quality of the data.

6.2.2 Game Variety and Exploration 游戏的多样性与探索

KataGo also differs slightly from AlphaZero and Leela Zero in the ways that it introduces entropy into self-play to encourage variety. Firstly, a wide variety of minor randomizations are applied to ensure a diversity of data with different rule sets and values of komi, as well as handicap games. See Appendix C for details.

KataGo also borrows the technique of branching the game to try an alternative line of play from the SAI project. In the SAI training process, this was primarily used to obtain data about the score values of positions by varying komi between branches[6], but here we adapt it instead as an aid for exploration. KataGo uses two branching mechanisms to ensure the neural net (1) has some experience in refuting unusual or bad moves, and (2) learns how to play openings resulting from unusual early opening moves:

- 1. In 2.5% of positions, the game is temporarily branched to try an alternative move drawn randomly from the raw policy of the net 70% of the time with temperature 1, 25% of the time with temperature 2, and otherwise with temperature infinity. A full search is performed to produce a policy training sample (the *MCTS* search winrate is used for the game outcome target and the score and ownership targets are left unconstrained). This ensures that there is a small percentage of training data on how to respond to or refute moves that a full search might not play. Recursively, a random quarter of these branches are continued for an additional move, otherwise they are terminated.
- 2. In 5% of games, the game is permanently branched after the first r turns where r is drawn from an exponential distribution with mean $0.025 * B^2$. Between 3 and 10 moves are chosen

卡塔围棋还与AlphaZero和Leela Zero略有不同,它将熵引入自我游戏,以鼓励多样性。首先,各种小的 随机化被应用,以确保不同的规则集和Komi值的数据的多样性,以及残局。

KataGo还借用了SAI项目中的分支对局技术来尝试另一种下法。在SAI的训练过程中,这主要是用来通过改变分支之间的komi来获得有关位置得分值的数据[6],但在这里我们将其改编为探索的辅助工 具。KataGo使用两个分支机制来确保神经网络(1)在反驳不寻常或不好的棋步方面有一些经验,以及(2) 学习如何下由不寻常的早期开局棋所产生的开局。

在2:5%的位置上,游戏被临时分支,以尝试从网的原始策略中随机抽出的替代棋步,其中70%的时间温度为1,25%的时间温度为2,否则温度为无。进行全面搜索以产生一个策略训练样本(MCTS搜索胜率被用于游戏结果目标,分数和所有权目标不受限制)。这确保了有一小部分关于如何应对或反驳全面搜索可能无法发挥的棋的训练数据。递归地,这些分支中的随机四分之一会继续进行额外的棋步,否则会被终止。

2. 在5%的游戏中,游戏在最初的r轮之后被永久地分支,其中r是从平均为0:025的指数分布中抽取的B2。统一随机地选择3到10步棋,每步棋都有一个神经网络评估,并下出神经网络最喜欢的棋。通过迭代查询神经网络的得分差异,然后将其添加到Komi中,调整Komi以补偿该棋的不利之处。然后,对局就会正常进行到结束。这确保总有一小部分棋局有不寻常的开局或定式,例如涉及5-4点的开局或基于中心的开局。

由于备用棋步往往是坏棋,分支对局可以偶尔探索这些棋步,而不会用受坏棋影响的对局结果来污染 价值训练目标,因为在分支点之前的所有位置仍然是针对原始博弈结果进行训练的。 uniformly at random, each given a single neural net evaluation, and the favorite by the neural net is played. Komi is adjusted to compensate the disadvantage of that move by iteratively querying the neural net for the score difference then adding it to komi. The game is then played to completion as normal. This ensures that there is always a small percentage of games with unusual openings or joseki, for example openings involving the 5-4 points or center-based openings.

Since alternate moves are often bad moves, branching the game enables occasionally exploring them without contaminating the value training targets with a game result affected by the bad move, since all positions prior to the branch point are still trained towards the original game result.

6.2.3 Minor Endgame Optimizations 小规模终局优化

KataGo also performs a few Go-specific optimizations to speed up play.

In Go, define a group of stones to be *pass-alive* if none of those stones can be captured by the opponent even if the opponent gets unboundedly many consecutive moves. This can be determined efficiently by Benson's algorithm [1]¹⁹. Furthermore, for each player $p \in \{Black, White\}$, define a maximal connected non-p region (possibly including stones of p's opponent) to be *pass-alive-territory* for p if the region is bordered by p and only p, and all bordering groups are pass-alive, and all but zero or one points of the region are adjacent to a bordering group.

Both AlphaZero and Leela Zero both only use the Tromp-Taylor rules for self-play learning in Go²⁰. In KataGo in addition to randomizing other aspects of the rules, we also deviate from the Tromp-Taylor rules for scoring in which, informally, all stones are considered "alive" if left at the end of the game. We use an alternative scoring rule under which any pass-alive-territory belongs to that player even if it contains dead opponent stones, allowing the player to omit the moves to capture those dead stones.

Under these scoring rules it is easy to prove that if every region of the board is pass-alive or passalive-territory for at least one player, optimal play consists of both players passing and ending the game. So under these rules as a provably-safe optimization in such a case, we immediately terminate the game.

Additionally, we add two minor heuristic optimizations: firstly, if the opponent has passed at least four times in a row, we prohibit moves in either player's pass-alive territory. Secondly, we add a tiny bias at the root of search against moves in areas that the ownership prediction of the net indicates that the opponent almost certainly owns, or that the current player almost certainly owns unless filling opponent liberties or connecting non-pass-alive groups. The bias is smaller than any in-game score increment so as to only introduce a preference when the bot otherwise considers moves equal. These heuristic optimizations mildly speed up the end of the game.

¹⁹See also: https://en.wikipedia.org/wiki/Benson%27s_algorithm_(Go)

²⁰No humans in practice use Tromp-Taylor rules, but they are computer-friendly for self-play and close enough to other rules that with minor hacks bots trained with them can be adapted for practical use. See: https://senseis.xmp.net/?TrompTaylorRules

与某些版本的AlphaZero和Leela Zero一样,KataGo执行门控。训练中的新候选神经网络首先要与当前用于自我游戏的网络进行测试,以确保新的候选神经网络在取代当前网络之前不会比它差很多。 KataGo的门槛相当低,以尽量减少延迟和开销。候选网络必须在与当前网络的200场比赛中至少赢得100场,才能被接受为自我比赛的新网络。使用300次访问(搜索直到树的大小为300),退火到400和500,同时自我发挥的访问也向上退火。此外,各种自我发挥的设置增加的探索被禁用,以最大限度地发挥强度。详见附录D。

6.2.4 Gating

Like some versions of AlphaZero and like Leela Zero, KataGo performs gating. New candidate neural nets from training are first tested against the current net being used for self-play to ensure that the new candidate is likely not much worse than the current net before replacing it.

KataGo's gating is fairly light so as to minimize latency and overhead. Candidate nets must win at least 100 out of 200 total games against the current net to be accepted as the new net for self-play. A fixed 300 visits are used (searching until the tree is size 300), annealing up to 400 and 500 at the same time as self-play visits are annealed upwards. Additionally, a variety of the self-play settings adding exploration are disabled in order to maximize playing strength. See Appendix D for details.

7 Experiments And Results

7.1 Testing Versus Leela Zero

KataGo's primary run took approximately one week, using $16 \times V100$ GPUs²¹ for self-play²², $2 \times V100$ for gating games, and $1 \times V100$ for training, and an additional $1 \times V100$ when a larger net was being concurrently trained to eventually overtake the smaller. We also increased the number of GPUs for self-play to $24 \times V100$ and to $32 \times V100$ at the time of annealing up to 900 and 1200 visits, respectively. The final 15-block neural net size was trained for about 270 million data samples, by which point about 160 million data samples had been generated from 2.5 million self-play games.

We then tested this run against Leela Zero:

- We sampled every fifth Leela Zero neural net from LZ30 up through LZ150, as well as LZ157 which is Leela Zero's strongest 15-block neural net prior to transitioning to larger sizes²³. This roughly matches KataGo's largest neural net size. We also sampled KataGo's neural net over the course of its main run.
- Between every pair of Leela Zero nets less than 35 versions apart, we played approximately 120 games to establish approximate relative strengths of the Leela Zero nets as a benchmark.
- For each KataGo net, we played batches of games versus random Leela Zero nets choosing them with probability roughly proportional to the predicted variance p(1-p) of the game result. The winning chance p was estimated from the Bayesian maximum likelihood Elo^{24} based on all game results between all versions so far. This ensured that most games would be with Leela Zero nets close in strength, but with plenty of variety.

Games were played on a 19x19 board with a fixed 7.5 komi under Tromp-Taylor rules, with a fixed 800 visits and time management disabled and resignation enabled at a threshold of 2% winrate. KataGo's score maximization utility was set to 0.25. To ensure additional game variety, both

 $^{^{21}}$ Nvidia Tesla V100 GPU

²²Playing roughly 3200 games in parallel (200 per GPU) to take advantage of batching of neural net queries.

²³On strong consumer hardware, LZ30 might be beginner level, LZ50 weak/mid club player level, LZ80 experienced amateur level, LZ110 pro strength, and LZ130 either strong pro strength or a little beyond.

²⁴We used a custom-implemented slight variant of https://www.remi-coulom.fr/Bayesian-Elo/

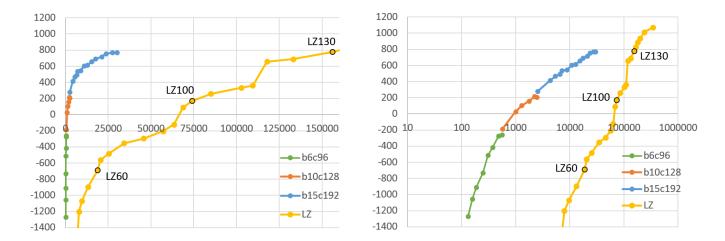


Figure 8: Relative 800-visit Elo strength of KataGo's main run's three net sizes (b6c96, b10c128, b15c192) vs. Leela Zero versions up through LZ157. X-axis is the cumulative self-play cost in millions of equivalent 20 block x 256 channel neural net queries, Y-axis is relative Elo. For Leela Zero, we ignored ELF games in computing cost. Left: linear scale. Right: log scale.

KataGo and Leela Zero were set to additionally randomize early in the game, Leela Zero with a temperature of 0.3 in the first 30 turns²⁵, and KataGo with a temperature of 0.3 decaying to 0.0 with a 30-turn halflife. Maximum-likelihood relative Elo ratings were computed using the final set of approximately 50000 games.

For both KataGo and Leela Zero, we estimated the cumulative self-play computation by crudely assuming that the evaluation of a neural net with b blocks and c channels has cost proportional to bc^2 and multiplying by number of neural net evaluations (assuming games are played in parallel so that batching reduces GPU overhead of small nets)²⁶. For KataGo we simply counted the neural net evaluations. For Leela Zero we estimated it by scanning the public training data and multiplying the number of rows by the known number of playouts or visits used at that time, discounting by 20% as a rough estimate of neural net caching for transpositions. For tree reuse by Leela Zero, we conservatively assumed 100% reuse of all visits in the top move summed across training rows and we did not attempt to estimate the cost of ELF games generated by Leela Zero²⁷.

Shown in Figure 8 is the result of plotting Elo ratings versus estimated computation for both. As is shown, the combined effect of KataGo's techniques results in much faster learning. The reduction in computation required is close to a factor of 100(!) for the early parts of the process, and still a factor of about 5 at the furthest point we were able to progress KataGo's main run, just below the strength of LZ130, Leela Zero's 131st neural net. We also ran an additional 500 games using 6400 visits per turn between KataGo's final net and LZ130, achieving 226/500 wins (45%) and confirming a strength slightly below but near LZ130 at larger numbers of visits as well.

²⁵For reference, the command line used for Leela Zero: ./leelaz --gtp --weights WEIGHTS.gz --threads 1 --visits 800 --resignpct 2 --noponder --timemanage off --randoment 30 --randomemp 0.3 --log lz.log ²⁶Since for a given number of blocks and channels our neural nets are very close in computational cost to Leela Zero nets, this metric was chosen as a very rough way to normalize out hardware and implementation differences.

²⁷Based on informal chat with some Leela Zero developers, starting around LZ132 the Leela Zero project also began using training data generated by the then-much-larger-and-stronger ELFv0 neural net from Facebook AI. In addition to possibly causing LZ132-LZ157 to be stronger than a 15-block net might achieve alone, we did *not* attempt to count the cost of this additional data.

Bot	Self-play 20b×256c Evals Used	Games	Elo	On good hardware, likely
Leela Zero LZ30	5800M	1.2M	-2307	Beginner
Leela Zero LZ80	46000M	4.0M	-295	Strong Club Player
Leela Zero LZ105	85000M	5.3M	259	Top Amateur
Leela Zero LZ130	157000M	7.1M	774	>= Strong Pro
Leela Zero LZ157	346000M	8.7M	1073	Superhuman
KataGo	562M	0.4M	-260	Strong Club Player
KataGo	2466M	1.0M	206	Top Amateur
KataGo	7111M	1.4M	534	Professional
KataGo	30000M	2.5M	767	>= Strong Pro

Table 4: Selected neural net versions from Leela Zero and from KataGo's main run, comparing the amount of self-play computation measured in equivalent 20 block x 256 channel neural net queries, again ignoring ELF games, against measured Elo ratings versus Leela Zero with 800 visits.

We did experience some diminishing returns near the end of KataGo's run, as is seen on the log-scale plot of Figure 8. It is certainly possible in longer runs that certain techniques would need to be adjusted to ensure maximal final strength. For example, perhaps playout or visit cap oscillation could need to be removed when fine-tuning near the end of a longer run for maximal-strength self-play. Alternatively, it is possible that auxiliary targets may consume a small part of the neural net's capacity, and reducing their weight later in training would improve strength by freeing some capacity for other targets. We did not test this. Our ablation runs in the next section also suggest that if strength only on 19x19 boards is desired, specializing to that size would also improve strength yet further.

7.2 Ablation Runs

We ran a variety of shorter ablation runs removing various major components and techniques presented in this paper to study the effect of their removal:

- NoAux Removes the ownership, score, and opponent policy auxiliary training targets. Also removes score maximization behavior, since the neural net can no longer predict score.
- NoPAux Removes the opponent policy auxiliary training target only.
- NoScore Removes score maximization behavior only.
- NoOsc600a Removes playout/visit oscillation, using a fixed 600 visits.
- NoOsc600b Removes playout/visit oscillation, using a fixed 600 visits, and doubles the training window size.
- NoOsc200 Removes playout/visit oscillation and reduces visits to a fixed 200 visits.
- NoGPool Removes global pooling from residual blocks. Removes global pooling from the policy head *except* for computing the "pass" output, as KataGo's policy head is otherwise fully convolutional, leaving no other way to compute the pass output. Pooling is *not* removed from the value head.

- NoGoFeat Removes all higher-level Go input features, including liberties, inescapable atari, pass-alive area, parity. Leaves only on-board, stones, illegal-ko location, history, and features indicating the rules. Also removes the Go-specific minor heuristics from section 6.2.3 involving passing and the tiny utility bias.
- NoSmall Removes training on small boards, self-play and gating only occur on 19x19 boards.

To evaluate these runs, we sampled neural nets from all of these runs together along with KataGo's main run. Then, as with testing against Leela Zero, we repeatedly iterated through all sampled versions playing games on 19x19 with a fixed 7.5 komi using 800 visits against random opponents proportionally to the variance p(1-p) of the game result. Again p was determined based on a maximum-likelihood Elo model all game results so far. Games were played in batches for GPU-efficiency. Maximum-likelihood relative Elo ratings were computed using the final set of approximately 76000 games (note that resulting Elos are not directly comparable with the Elos versus Leela Zero in section 7.1).

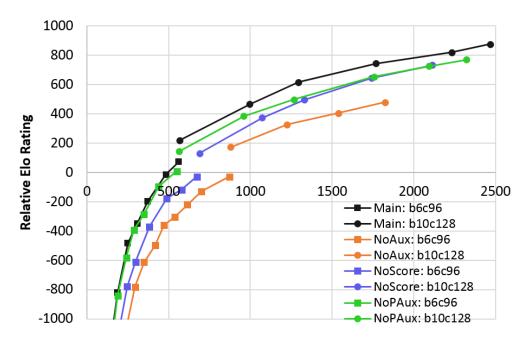


Figure 9: KataGo's main run versus NoAux and NoPAux and NoScore. X-axis is the cumulative self-play cost in millions of equivalent 20 block x 256 channel neural net queries.

As shown in Figure 9, removing auxiliary training targets and score maximization resulted in a noticeable drop in learning efficiency, confirming that at least up to the expert amateur level of the 10-block 128-channel neural net, the targets provide useful regularization. Removing the auxiliary policy target alone also harmed learning, indicating its usefulness separately from the other targets. And removing score maximization behavior alone also harmed learning. Figure 10 shows that its removal significantly increased the average entropy of the policy training target distribution, consistent with one of our original motivations for score maximization as a way to keep the policy target sharp and informative. Its effect on the ownership target was less clear.

As shown in Figure 11, removing playout oscillation resulted in a massive drop in learning efficiency. Since KataGo's current hyperparameters are adapted to the data generation rate expected from

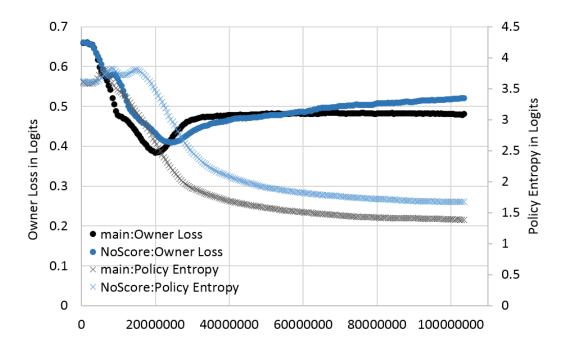


Figure 10: Training ownership loss and entropy of the policy target distribution, over the course of training the 6-block 96-channel neural net for main and NoScore runs. X-axis is the number of training samples.

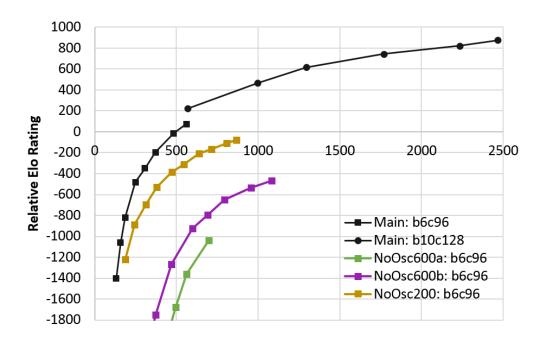


Figure 11: KataGo's main run versus NoOsc runs. X-axis is the cumulative self-play cost in millions of equivalent 20 block x 256 channel neural net queries.

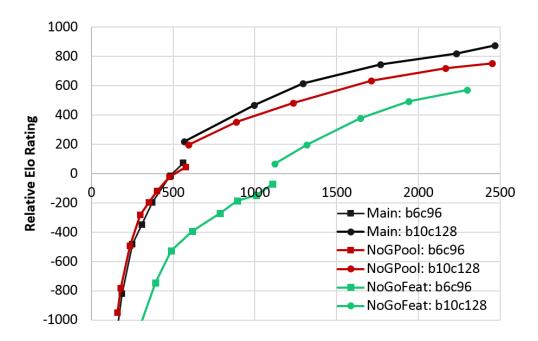


Figure 12: KataGo's main run versus NoGPool and NoGoFeat. X-axis is the cumulative self-play cost in millions of equivalent 20 block x 256 channel neural net queries.

oscillation, likely this drop could be reduced by hyperparameter re-tuning (indeed, doubling the training window mitigated a fraction of the drop by compensating for the reduced amount of value data). However, the magnitude of the drop and the fact that oscillation outperformed both a small (200) and larger (600) fixed number of visits is evidence that the technique is beneficial, at least this early in training.

The removal of global pooling shown in Figure 12 was interesting. Removal actually accelerated the earliest parts of learning but resulted in a longer-term lag. The long-term lag makes sense since at strong levels, distinguishing board sizes and other global context should be valuable. But perhaps global context is not relevant when play is still weak, or perhaps it hampers early learning by making it easy for the neural net to distinguish between board sizes, reducing transfer of learning from smaller boards. More tests would be needed to investigate this or other hypotheses.

Also in the same Figure 12, we show the result of removing higher-level features in KataGo that are arguably less in the spirit of "learning from zero", namely the Go-specific input features and some of the minor optimizations. Unsurprisingly, we observe a large drop in training efficiency, but far less than the total speedup obtained. Alongside the other ablation studies, this clearly indicates the value of the other improvements beyond merely specialized Go-specific input features and heuristics.

Lastly, we find in Figure 13 training only on 19x19 boards instead slightly slows early learning but achieves a slightly higher strength on 19x19, growing more over time (all testing games for measuring Elo were played only on 19x19). The fact that learning is slightly slower early and the final gain is gradual indicates that there is much shared learning between board sizes, since in KataGo's main run while 19x19 is upweighted to be a common size it is not even a majority of the data. It also suggests that at the cost of specializing to only 19x19, if desired we could also reach somewhat higher strengths than KataGo's main run did in the same amount of compute.

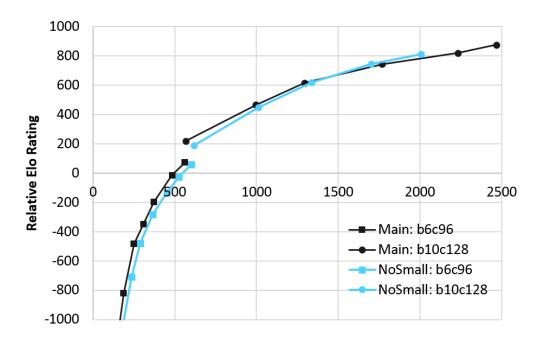


Figure 13: KataGo's main run versus NoSmall. X-axis is the cumulative cost self-play in millions of equivalent 20 block x 256 channel neural net queries.

8 Conclusions And Future Work

In this paper, we introduced a variety of techniques and methods for improving self-play learning in Go, demonstrating a gap between basic AlphaZero-like training and what could be possible with better methods. Our bot KataGo, up to the point we were able to test, achieves a substantial improvement in learning efficiency of more than 5x over the open-source Leela Zero in reaching a strong level of play, and can handle multiple board sizes and rulesets with a single set of learned weights. The speedup in the very earliest stages is even greater, such that with our released code, training a full 19x19 Go bot from zero up to at least moderate amateur strength may now be within the reach of individual consumer hardware!

However, we were unable to yet test these techniques in runs up to the full length of AlphaZero or of later replications such as that of Leela Zero's full run or Elf OpenGo. It is possible that some of the techniques presented will need to be adjusted when fine-tuning strength in a longer run, and future experimentation down those lines would be interesting and exciting. Moreover as we have discussed, many could have application to other games or to other broader problems in reinforcement learning. It is our hope that by presenting these ideas and their effective use so far in KataGo, we lay some groundwork for future research.

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以下是对KataGo的神经网结构的详细分解。 神经网的输入由两个张量组成。第一个大小为B*B*Cspatial,其中B是棋盘的大小,Cspatial=22是空间输入通道的数量。第二个是一个长度为Cglobal的向量,其中Cglobal=14是全局输入通道的数量,其条目是整个游戏状态的属性,而不是棋盘上的特定位置。 神经网由一个主干组成,上面连接着多个头,每个头为不同的目的产生不同的输出。所有头的价值相关预测都是从当前玩家的角度出发。·

Appendix A Neural Net Architecture

残差卷积神经网络——其中的策略和价值网络被用于评估棋局,以进行下一步落子位置的先验概率估算。

The following is a detailed breakdown of KataGo's neural net architecture. ²⁸

The input to the neural net consists of two tensors. The first is size $B \times B \times C_{\text{spatial}}$ where B is the size of the board and $C_{\text{spatial}} = 22$ is the number of spatial input channels. The second is a vector of length C_{global} where $C_{\text{global}} = 14$ is the number of global input channels, whose entries are properties of the whole game state rather than of specific locations on the board.

The neural net consists of a main trunk, upon which multiple heads are attached, each head producing a different output for a different purpose. All value-related predictions by all heads are from the perspective of the current player.

The trunk consists of:

对空间输入张量进行5x5卷积,输出C通道,同时对全局输入张量进行矩阵乘法,输出C通 道。

通道加法,其中来自转换后的全局输入的C通道被作为偏置添加到5x5卷积的C通道上。

输入主干网络 前的初步数据 处理

正常的残差卷积

- A 5x5 convolution of the spatial input tensor outputting C channels, and in parallel, a matrix multiplication of the global input tensor outputting C channels.
- A channelwise addition where the C channels from the transformed global input are added as biases to the C channels of the 5x5 convolution.
- - A batch-normalization layer.
 - A ReLu activation function.
 - A 3x3 convolution outputting C channels.
 - A batch-normalization layer.
 - A ReLu activation function.
 - A 3x3 convolution outputting C channels.
 - A skip connection from the start of the block that is added elementwise with the result.
- 全局池化-残差卷积 The remaining two blocks (positioned about halfway and three-quarters-way deep in the stack) consist of the following in order:

 剩下的两个区块(位于堆栈中大约一半和四分之三深的位置)
 - A batch-normalization layer.
 - A ReLu activation function.
 - A 3x3 convolution outputting C channels.
 - A global pooling bias structure (described below) that globally pools C_{pool} of the channels to bias the other $C C_{\text{pool}}$ channels.
 - A batch-normalization layer.
 - A ReLu activation function.
 - A 3x3 convolution outputting C channels.
 - A skip connection from the start of the block that is added elementwise with the result.

²⁸In the source code, there is an additional output head not described here that was used to support a regularization term for Japanese rules, but both it and Japanese rules were unused for the experiments in this paper.

数据经过主干 神经网络block块 区域后处理

- At the end of the stack of blocks, a batch-normalization layer.
- A ReLu activation function.

The policy head consists of: policy head: 策略网路 head:头,脑袋 策略大脑、策略网路

从主干网络一分为2 分出一个策略头、 一个价值网络头

• A global pooling bias structure (described below) that globally pools the output of G to bias the output of P. —个全局汇集偏置结构(如下所述),全局汇集G的输出来偏向P的输出。

• A batch-normalization layer.

global pooling "就是pooling的滑窗size 和整张feature map的size一样大。这样,每个W×H×CWtimes H\times CW×H×C的feature map输入就会被转化为1×1×C1\times 1\times C1×1×C输出。因此,其实也等同于每个位置权重都为1/(W×H)1/(W×H)1/(W\times H)1/(W×H)的FC层操作。

- A ReLu activation function.
- A 1x1 convolution with 2 channels, outputting two policy distributions in logits over moves on each of the locations of the board. The first channel is the predicted policy $\hat{\pi}$ for the current player. The second channel is the predicted policy $\hat{\pi}_{opp}$ for the opposing player on the subsequent turn.
- In parallel, a matrix multiplication of the globally pooled values of G outputting 2 values, which are the logits for the two policy distributions for making the pass move for $\hat{\pi}$ and $\hat{\pi}_{\text{opp}}$, as the pass move is not associated with any board location.

同时,对G的全局集合值进行矩阵乘法,输出2个值,这是为pi和pi_opp做跳过一手棋的两个政策分布的对数,因为跳过一手棋不与任何棋盘位置相关。

The value head consists of: value head:价值网路 head:头,脑袋 价值评估大脑、评估网路

- A 1x1 convolution outputting C_{head1} channels ("V").
- A global pooling layer (described below) of V outputting $3C_{\text{head1}}$ values (" V_{pooled} ").

• A game-outcome subhead consisting of:

价值头下面又分成² 多个子级的评估网络

头

- A fully-connected layer from V_{pooled} including bias terms outputting C_{head2} values.
- A ReLu activation function.
- A fully-connected layer from V_{pooled} including bias terms outputting 9 values.
 - * The first 3 values are a distribution in logits whose softmax \hat{z} predicts among the three possible game outcomes win, loss, and no result (the latter being possible under non-superko rulesets in case of long-cycles).
 - * The fourth value is multiplied by 20 to produce a prediction $\hat{\mu}_s$ of the final score difference of the game in points²⁹.
 - * The fifth value has a softplus activation applied and is then multiplied by 20 to produce an estimate $\hat{\sigma}_s$ of the standard deviation of the predicted final score difference in points.
 - * The sixth through ninth values have a softplus activation applied are predictions \hat{rv}_i of the expected variance in the MCTS root value for different numbers of playouts³⁰.
 - * All predictions are from the perspective of the current player.

- An ownership head consisting of:
 - A 1x1 convolution of V outputting 1 channel.
 - A tanh activation function.
 - The result is a prediction \hat{o} of the expected ownership of each location on the board, where 1 indicates ownership by the current player and -1 indicates ownership by the opponent. 其结果是对棋盘上每个位置的预期所有权进行预测^o。 其中,1表示当前玩家的所有权,-1表示对手的所有权。
- A final-score-distribution subhead consisting of:

最终分数分布的子网路

- A scaling component:
 - * A fully-connected layer from V_{pooled} including bias terms outputting C_{head2} values.
 - * A ReLu activation function.
 - * A fully-connected layer including bias terms outputting 1 value (" γ ").
- For each possible final score value s:

$$s \in [-S + 0.5, -S + 1.5, \dots, -1.5, -0.5, 0.5, 1.5, \dots, S - 1.5, S - 0.5]$$

where S is a an upper bound for the plausible final score difference of any game³¹, in parallel:

* The $3C_{\text{head1}}$ values from V_{pooled} are concatenated with two additional values:

$$(0.05 * s, Parity(s) - 0.5)$$

0.05 is an arbitrary reasonable scaling factor so that these values vary closer to unit scale. Parity(s) is the binary indicator of whether a score value is normally possible or not due to parity of the board size and komi³².

- * A fully-connected layer (sharing weights across all s) from the $3C_{\text{head1}} + 2$ values including bias terms outputting C_{head2} values.
- * A ReLu activation function.
- * A fully-connected layer (sharing weights across all s) from V_{pooled} including bias terms, outputting 1 value.
- The resulting 2S values multiplied by softplus(γ) are a distribution in logits whose softmax \hat{p}_s predicts the final score difference of the game in points. All predictions are from the perspective of the current player.

A global pooling layer in KataGo takes a tensor with C channels (shape $B \times B \times C$) and outputs a vector of length 3C containing:

²⁹20 was chosen as an arbitrary reasonable scaling factor so that on typical data the neural net would only need to output values around unit scale, rather than tens or hundreds.

³⁰In training the weight on this head is negligibly small. It is included only to enable future research on whether MCTS can be improved by biasing search towards more "uncertain" subtrees.

 $^{^{31}}$ In KataGo, we set S = 19 * 19 + 60, since 19 is the largest standard board size, and the extra 60 conservatively allows for the possibility that the winning player wins all of the board and has a large number of points from komi.

³²In Go, usually every point on the board is owned by one player or the other in a finished game, so the final score difference varies only in increments of 2 and half of values only rarely occur. Such a parity component is very hard for a neural net to learn on its own. But this feature is mostly for cosmetic purposes, omitting it should have little effect on overall strength).

- The mean of each channel.
- The mean of each channel multiplied by $\frac{1}{10}(B B_{\text{mid}})$
- The maximum of each channel.

where $B \in [B_{\min}, B_{\max}] = [9, 19]$ is the length of the board and $B_{\min} = \frac{1}{2}(B_{\min} + B_{\max})$. B_{\min} is subtracted to improve orthogonality, and $\frac{1}{10}$ is a arbitrary reasonable scaling constant so that the resulting values remain near unit scale.

In the value head, the third item is replaced with:

• The mean of each channel multiplied by $\frac{1}{100}((B-B_{\rm avg})^2-\sigma^2)$

where $\sigma^2 = \frac{1}{11} \sum_{b=9}^{19} (b - B_{\text{avg}})^2$. This is since the value head computes values, like score difference, that need to scale the mean quadratically with board length. $\frac{1}{100}$ is an arbitrary reasonable scaling constant to ensure unit-scale magnitudes, and subtracting σ^2 is to improve orthogonality with the other channels.

A global pooling bias structure takes input tensors X (shape $B \times B \times C_X$) and G (shape $B \times B \times C_G$) and consists of:

- A batch normalization layer and ReLu activation applied to G (output shape $B \times B \times C_G$).
- A global pooling layer on the result (output shape $3C_G$).
- Multiplication by a matrix of size $3C_G \times C_X$ (output shape C_X).
- Channelwise addition with X, treating the C_X different values as per-channel bias terms (output shape $B \times B \times C_X$).

Three different neural net sizes are used for the experiments in this paper. The values of all the above constants for these three sizes can be found in Table 5.

Size	$6b \times 96c$	$10b\times128c$	15b×192c
N	6	10	15
C	96	128	192
C_{pool}	32	32	64
$C_{ m head1}$	32	32	32
$C_{ m head2}$	48	64	80

Table 5: Architectural constants for various neural net sizes.

Appendix B Loss Function

The loss function for neural net training in KataGo is the sum of:

• Game outcome value loss:

$$c_{\text{value}} \sum_{r \in \{\text{win,loss}\}} z(r) \log(\hat{z}(r))$$

where z is a one-hot encoding of whether the game was won or lost by the current player³³, \hat{z} is the neural net's prediction of z, and $c_{\text{value}} = 1.5$.

• Policy loss:

$$-\sum_{m \in moves} \pi(m) \log(\hat{\pi}(m))$$

where π is the target policy distribution and $\hat{\pi}$ is the predicted policy distribution.

• Opponent policy loss:

$$-w_{\text{opp}} \sum_{m \in \text{moves}} \pi_{\text{opp}}(m) \log(\hat{\pi}_{\text{opp}}(m))$$

where π_{opp} is the target opponent policy distribution, $\hat{\pi}_{\text{opp}}$ is the predicted opponent policy distribution, and $w_{\text{opp}} = 0.15$.

• Ownership loss:

$$-w_o \sum_{l \in \text{board}} \frac{1 + o(l)}{2} \log \left(\frac{1 + \hat{o}(l)}{2} \right) + \frac{1 - o(l)}{2} \log \left(\frac{1 - \hat{o}(l)}{2} \right)$$

where $o(l) \in \{-1, 1\}$ is the actual final owner of board location l, $\hat{o}(l) \in [-1, 1]$ is the neural net's prediction, and $w_o = 1.5/B^2$ where B is the length of the board.

• Score belief loss ("pdf"):

$$-w_{\text{spdf}} \sum_{x \in \text{possible scores}} p_s(x) \log(\hat{p}_s(x))$$

where $p_s(x)$ is a one-hot encoding of whether the final score difference is exactly x, and $\hat{p}_s(x)$ is the neural net's predicted probability that the final score difference is exactly x, and $w_{\rm spdf} = 0.02$.

• Score belief loss ("cdf"):

$$w_{\text{scdf}} \sum_{x \in \text{possible scores}} \left(\sum_{y < x} p_s(y) - \hat{p}_s(y) \right)^2$$

where $w_{\text{scdf}} = 0.02$

• Root variance loss:

$$w_{\text{rv}} \sum_{i=0}^{3} (\text{rv}_i(y) - \hat{\text{rv}}_i(y))^2$$

where rv_i are the recorded values of variance in the MCTS root value between 1 and $\{4, 16, 64, 256\}$ visits, $\hat{\text{rv}}_i$ are the neural net's predictions of these values to be used for future research, and $w_{\text{rv}} = 0.2$ (in practice, the variances are small and therefore this loss term is mostly negligible).

• Score belief mean self-prediction:

$$-w_{\rm sbreg}$$
Huber $(\hat{\mu}_s - \mu_s, \, \delta = 10.0)$

where $w_{\text{sbreg}} = 0.004$ and

$$\mu_s = \sum_x x \hat{p}_s(x)$$

and Huber (x, δ) is the *Huber loss function* equal to the squared error loss $f(x) = 1/2x^2$ except that for $|x| > \delta$, instead Huber $(x, \delta) = f(\delta) + (|x| - \delta) \frac{df}{dx}(\delta)$. This avoids some cases of divergence in training due to large errors just after initialization.

Note that neural net is predicting itself - i.e. this is a regularization term for an otherwise unanchored output $\hat{\mu}_s$ to roughly equal to the mean score implied by the neural net's full score belief distribution. The neural net easily learns to make this output highly consistent with its own score belief³⁴.

• Score belief standard deviation self-prediction:

$$-w_{\rm sbreg}$$
Huber $(\hat{\sigma}_s - \sigma_s, \, \delta = 10.0)$

where

$$\sigma_s = \left(\sum_x (x - \mu)^2 \hat{p}_s(x)\right)^{1/2}$$

Similarly, the neural net is predicting itself - i.e. this is a regularization term for an otherwise unanchored output $\hat{\sigma}_s$ to roughly equal to the standard deviation of the neural net's full score belief distribution. The neural net easily learns to make this output highly consistent with its own score belief³⁴.

• Score belief scaling penalty:

$$w_{\rm scale} \gamma^2$$

where γ is the activation strength of the internal scaling of the score belief and $w_{\text{scale}} = 0.0005$. This prevents some cases of training instability involving the multiplicative behavior of γ on the belief confidence where γ grows too large.

• L2 penalty:

$$c||\theta||^2$$

where θ are the model parameters and c = 0.00003, so as to bound the weight scale and ensure that the effective learning rate does not decay due to batch normalization.

³⁴These are partly for implementation convenience. KataGo's play engine uses a separate GPU implementation so as to run independently of TensorFlow, and this allows us to avoid implementing the score belief head. Also for technical reasons relating to dynamic score utility and tree re-use, using only the first and second moments instead of the full distribution is convenient.

Appendix C Game Initialization

Aside from the more interesting game branching mechanism described in section 6.2.2, KataGo randomizes in a variety of minor ways to ensure diverse training data. We enumerate these minor ways here:

- Since KataGo is designed to support multiple rulesets, games are randomized uniformly between positional versus situational superko rules, and between suicide moves allowed versus disallowed. Although KataGo supports it, for this paper simple ko rules are not used.
- As mentioned earlier in section 4.3, games are randomized in board size from 9 to 19 with frequency weights 1, 2, ..., 11 but with the weight on size 19 further multiplied by 3, 5, or 10 as training progresses.
- To enable experience with different values of komi, rather than using a fixed komi of 7.5, komi is randomized by drawing from a normal distribution with mean 7 and standard deviation 1 truncated to 3 standard deviations, and rounding to the nearest integer or half-integer. However, 5% of the time, a standard deviation of 10 is used instead. This ensures that almost all games are played under close-to-fair conditions for maximally informative learning, but that there is still some data with much more unusual values of komi.
- To enable experience with handicap game positions, 5% of games are played as handicap games, where Black gets a random number of additional free moves at the start of the game, chosen randomly proportionally to the raw policy distribution of the neural net. Of those games, 90% use the neural net to adjust komi to compensate White for Black's advantage. This is done after handicap placement by iteratively several times performing a neural net query for the expected final score difference given the placement, and then adding that amount to komi. The maximum number of free Black moves is 0 (no handicap) for board sizes 9 and 10, 1 for board sizes 11 to 14, 2 for board sizes 15 to 18, and 3 for board size 19.
- To initialize each game and ensure opening variety, the first r moves of a game are played randomly directly proportionally to the raw policy distribution of the net, where r is drawn from an exponential distribution with mean $0.04 * B^2$. where B is the length of the board.
- During the game, moves are selected proportionally to the target-pruned MCTS playout distribution raised to the power of 1/T where T is a temperature constant. T begins at 0.8 and decays smoothly down to 0.2 based on the turn number, with a halflife in turns equal to the length of the board B.

Appendix D Gating Game Initialization

Compared to the game initialization and randomization described in Appendix C, the following changes are made for gating games:

规则和棋盘大小仍然是随机的,但Komi不是随机的,是7.5的。

- The rules and board size are still randomized but komi is not randomized and is fixed at 7.5.
- Handicap games are disabled.
- From the first turn, moves are played using full search rather than using the raw policy to 从第一轮开始了就使用完全搜索来下棋,而不是使用原始策略来下play some of the first moves.
- The temperature T for selecting a move based on the MCTS playout distribution starts at 0.5 instead of 0.8.

搜索树重复利用

- Dirichlet noise and forced playouts and visit cap oscillation are disabled, tree reuse is enabled.
- The root uses $c_{\rm FPU} = 0.2$ just the same as the rest of the search tree instead of $c_{\rm FPU} = 0.0$.
- Since there is no need to complete the game to obtain ownership and score targets, resignation is enabled, occurring if both sides agree that for the last 5 turns, the worst MCTS winrate estimate p for the losing side has on each turn been less than 5%.

由于不需要完成游戏来获得所有权和得分目标,因此,如果双方都同意在过去5个回合中,失败一方的最差MCTS胜 率估计值p在每个回合中都小于5%,那么就可以认输。