Learning proofs for the classification of nilpotent semigroups

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Abstract

PRELIMINARY VERSION for Git-Hub

1 Introduction

We are interested in the classification of finite semigroups. Distler [4, 5] has provided a list of isomorphism classes for sizes $n \leq 10$, but at great computational expense. The question we pose here is whether AI can learn to do a classification proof for these objects.

Let's point out right away that the process we look at here will not, in its current state, be useful for improving the computational time for a classification proof. We are able to find proofs with small numbers of nodes, however the training time necessary to do that is significantly bigger than the gain with respect to a reasonable benchmark process. Therefore, this study should be considered more for what it says about the general capacity of a deep learning process to learn how to do proofs.

Unsurprisingly, the motivation for this question is the recent phenomenal success obtained by Alpha Go and Alpha Zero at guiding complex strategy games. If we think of a mathematical proof as a strategy problem, then it seems logical to suppose that the same kind of technology could guide the strategy of a proof.

In turn, this investigation serves as a convenient and fun way to experiment with some basic Deep Learning programming.

The problem at hand is that of determining the list of isomorphism classes of semigroups of a given kind. We recall that a semigroup consists of a set A and a binary operation

$$A \times A \to A \quad \text{denoted} \quad (x, y) \mapsto x \cdot y$$

subject only to the axiom that it is associative $\forall x, y, z \in A,\ x \cdot (y \cdot z) = (x \cdot y) \cdot z$. For us, the set A will be finite, typically having from 7 to 10 (or maybe 11) elements.

We envision a simple format of the classification proof, where at each step we make some *cuts*, branching according to the possible hypotheses for the values of a single multiplication $x_i \cdot y_i$. The basic strategy question is which location (x_i, y_i) to choose at each stage of the proof. Once the possible cuts have been exhausted then we have a classification.

We don't worry here about filtering according to isomorphism classes, however we use the symmetry by starting with an initial hypothesis about the possible multiplication operations; the set of these hypotheses is filtered by a sieve under the symmetric group action. Typically, our proof learning process will then concentrate on a single instance denoted σ of this collection of possible initial conditions.

We describe the learning setup used to try to learn proofs, and make comments on the choice of network architecture and sampling and training processes. At the end, we show some graphs of the result of the learning process on specific proof problems.

For a small initial condition corresponding to certain semigroups of size 7, we can find in another way the precise lower bound for the size of the proof. Our learning framework is able to attain proofs of the lower-bound size. For larger cases it isn't practically possible to obtain a proven lower bound so we can only show the progress that is attained, leaving it to speculation for the question of how close we are getting to the theoretical lower bound.

We now discuss the framework in somewhat greater detail. We are going to be classifying *nilpotent semigroups*. It is useful to understand the role played by nilpotent semigroups in the classification of finite semigroups.

They are representative of the phenomena that lead to large numbers of solutions. In order to understand this, it is good to look at one of the main constructions of a large number of semigroups.

We consider a filtered nilpotent semigroup A of size $n \geq 3$ with filtration having three steps as follows:

$$F^0 A = A = \{0, \ldots, n-1\}, \quad F^1 A = \{0, 1\}, \quad F^2 A = \{0\}.$$

It means that $x \cdot y \in \{0, 1\}$, and if $x = 0$ or $x = 1$ or $y = 0$ or $y = 1$ then $x \cdot y = 0$. Clearly, for any multiplication table satisfying these properties we have $(x \cdot y) \cdot z = 0$ and $x \cdot (y \cdot z) = 0$ for any $x, y, z \in A$. Therefore, any multiplication table satisfying these properties is automatically associative. To specify the table, we must just specify $x \cdot y \in \{0, 1\}$ for

$x, y \in F^0A - F^1A = \{2, \ldots, n-1\}$. There are

$$2^{(n-2)^2}$$

possibilities. For example with $n = 6$ this is $2^16 = 65536$ possibilities. For $n = 10$ we have 2^{64} possibilities.

This example illustrates an important phenomenon, and along the way shows that we can expect the nilpotent cases of all kinds to occupy an important place in the classification. On the other hand, in the nilpotent case the choice of a filtration gives a somewhat natural ordering on the objects, allowing to consider that the order is not completely arbitrary and that it could be used in the deduction procedure. One *caveat* here is of course that in general there might be several different full nilpotent filtrations adapted to the same multiplication, so as n gets bigger we will want to refine things more. For the case $n = 6$ the full nilpotent filtration convention leads to a reasonable problem.

The next step, in order to understand both the proof mechanism and the encoding of data to feed to the machine, is to discuss *multiplexing*. This is a very standard procedure. To give a simple example, suppose we want to make a neural network to predict traffic on a road. It will depend on the day of the week. If we give as input data a number $d \in \{0, \ldots, 6\}$ it isn't going to work very well. A much better solution is to give as input data a vector $v \in \mathbb{Z}^7$ with

$$v = (v_0, \ldots, v_6), \quad v_i \in \{0, 1\}, \quad v_0 + \ldots + v_6 = 1.$$

The last two conditions mean that there is exactly one value that equals 1, the rest are 0. We have transformed our integer data from a *quantity* to a *location*. With the location data, the machine could make a different calculation for each day of the week and is much more likely to find a good answer. Indeed if we give a number input a sufficiently deep machine would very likely first just transform it to a place input and then work with that.

In our situation, the analogous point is that we don't want to give the numerical data of the values $A.t[x][y]$ in the multiplication table. These are numerical values in $\{0, \ldots, n-1\}$ but as we have seen above, their ordering is only somewhat canonical in the nilpotent case, and in the general non-nilpotent case it might be highly indeterminate. Therefore, we *multiplex* the multiplication table into an $n \times n \times n$ tensor $A.m[x][y][z]$ with the rule

$$A.m[x][y][z] = 1 \Leftrightarrow x \cdot y = z, \quad A.m[x][y][z] = 0 \text{ otherwise.}$$

Recall here that the indices x, y, z take values in $0, \ldots, n-1$. A more mathematical notation

would be $M_{x,y,z}$ but let's stick to the notation $A.m[x][y][z]$ that is going to be closer to the programming language.

We'll call the tensor $A.m$ the *mask*. This representation has some nice properties. The first of them is that it allows us to encode not only the multiplication table itself that we are looking to classify, but also whole collections of multiplication tables. A *mask* is an $n \times n \times n$ tensor $A.m$ with entries denoted $A.m[x][y][z]$, such that the entries are all either 0 or 1. A mask is transformed into a condition about multiplication tables as follows:

$$A.m[x][y][z] = 0 \quad \text{means} \quad x \cdot y \neq z$$

whereas

$$A.m[x][y][z] = 1 \quad \text{means} \quad x \cdot y \quad \text{might be} \quad z$$

Given a mask $A.m$, a table $A.t$ (that is, an $n \times n$ array whose entries $A.t[x][y]$ are in $0, \ldots, n-1$) is said to *satisfy* $A.m$ if, for all $x, y \in \{0, \ldots, n-1\}$ if we set $z := A.t[x][y]$ then $A.m[x][y][z] = 1$.

Geometrically we may view the mask as a subset of a 3-dimensional grid (the subset of points where the value is 1) and a table, viewed as a section from the 2-dimensional space of the first two coordinates into the 3-dimensional space, has to have values that land in the subset in order to satisfy the mask.

For a given mask $A.m$ there is therefore a set of associative multiplication tables $A.t$ that satisfy $A.m$.

We may formulate our original problem in this way: there is a mask $Q(\text{nil}, n).m$ of size n corresponding to the conditions in Definition ???. Precisely, we have

$$Q(\text{nil}, n).m[x][y][z] = 1 \text{ if } z = 0 \text{ or } z < \min(x, y), \quad Q(\text{nil}, n).m[x][y][z] = 0 \text{ otherwise.}$$

A table $A.t$ is a solution to our Problem ??? if and only if it satisfies the mask $Q(\text{nil}, n).m$.

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2 Nilpotent semigroups

By a ^{0}*semigroup* we mean a semigroup with a distinguished element 0 with the properties $0x = x0 = 0$ for all x. The case of semigroups (without 0) may be recovered by the operation of formally adding on a 0 denoted $A \mapsto A^0 := A \sqcup \{0\}$.

If A is a set we denote by A^0 the set $A \sqcup \{0\}$ considered as an object of the category of pointed sets. Given pointed sets $(A, 0)$ and $(B, 0)$ we denote the *product* as

$$(A, 0) \otimes (B, 0) := (A - \{0\}) \times (B - \{0\}) \sqcup \{0\}.$$

This is the cartesian product in the category of pointed sets. The sum in that category is

$$(A, 0) \vee (B, 0) := (A - \{0\}) \sqcup (B - \{0\}) \sqcup \{0\}.$$

The category of pointed sets with these operations is sometimes known as the *category of* $\mathbb{F}_1$*-modules* and we follow the line of motivation implied by this terminology. In particular,

an $\mathbb{F}_1$-algebra is going to be a pointed set $(A, 0)$ together with an associative operation

$$(A, 0) \otimes (A, 0) \to (A, 0).$$

This is equivalent to the notion of a ^{0}semigroup so an alternate name for this structure is "$\mathbb{F}_1$-algebra".

Whereas conceptually we think primarily of pointed sets, in practical terms it is often useful to consider only the subset of nonzero elements, so these two aspects are blended together in the upcoming discussion.

A finite semigroup X is *nilpotent* if it has a 0 element and there is an n such that $x_1 \cdots x_n = 0$ for any $x_1, \ldots, x_n$.

Note in particular that a nilpotent semigroup is by definition also a ^{0}semigroup so we can say "nilpotent semigroup" in place of "nilpotent ^{0}semigroup".

Suppose X is a nilpotent semigroup. We define X^k to be the set of products of length k. We have $X^i = \{0\}$ for $i \geq n$ (the n above). By definition $X^1 = X$. We have

$$X^{i+1} \subset X^i$$

and these inclusions are strict. That implies that we can take $n = |X|$ in the nilpotency condition.

We introduce the *associated-graded semigroup* $Gr(X)$ defined as follows: the underlying set is the same, viewed as decomposed into pieces

$$Gr(X) := X = \{0\} \cup \bigcup_{i \geq 1} (X^i - X^{i+1}).$$

Put $Gr^i(X) := (X^i - X^{i+1})$, and $Gr^i(X)^0 := Gr^i(X) \cup \{0\}$. This notion keeps with the $\mathbb{F}_1$-module philosophy.

In the current version of this project, we classify semigroups that are already their own associated-gradeds. This amounts to saying that the product of two elements in $(X^i - X^{i+1})$ and $(X^i - X^{i+1})$ is either in $(X^{i+j} - X^{i+j+1})$ or is equal to zero. For the 4-nilpotent case, one can recover the general classification by just lifting all products that are equal to zero, into arbitrary elements of X^3.

2.1 The 4-nilpotent case

We consider the following situation: we have sets A and B of cardinalities denoted a and b respectively, and we look for a multiplication operation

$$m : A \times A \to B^0,$$

recall $B^0 := B \sqcup \{0\}$. We require that B be contained in the image (it isn't necessary to have 0 contained in the image, that might or might not be the case).

Such an operation generates an equivalence relation on $(A \times A \times A)^0$ in the following way. If $m(x,y) = m(x',y')$ then for any z we set $(x,y,z) \sim (x',y',z)$ and $(z,x,y) \sim (z,x',y')$. Furthermore, if $m(x,y) = 0$ then we set $(x,y,z) \sim 0$ and $(z,x,y) \sim 0$.

Let Q be the set of nonzero equivalence classes (it could be empty). We obtain a graded semigroup structure on

$$A^0 \vee B^0 \vee Q^0.$$

Suppose given a graded semigroup of the form $A^0 \vee B^0 \vee P^0$. Let m be the multiplication operation from $A \times A$ to B^0 and suppose its image contains B. This yields Q^0. There is a unique map $Q^0 \to P^0$ inducing a morphism of graded semigroups.

Because of this observation, we would like to classify multiplication maps $m : A \times A \to B^0$ such that the quotient $Q := A^3/\sim$ has at least two elements.

A few further restrictions are discussed in §4.1 below.

Given a multiplication operation satisfying the conditon $|Q| \geq 2$, we can consider a quotient $Q^0 \to I^0 = \{0,1\}$ that sends Q surjectively to I^0. Therefore, we try to classify graded semigroups of the form

$$A^0 \vee B^0 \vee I^0$$

which is to say, 4-nilpotent graded semigroups of size vector $(a,b,1,1)$.

A next question is the choice of ordering of the sets A and B. For the computer program, a set with a elements is $A = \{0,\ldots,a-1\}$. Similarly $B = \{0,\ldots,b-1\}$. We let the "zero" element of B^0 correspond to the integer b so $B^0 = \{0,\ldots,b\}$ containing the subset B indicated above. We'll denote this element by 0_B in what follows, in other words 0_B corresponds to the integer $b \in \{0,\ldots,b\}$.

Our structure is therefore given by the following operations:

$$\mu : A \times A \to B^0$$

$$\phi : A \times B^0 \to I^0$$

and

$$\psi : B^0 \times A \to I^0$$

with the last two satisfying $\phi(x, 0_B) = 0$ and $\psi(0_B, x) = 0_I$ for all $x \in A$.

3 A sieve reduction

The classification proof setup that we have adopted is to fix the ϕ matrix and divide by permutations of A and B. That is to say, $\mathscr{S}_a \times \mathscr{S}_b$ acts on the set of matrices (i.e. $a \times b$ matrices with boolean entries) and we choose a representative for each orbit by a sieve procedure. This results in a reasonable number of cases, and the sieve procedure also gives a light property of ordering on the elements of A that seems somewhat relevant.

Once this matrix is fixed, we search for matrices m. We get some conditions on the matrix ψ and these are combined into a ternary operation

$$\tau : A \times A \times A \to I^0.$$

The proof is by cuts on the possibilities for the matrix μ, and the leaf of the proof tree is declared to be 'done' when μ is determined. It doesn't seem to be necessary or particularly useful to make cuts on the possibilities for the matrices ψ or τ although this could of course be envisioned.

Another possibility, for absorbing the $\mathscr{S}_a \times \mathscr{S}_b$ action, would be to declare that the values of m in B should be lexicographically ordered as a function of $(x, y) \in A \times A$, and then choose representatives for the initial elements under the $\mathscr{S}_a$ action. Many attempts in this direction were made, but in the end, this seemed to be less useful than the current setup.

We therefore start with a set Σ of input data. Each datum in Σ consists of a representative for the equivalence class of a function $\phi : A \times B^0 \to I^0$ (such that $A \times \{0_B\}$ maps to 0_I) under the action of the group $\mathscr{S}_a \times \mathscr{S}_b$. The equivalence class is chosen in a way that generally puts the 1's in this matrix towards lower indices in A and towards the higher indices in B.

The other blocks of the input datum, for the right multiplication $\psi : B^0 \times A \to I$ and the product $\mu : A \times A \to B^0$, are left free.

Here is a table of the sizes $|\Sigma|$, that is to say the numbers of equivalence classes, in terms of a and b. This is the table of [8], see the references on that page, and others such as [7].

$a \setminus b$	2	3	4	5	6
2	7	13	22	34	50
3	13	36	87	190	386
4	22	87	317	1053	3250
5	34	190	1053	5624	28576
6	50	386	3250	28576	$251610^{(*)}$

$(*)$ my program ran out of memory to compute this for $(6, 6)$, the value is taken from [8].

We are not interested in the function that sends everything to 0_I. Furthermore we typically don't consider the first few elements of Σ that correspond to cases where $\phi(x, y) = 0_I$ for all but one value of x. These correspond to initial conditions with a large symmetry group, that are partially absorbed by the symmetry consideration that is explained next. The cases that aren't covered by the symmetry consideration should be treated by also specifying the matrix ψ; we don't pursue that at the present time.

We exploit the symmetry obtained by interchanging the order of multiplication: given a semigroup M we obtain the opposite semigroup M^o with the same set but composition $*$ defined in terms of the composition $\cdot$ of M, by

$$x * y := y \cdot x.$$

This interchanges the matrices ϕ and ψ, notably.

We define an additional filter "half-ones" (cf 4.1) to make the following assumption:
—That the number of nonzero entries of the matrix ψ is $\leq$ the number of nonzero entries of ϕ. (The latter number being fixed by the choice of element $\phi \in \Sigma$).

3.1 Initial data for $(3, 2)$

For reference we record here the left multiplication matrices for the 13 initial instances in Σ given by the sieve for $(a, b) = (3, 2)$. Recall that the left multiplication is the product $A \times B^0 \to I$, but the product with the zero element (numbered as $2 \in B^0$ here) is zero so we only need to include the first two columns. This is a 3×2 matrix. The entry L_{ij} is the product $i \cdot j$ for $i \in A$ and $j \in B$ ($i \in \{0, 1, 2\}$ and $j \in \{0, 1\}$).

$$L(\sigma = 0) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad L(\sigma = 1) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad L(\sigma = 2) = \begin{bmatrix} 0 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$L(\sigma = 3) = \begin{bmatrix} 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \quad L(\sigma = 4) = \begin{bmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad L(\sigma = 5) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$L(\sigma = 6) = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad L(\sigma = 7) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \quad L(\sigma = 8) = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

$$L(\sigma=9)=\begin{bmatrix}1&1\\1&1\\0&0\end{bmatrix}\quad L(\sigma=10)=\begin{bmatrix}1&1\\1&0\\0&1\end{bmatrix}$$

$$L(\sigma=11)=\begin{bmatrix}1&1\\1&1\\0&1\end{bmatrix}\quad L(\sigma=12)=\begin{bmatrix}1&1\\1&1\\1&1\end{bmatrix}$$

4 The classification task

Given three sets X, Y, Z, a *mask* for a function $X \times Y \to Z$ is a boolean tensor $m : X \times Y \times Z \to \{0, 1\}$. A function $f : X \times Y \to Z$ is covered by m, if $m(x, y, f(x, y)) = 1$ for all x, y.

The statistics of m denoted $\mathrm{stat}(m)$ is the function $X \times Y \to \mathbb{N}$ sending (x, y) to the number of z with $m(x, y, z) = 1$, i.e. it is the sum of m along the Z axis.

If $\mathrm{stat}(m)(x, y) = 0$ for any pair (x, y) then there doesn't exist a covered function. Thus, we say that m is *possible* if $\mathrm{stat}(m) > 0$ at all x, y.

If $\mathrm{stat}(m)(x, y) = 1$ it means that there is a single value z such that $m(x, y, z) = 1$. This means that if f is a covered function, we know $f(x, y) = z$.

We say that the mask is *done* if $\mathrm{stat}(m)(x, y) = 1$ for all x, y. In this case it determines a unique function f.

Given masks m, m' we say that $m \subset m'$ if $m(x, y, z) = 1 \Rightarrow m'(x, y, z) = 1$.

We now get back to our classification task. A *position* is a quadruple of masks $p = (m, l, r, t)$ where m is a mask for the function $\mu : A \times A \to B^0$, l is a mask for ϕ, r is a mask for ψ, and t is a mask for $\tau : A \times A \times A \to I^0$ (a mask for a ternary function being defined analogously).

We say that a position p is a subset of another position p' if $m \subset m'$, $l \subset l'$, $r \subset r'$ and $t \subset t'$.

Given a point $\phi \in \Sigma$, the mask l is required to be equal to the done mask determined by this function.

Let $\mathcal{P}$ be the set of positions and let $\mathcal{P}_{\Sigma n'}$ be the set of positions corresponding to any subset $\Sigma' \subset \Sigma$. Let $\mathcal{P}_\phi = \mathcal{P}_{\{\phi\}}$ be the set of positions corresponding to a point $\phi \in \Sigma$.

A position $(m, l, r, t) \in \mathcal{P}$ is *impossible* if any of the masks m, l, r, t are not possible i.e. have a point where the statistics are 0.

A position is *realized* if there is a collection of functions covered by the masks that form a graded nilpotent semigroup. We may also impose other conditions on the realization such

as discussed above.

We'll define a function

$$\text{process} : \mathcal{P} \to \mathcal{P}$$

such that process$(p) \subset p$, and such any realization of p is also a realization of process(p). The process function is going to implement some basic steps of deductions from the associativity condition.

The function is repeated until it makes no further changes, so that process(process(p)) = process(p).

We also define a function

$$\text{filter} : \mathcal{P} \to \{\text{active}, \text{done}, \text{impossible}\}$$

by saying that filter(p) is impossible if any of the following hold:
—any of the masks in p is not possible (i.e. there is a column containing all $False$'s);
—the mask r contains uniquely defined entries with values $\neq 0_I$ in number larger than the number of nonzero entries of ϕ, so that a realization would have to contradict our assumption ???;
—in §4.1 we introduce two additional filters that could also be imposed.

We say that filter(p) is done if the mask m is done. Note here that we aren't necessarily requiring r or t to be done (l is automatically done since it corresponds to the function ϕ).

We say that filter(p) if it is neither impossible or done.

The initial position corresponding to $\phi \in \Sigma$ consists of setting the mask l to be the done mask corresponding to the function ϕ, and setting m, r and t to be full masks i.e. ones all of whose values are 1.

The goal is to classify the done positions that are subsets of the initial position.

We do a proof by *cuts*. A cut at a position p corresponds to a choice of $(x, y) \in A \times A$, leading to the position leaves $p_1, \ldots, p_k$ that correspond to choices of $z_1, \ldots, z_k$ such that $m(x, y, z_i) = 1$. In each position p_i the column (x, y) of m is replaced by a column with a unique 1 at position z_i, the rest of m remains unchanged. The generated positions are then processed.

Clearly we only want to do this if $\text{stat}(m)(x, y) \geq 2$. Such a choice is available any time filter(p) is active.

A partial classification proof consists of making a series of cuts, leading to a proof tree (see below). Each leaf is filtered as active, done or impossible. The proof is complete when

all the leaves are filtered as done or impossible. The data that is collected is the set of done position at leaves of the tree. These are the done positions subsets of the initial position.

4.1 Additional filters

In view of the size of certain proof trees that occur, it has shown to be useful to introduce some additional filters. They should be considered as acceptable in view of the classification problem.

One filter that we call the "profile filter" asks that there shouldn't be two elements that have the same multiplication profile, i.e. that provide the same answers for all multiplications with other elements. In other words, if there exist distinct elements $x \neq x'$ such that $x \cdot y = x' \cdot y$ and $y \cdot x = y' \cdot x$ then this filter marks that case as "impossible". The reasoning is that such examples can be obtained from the classification for smaller values of n by simply doubling an object into two copies of itself as far as the multiplication table is concerned.

The other filter called "half-ones" imposes the condition that we discussed previously, saying the number of nonzero entries of the right-hand multiplication matrix ψ should be $\leq$ the number of nonzero entries of the left-hand one ϕ, which we recall is fixed by the choice of instance in Σ.

Entries are provided in the 'Parameters' section to turn these filters off or on. By default they are turned on, and our discussion of numbers of proof nodes below will assume they are turned on unless otherwise specified.

5 Proof tree

A proof by cuts leads to a proof tree $\mathscr{T}$. This is defined in the following way. The definition will be inductive: we define a notion of partial proof tree, how to extend it, and when it becomes complete.

The tree has nodes connected by edges, viewed in a downward manner: each node (apart from the root) has one incoming edge above it and some outgoing edges below. The leaf nodes are those having no outgoing edges.

Each node is going to have a position attached to it. Each non-leaf node, also called 'passive', has a pair $(x, y) \in A \times A$ called the 'cut' associated to it.

The root node corresponds to the initial position, which in our setup comes from the chosen matrix $\phi \in \Sigma$. Call this position $p_{\mathrm{root}}(\phi)$.

The leaf nodes are classified into 'active', 'done' and 'impossible' cases. These depend on the position p associated to the node, via the function filter(p) that determines the case.

The proof tree is said to be complete if all the leaf nodes are either done or impossible.

If a partial proof tree is not complete, then it can be extended to a new tree in the following way. Choose an active leaf node corresponding to position $p = (m, l, r, t)$ and choose a cut $(x, y) \in A \times A$. This should be chosen so that $k := \mathrm{stat}(m)(x, y) \geq 2$, such a choice exists because if not then the position would be classified as impossible or done.

Let $z_1, \ldots, z_k$ be the values such that $m(x, y, z_i) = 1$.

The pair (x, y) is going to be the one associated to the corresponding node in the new tree. The new tree is the same as the previous one except for the addition of k new nodes below our chosen one, with positions $p_1, \ldots, p_k$. These positions are determined as follows. Let $l'_i = l$, $r'_i = r$ and $t'_i = t$. Let m'_i be the same matrix as m but with the column $m'_i(x, y, -)$ replaced by a column with a single 1 at location z_i. This defines positions $p'_1, \ldots, p'_k$. We then set $p_i := \mathrm{process}(p'_i)$.

Proposition 5.1. *Suppose M is a semigroup structure covered by a position p at a node of the tree. Then it is covered by exactly one of the new nodes $p_1, \ldots, p_k$. Therefore, if M is a semigroup structure covered by the root position $p_{\mathrm{root}}(\phi)$, it is covered by exactly one of the positions corresponding to leaf nodes of the tree.*

Proof. With the above notations at a node corresponding to position p, if $M = (\mu, \phi, \psi, \tau)$ is a semigroup structure covered by p then $\mu(x, y) \in \{z_1, \ldots, z_k\}$. In view of the replacement of the column $m(x, y, -)$ by k columns corresponding to the values z_i, it follows that μ is covered by exactly one of the masks m'_i. As the other ones l', r', t' are the same as before, we get that M is covered by exactly one of the positions p'_i. Then, the property of the process function implies that M is covered by exactly one of the positions p_i. This proves the first statement; the second one follows recursively. □

Remark: There is no semigroup structure satisfying our assumptions and covered by an impossible node. Thus, given a completed proof tree, the admissible semigroup structures with given ϕ are covered by the done nodes of the tree.

Remark: We note that a single done node could cover several structures, since we are only requiring that the mask m be done; the mask r could remain undone and correspond to several different functions ψ. This phenomenon is rare.

We will be interested in counting the cumulative number of nodes over the full tree when the proof is completed. By this, we mean to count the passive nodes, but not the done

or impossible ones. The count does include the root (assuming it isn't already done or impossible, which could indeed be the case for a small number of instances of our initial conditions usually pretty far down in the sieve).

6 The best possible choice of cuts

In order to create a proof, one has to choose the cuts $\mathrm{cut}(p) = (x, y)$ for each position p. The *minimization criterion* is that we would like to create a proof with the smallest possible number of total nodes. This count can be weighted in a distinct way for the done and impossible nodes. Let $|\mathscr{T}|$ denote this number, possibly with weights assigned to the done and impossible nodes. For the purposes of our discussion, these weights are assumed to be zero, although a very small weight is included in the implemented program with the idea that it could help the learning process.

If v is a node of the proof tree, let $\mathscr{T}(v)$ denote the part of the proof tree under v, including v as its root node.

If p is a position, let $\mathscr{T}^{\min}(p)$ denote a minimal proof tree whose root has position p. (There could be more than one possibility.) We define the minimal criterion at p to be

$$\mathscr{C}^{\min}(p) := |\mathscr{T}^{\min}(p)|.$$

Suppose p is an active position and (x, y) is an allowable cut for p. Let $p_1, \ldots, p_k$ be the new positions generated by this cut. Define

$$\mathscr{C}^{\min}(p; (x, y)) := \mathscr{C}^{\min}(p_1) + \cdots + \mathscr{C}^{\min}(p_k).$$

Lemma 6.1. *If $\mathscr{T} = \mathscr{T}^{\min}(p)$ is a minimal proof tree and v is a node of $\mathscr{T}$ with position q then*

$$\mathscr{T}(v) = \mathscr{T}^{\min}(q)$$

is a minimal proof tree for the position q.

If $\mathscr{T}^{\min}(p)$ is a minimal proof tree with root node having position p, which we assume is active, and if (x, y) is the cut at this root node, then

$$\mathscr{C}^{\min}(p) = 1 + \mathscr{C}^{\min}(p; (x, y)).$$

Proof. For the first statement, if one of the sub trees were not minimal it could be replaced by a smaller one and this would decrease the global criterion for $\mathscr{T}$, contradicting minimality of $\mathscr{T}$. Thus, the sub-trees are minimal.

For the second part, say the nodes below p correspond to positions $p_1, \ldots, p_k$. The tree $\mathscr{T}^{\min}(p)$ is obtained by joining together the sub-trees (that are minimal by the first part) $\mathscr{T}^{\min}(p_i)$ plus one additional node at the root. This gives the stated count. □

Define the *minimizing strategy* as being a function $\mathrm{cut}^{\min}(p) = (x, y)$ where (x, y) is a choice that achieves the minimum value of $\mathscr{C}^{\min}(p; (x, y))$ over allowable cuts (x, y) at p. We say "a function" here because there might be several choices of (x, y) that attain the minimum so the strategy could be non-unique.

The fact that the minimization criterion is additive in the nodes below a given node, implies the following—rather obvious—property that says that if you make a best possible choice at each step along the way then you get a best possible global proof.

Corollary 6.2. *If $\mathscr{T}$ is a proof tree obtained by starting with root node position p and following a minimizing strategy at each node, then $\mathscr{T} = \mathscr{T}^{\min}(p)$ is a minimal proof tree for p.*

Proof. We'll prove the following statement: suppose given two different proof trees $\mathscr{T}$ and $\mathscr{T}'$ that both satisfy the property that they follow a minimizing strategy at each node, then $|\mathscr{T}| = |\mathscr{T}'|$ and both trees are minimal.

We prove this statement by induction. It is true tautologically at a position that is done or impossible. Suppose v is a position, and suppose $v_1, \ldots, v_k$ and $v'_1, \ldots, v'_{k'}$ are the nodes below v in $\mathscr{T}$ and $\mathscr{T}'$ respectively. Let $p_1, \ldots, p_k$ and $p'_1, \ldots, p'_{k'}$ denote the corresponding positions. We know by the inductive hypothesis that $\mathscr{T}(v_i)$ and $\mathscr{T}'(v'_j)$ are minimal trees (because they follow the minimizing strategy), hence

$$|\mathscr{T}(v_i)| = |\mathscr{T}^{\min}(p_i)| = \mathscr{C}^{\min}(p_i)$$

and the same for $|\mathscr{T}'(v'_j)|$. We conclude that

$$|\mathscr{T}(v_1)| + \cdots + |\mathscr{T}(v_k)| = \mathscr{C}^{\min}(p_1) + \cdots + \mathscr{C}^{\min}(p_k) = \mathscr{C}^{\min}(p; (x, y)),$$

and again similarly for the v'_j. But

$$|\mathscr{T}(v)| = 1 + |\mathscr{T}(v_1)| + \cdots + |\mathscr{T}(v_k)|$$

so combining with the lemma we get

$$|\mathscr{T}(v)| = 1 + \mathscr{C}^{\min}(p; (x, y)).$$

Similarly

$$|\mathscr{T}'(v)| = 1 + \mathscr{C}^{\min}(p;(x',y')).$$

The minimizing strategy says that these are both the smallest values among all choices of cuts (x,y). In particular they are equal, which shows that $|\mathscr{T}(v)| = |\mathscr{T}'(v)|$. If we now consider a minimal tree $\mathscr{T}^{\min}(p)$ starting from the position p corresponding to v, it starts with a cut (x'',y'') and we have

$$|\mathscr{T}^{\min}(p)| = 1 + \mathscr{C}^{\min}(p;(x'',y''))$$

by the lemma. But this value has to be the smallest value among the choices of cuts (x,y) otherwise its value could be reduced which would contradict minimality of $\mathscr{T}^{\min}(p)$. Thus, it is equal to the values for (x,y) and (x',y') above, that is to say

$$\mathscr{C}^{\min}(p;(x'',y'')) = \mathscr{C}^{\min}(p;(x,y)) = \mathscr{C}^{\min}(p;(x',y')).$$

Therefore

$$|\mathscr{T}^{\min}(p)| = |\mathscr{T}(v)| = |\mathscr{T}'(v)|.$$

This shows that $\mathscr{T}(v)$ and $\mathscr{T}'(v)$ are also minimal trees. This completes the proof of the inductive statement.

The inductive statement at the root gives the statement of the corollary. □

7 Neural networks

The model to be used for learning proofs will consist of a pair of networks (N, N_2) that provide approximations to ideal functions $\widehat{N}$ and $\widehat{N}_2$ defined as follows:

$$\widehat{N}(p) := \log_{10} \mathscr{C}^{\min}(p)$$

$$\widehat{N}_2(p;(x,y)) := \log_{10} \mathscr{C}^{\min}(p;(x,y)).$$

We then follow the strategy

$$\mathrm{cut}^{N_2}(p) := (x,y) \text{ attaining a minimum of } N_2(p;(x,y)).$$

Clearly, if N_2 accurately coincides with $\widehat{N}_2$ then $\mathrm{cut}^{N_2}(p) = \mathrm{cut}^{\min}(p)$ and we obtain a minimizing strategy.

The neural networks are trained in the following manner. First suppose we are given N_2. Then, let $\mathscr{T}^{N_2}(p)$ be the proof tree obtained by following the cut strategy $\mathrm{cut}^{N_2}(p)$ (in case of a tie, unlikely because the values are floating-point reals, the computer determines the minimum here by some algorithm that we don't control).

Then set $\mathscr{C}^{N_2}(p) := |\mathscr{T}^{N_2}(p)|$ and let

$$\widetilde{N}[N_2](p) := \log_{10} \mathscr{C}^{N_2}(p).$$

On the other hand, suppose we are given N. Then for any position p and allowable cut (x, y), let $p_1, \ldots, p_k$ be the generated positions. We define

$$\widetilde{N}_2[N](p; (x, y)) := \log_{10}(1 + 10^{N(p_1)} + \ldots + 10^{N(p_k)}).$$

We would like to train N and N_2 conjointly to approximate the values of $\widetilde{N}[N_2](p)$ and $\widetilde{N}_2[N](p; (x, y))$ respectively. The training process is iterated to train N, then N_2, then N, then N_2 and so forth.

Theorem 7.1. *If such a training is completely successful, that is to say if we obtain N, N_2 that give perfect approximations to their target values, then*

$$N(p) = \widehat{N}(p) \quad \textit{and} \quad N_2(p; (x, y)) = \widehat{N}_2(p; (x, y)),$$

and $\mathrm{cut}^{N_2}(p) = \mathrm{cut}^{\min}(p)$. *Then, the proof tree created using the strategy dictated by N_2 is a minimal one.*

Proof. We define the following inductive invariant $D(p)$ for any position p: let $D(p)$ be the maximum depth of any proof tree starting from p. We note that if (x, y) is any cut allowable at p and if $p_k(x, y)$ denote the new positions after making that cut (and processing) then $D(p_k(x, y)) < D(p)$. Indeed, given a proof tree for $p_k(x, y)$ with depth $D(p_k(x, y))$ we can plug it into a proof tree for p that has depth $D(p_k(x, y)) + 1$.

The possible proof trees have bounded depth, indeed after at most a^2 cuts all of the values in the multiplication table are determined and any resulting position must be done or impossible. Therefore the maximal value $D(p)$ is well-defined and finite.

We may now proceed to prove the theorem by induction on the invariant $D(p)$. For a given position p, consider all the cuts (x, y) allowable at p. For each cut, we obtain new positions $p_k(x, y)$. The tree $\mathscr{T}^{N_2}(p_k(x, y))$ has size $\mathscr{C}^{N_2}(p_k(x, y)) := |\mathscr{T}^{N_2}(p_k(x, y))|$, the $\log_{10}$ of which is equal to

$$\widetilde{N}[N_2](p_k(x, y)) := \log_{10} \mathscr{C}^{N_2}(p_k(x, y)) = \log_{10} |\mathscr{T}^{N_2}(p_k(x, y))|.$$

By the inductive hypothesis, which applies since $D(p_k(x,y)) < D(p)$, we have

$$\widetilde{N}[N_2](p_k(x,y)) = N(p_k(x,y)).$$

Putting this into the definition of $\widetilde{N}_2[N]$ we get

$$\widetilde{N}_2[N](p;(x,y)) := \log_{10}(1+10^{N(p_1(x,y))}+\ldots+10^{N(p_k(x,y))}) = \log_{10}\left(1+\sum|\mathscr{T}^{N_2}(p_j(x,y))|\right).$$

In other words, $10^{\widetilde{N}_2[N](p;(x,y))}$ is the size of the tree that is generated below position p if we choose the cut at (x,y).

As the target value for $N_2(p;x,y)$ is $\widetilde{N}_2[N](p;(x,y))$, our hypothesis now says that the size of the tree generated by cutting at (x,y) is $10^{N_2(p;x,y)}$. This shows that

$$N_2(p;(x,y)) = \widehat{N}_2(p;(x,y)).$$

Now, the strategy of the proof is to choose the (x,y) that minimizes $N_2(p;x,y)$. By the previous discussion, this is also the cut that minimizes the size of the proof tree. This shows that $\mathrm{cut}^{N_2}(p) = \mathrm{cut}^{\min}(p)$.

Therefore, the proof tree created starting from p and following our strategy, is a minimal one. Therefore,

$$\widetilde{N}[N_2](p) = \widehat{N}(p),$$

and in turn by the hypothesis that N predicts its target value we get

$$N(p) = \widehat{N}(p).$$

This completes the inductive proof of the statements of the theorem. It follows that the proof tree obtained by choosing cuts according to the values of N_2, is a minimal one. □

7.1 Modification by adding the rank

In our current implementation, we modify the above definitions by an additional term in the function $\widehat{N}_2$, hence in the training for N_2. Let $R(p;(x,y))$ be the normalized rank of (x,y) among the available positions, ordered according to the value of $\widetilde{N}_2[N](p;(x,y))$. The normalization means that the rank is multiplied by a factor so it extends from 0 (lowest rank) to 1 (highest rank). We then put

$$\widetilde{N}_2^R[N](p;(x,y))(p;(x,y)) := \widetilde{N}_2[N](p;(x,y))(p;(x,y)) + R(p;(x,y)).$$

The network N_2 is trained to try to approximate this function.

Clearly, the theorem works in the same way: if N gives a correct approximation to the theoretical value then the element of rank 0 corresponds to the minimal value, and this will also be the minimal value of $\widetilde{N}_2^R[N]$. (??? explain in more detail ???).

This modification is based on the idea of including an element of classification in our training for N_2. A pure classification training would be to try to train by cross-entropy to choose the value of (x, y) that is minimal for $\widetilde{N}[N_2](p)$. This was tried but not very successfully, the problem being that information about lower but non-minimal values, that could be of use to the model, is lost in this process. Adding the rank to the score includes a classification aspect, while also not neglecting the non-minimal but lower values, and expands the values of the function we are trying to approximate in the lower ranges (one problem being that the smaller score values can group very near to the minimal value).

It is clearly more difficult to approximate the function with addition of the rank, and this is reflected in the plots of network output along the training process; but due to the combination of the two terms, we also need less accuracy in order to work towards a minimal proof.

8 Samples

Once we are given N, obtaining the sample data for training N_2 to approximate $\widehat{N}_2(p; (x, y))$ is relatively straightforward. Namely, we suppose given some sample positions p, then we choose samples $(p; (x, y))$ (it might not be necessary to include all values of (x, y) for a given p) and the calculation of $\widetilde{N}_2[N](p; (x, y))$ then just requires applying N to the associated positions $p_1, \ldots, p_k$. We note here that these are obtained from the raw positions $p'_1, \ldots, p'_k$ (column replacements) by an application of $p_i := \text{process}(p'_i)$ so some computation is still involved but in a limited way.

On the other hand, given N_2 to obtain sample data for $\widetilde{N}[N_2](p)$ according to our definition, requires a lot of computation. This is because in the definition of $\widetilde{N}[N_2](p)$ we need to calculate $\mathscr{C}^{N_2}(p) := |\mathscr{T}^{N_2}(p)|$ which means calculating the whole proof tree $\mathscr{T}^{N_2}(p)$. It isn't feasible to do this. We propose here two methods to get around this difficulty. They both involve further approximation and a recurrent or reinforcement-learning aspect.

8.1 First method

The first method is to calculate a pruned proof tree $\overline{\mathscr{T}}^{N_2}(p)$. Here, we only make a choice of cuts (according to the N_2-determined strategy $p \mapsto \mathrm{cut}^{N_2}(p)$) to extend the proof tree on some of the active nodes, and prune some other nodes at each stage. In the program it is called "dropout", in other words we drop some of the active nodes. Typically, we fix a number D and at each iteration, treat at most D active nodes and 'drop' the remaining ones. The main way of choosing these is to choose randomly, however we also envision an adaptive choice of the nodes to keep in order to address the issue of imbalanced properties of resulting positions, this will be discussed later.

The proof is then completed significantly faster (typically $D = 100$, 500 or 1000, the proof might finish after around 20 steps so we will have treated on the order of 10000 nodes rather than around 1000000 for a full proof, gaining a factor of 100). Along the way, this process also permits to try to gain an estimate of the size of the fully completed proof from doing only a very partial one.

Now we have a proof $\overline{\mathscr{T}} = \overline{\mathscr{T}}^{N_2}(p)$ in which each node v has a position $p(v)$ and a subproof $\overline{\mathscr{T}}(v)$. We would like to define $\widetilde{N}[N_2](p(v))$ by estimating the value for the full proof

$$\mathscr{C}^{N_2}(p(v)) = |\mathscr{T}^{N_2}(p(v))|.$$

The proof $\overline{\mathscr{T}}(v)$ has a certain number of nodes that remain active since they were dropped; the idea of the estimation is to use the network N itself to provide an estimate. Namely, if v' is a dropped (hence still active) node in $\overline{\mathscr{T}}(v)$ then we add

$$10^{N(p(v'))}$$

into the estimation of the size of $\mathscr{T}^{N_2}(p(v))$. This is to say that

$$|\mathscr{T}^{N_2}(p(v))|^{\mathrm{estimated}} := |\overline{\mathscr{T}}(v)| + \sum_{v'} 10^{N(p(v'))}$$

where the sum is over the dropped nodes v' that are leaves of $\overline{\mathscr{T}}(v)$. We now add the pair

$$\left(p(v), \log_{10}\left(|\mathscr{T}^{N_2}(p(v))|^{\mathrm{estimated}}\right)\right)$$

as a sample point in the training data for N.

8.2 Second method

The second method is a one-step version of the first method. Given a position p, we use N_2 to choose the N_2-minimizing cut (x, y) for p. Let $p_1, \ldots, p_k$ be the positions that are generated from the cut (including doing processing i.e. $p_i = \text{process}(p'_i)$ from the raw positions $p'_1, \ldots, p'_k$). Then we put

$$\widetilde{N}[N_2](p)^{\text{estimated}} := \log_{10}\left(1 + 10^{N(p_1)} + \cdots + 10^{N(p_k)}\right)$$

where more precisely if p_i is either done or impossible then the term $10^{N(p_i)}$ is replaced by the corresponding weight value that we are assigning to this case. We then add the pair

$$\left(p(v), \widetilde{N}[N_2](p)^{\text{estimated}}\right)$$

as a sample point in the training data for N.

9 Sampling issues

The first method of generating samples has the property that the generated samples are in the set of positions that are encountered in an N_2-minimizing proof. Notice that the pruned proof tree $\overline{\mathscr{T}}$ would be a part of a full proof tree made using the N_2-minimizing choice of cuts $\text{cut}^{N_2}(p)$ at each position p. This is both useful and problematic. Useful, because in calibrating a minimal proof we are most interested in the positions that occur in that proof. But problematic because it means that we don't see other positions p that might arise in a better strategy. Therefore, some exploration is needed.

The possibility of doing exploration is afforded by the second sampling method. Indeed, it can be done with the same computation cost starting at any position p. Therefore, we can add samples starting from a wide range of positions.

In practice what we do is to add to our pool of positions a random sampling of all the generated positions p_i that come from various choices of cuts (x, y) that might not be the best possible ones. These may be obtained for example when we are doing the computations of samples for training N_2.

The drawback of the second method is that it is entirely reinforcement-based, in other words it doesn't see to the end of the proof (the importance of doing that was first mentioned to me by D. Alfaya). Theoretically, in the long term after a lot of training, a pair of networks trained only using the second sampling method should generate the correct values, however

it seems useful to include samples taken according to the first method too as a way of accelerating training.

The reader will be asking, why not combine the two methods and run a pruned proof for some steps starting from a position p and collect the sampling data from there. This is certainly another possibility, I don't know whether it can contribute an improvement to the training.

We next comment on the adaptive dropout mentioned above. In this problem, some positions generate a very significantly longer proof than others. Those are the ones that lead to large outcomes in the global proof, so it is better if the neural networks concentrate their training on these cases to some extent. Therefore, in making a pruned proof tree $\overline{\mathscr{T}}$ it will be useful to prune in a way that keeps the nodes that are expected to generate larger sub-trees. This is measured using the existing network N. Thus, in pruning we prioritize (to a certain extent) keeping nodes v that have higher values of $N(p(v))$. These adaptive dropout proof trees are more difficult to use for estimating the global size of the proof, or at least I didn't come up with a good method to do that. Thus, the regular stochastic dropout method is also used, and sampling data is generating using the first sample method from both kinds of proofs.

The stochastic dropout proof trees are used to estimate the size of the N_2-minimizing proof and choose when to apply "early stopping" of the training process. When the estimated size goes below a specified threshold, the training process is stopped and we check how good is our strategy by doing a full proof. This allows us to search for a minimal proof in spite of an oscillatory behavior that will be discussed later.

10 Network architecture

We describe here the architectures that are used for the neural networks N and N_2. We didn't do any systematic hyperparameter search over the possible architectures or possible parameters for the architectures. It could be said, however, that in the course of numerous iterations of this project, various architectures were tried and the one we present here seems to be a reasonably good choice with respect to some previous attempts. It is of course likely that a good improvement could be made.

The input in each case is the position $p = (m, l, r, t)$ consisting of four boolean tensors of sizes $a \times a \times (b+1)$, $a \times (b+1) \times 2$, $(b+1) \times a \times 2$ and $a \times a \times a \times 2$ respectively. Recall that we are interested in the set B^0 that has $(b+1)$ elements. Also, $[I^0| = 2$ explaining the

values of 2 in the last three tensors.

We remark that l is included even though it isn't the subject of any computation (as it corresponds to the fixed input ϕ at the root of the tree) because the neural network will be asked to treat several different initial values ϕ at the same time.

The tensors are taken of type `torch.bool` but are converted to `torch.float` at the start of N and N_2.

We recall that the neural network treats a minibatch all at once, so the tensors have an additional dimension at the start of size $B :=$`batchsize`.

The output of N is a scalar value, so with the batch it is a tensor of size `batchsize`. The output of N_2 is a tensor of size $a \times a$ whose value at $(x, y) \in A \times A$ represents the predicted value if the cut (x, y) is chosen. Here again an additional dimension of size `batchsize` is appended at the start, so the output of N_2 is, in all, a tensor of size `batchsize`$\times a \times a$.

10.1 Input tensor

We would like to input the tensors m, l, r, t. These have sizes as follows, where B denotes the batchsize.

$$\begin{aligned} \text{size } m &= B \times a \times a \times (b+1) \\ \text{size } l &= B \times a \times (b+1) \times 2 \\ \text{size } r &= B \times (b+1) \times a \times 2 \\ \text{size } t &= B \times a \times a \times a \times 2 \end{aligned}$$

We would like to combine these together into an input vector that will make sense for learning.

As input into a fully connected layer, these tensors could just be flattened into vectors (i.e. tensors of size $B \times v$) and concatenated. This would give an input of length

$$v = a^2(b+1) + 4a(b+1) + 2a^3.$$

In order to preserve more of the tensor structure, we prepare the tensors for input into a 2-dimensional convolution layer. For this, we transform them into tensors of size $B \times f \times a \times a$ by placing the dimensions that are different from a into the first "feature" variable, including the middle dimension of t here also, and expanding the l and r tensors by a factor of a to give them a size that is a multiple of $a \times a$. We then concatenate these along the feature dimension.

More precisely, m will have $(b+1)$ features, l and r have $2(b+1)$ features, and t has $2a$ features. Thus our input tensor is of size $B \times f \times a \times a$ where B is the batchsize and

$$f = 5(b+1) + 2a.$$

The choice of method to prepare the input tensor is the first necessary design choice. Many possibilities were envisioned, including concatenation of various permutations of these tensors, and convolution layers of dimension 1, 2 or 3.

The method we choose to use depends of course on the processing to follow. The preparation method discussed above is not necessarily the best one but it seems to work pretty well.

10.2 Data flow

The basic trade-offs that need to be considered are the question of how data flows through the layers, versus computational time for a forward pass, and also training time needed for calculation of the gradients and back-propagation.

We may illustrate this by looking at the idea of starting with a fully-connected or *linear* layer. Let's consider for example the case $(a, b) = (5, 3)$. Then the fully flattened input dimension from above is $v = a^2(b+1) + 4a(b+1) + 2a^3 = 430$. A fully connected layer towards n neurons that would be declared as follows:

```
self.linA = nn.Linear(430,n)
```

is going to involve $430n$ weight parameters (plus n bias parameters that we don't worry about). If we take, say $n = 100$ this gives 43000 parameters for this layer only. Furthermore, the problem of size of data goes down from 430 to 100 so it persists. On the other hand, we could take for example $n = 32$ and this would give 13760 weight parameters and yield a very manageable size of tensor to deal with further. The problem here is that it is trying to pack all the information from 430 values (that are either 0 or 1) into a 32 dimensional space. All further operations will depend only on the 32 parameters.

This constricts the flow of data into the network, something that we would like to avoid. A similar consideration applies at the output stage. In the middle, some constriction might even be desireable as long as the data can also take a different path by "skip connections".

10.3 Convolution layers

It seems that we should be able to do better. If we start with a convolutional layer, we notice (in the same example $(a, b) = (5, 3)$) that the number of features is $f = 5(b + 1) + 2a = 30$ spread over a 5×5 array. The first convolutional layers can therefore with no problem maintain or even increase this number of features.

The price here is that our set of $a = 5$ vectors has an ordering that is not based on any strong natural consideration. Therefore, the convolutional aspect needs to be higher in order to obtain a good mixing between the features at different locations (x, y).

It turns out that a weak ordering property is in fact obtained by our sieve process of choice of the initial matrix ϕ: the sieve process that we use will make a choice of ordering for each equivalence class of input, and our implementation has the property that it tends to put more 1's as we go towards one of the corners of ϕ. This is admittedly not a very convincing justification for why it would be natural to use a convolutional structure, so there is undoubtedly room for having a better architecture that takes into account the tensor property but without requiring an ordering ("graph neural networks" GNN could come to mind, see for example [6] and the references therein).

In order to mix the values between different locations, we choose to use alternating convolution windows of sizes $[5, 1]$ and $[1, 5]$. In a window of size $[5, 1]$ it means that the feature values at location (x, y) are combined with those of locations $(x-2, y), (x-1, y), (x, y), (x+1, y), (x+2, y)$. Window size $[1, 5]$ means the same but with y. In our use cases, the number of values is a, usually ≤ 5.

An additional trick is available to reduce the number of parameters: grouped convolution places the features into groups and applies a different convolution to each group. A grouped $2d$ convolution with a window of size $[5, 1]$ (that is to say, extending by 2 elements in each direction in the y variable), with $8n$ input features, $8n$ output features and n groups, has

$$n \cdot 8 \cdot 8 \cdot 5 = 320n$$

parameters, whereas the same non-grouped version would have $320n^2$ parameters. The use of grouped convolution can allow us to maintain a good size of data flow through a layer, while diminishing the number of parameters and thereby improving the computational and training time.

The grouped convolution layer of the previous paragraph is declared as follows.

```
self.convA = nn.Conv2d(8*n,8*n,[5,1],padding = [2,0],padding_mode = 'circular',groups = n)
```

We note that the group idea can also be applied in a linear layer, by writing the linear layer as a $1d$ convolution that is going to be applied on a trivial one-element array.

11 Learning runs

In this section we show the plots of results of some runs of our network on various cases. The value of σ indicates the choice of initial instance $\phi \in \Sigma$. The captions include information on the number of trainable parameters in the global and local networks, and the numbers of iterations in the loops of training operations and sample proofs.

11.1 Training segments

Each phase of training involves a succession of loops with various mini-batch sizes and numbers of gradient descent steps per minibatch. A given "training segment" involves the the following steps:

global network N		
mini-batches	minibatch size	descent steps per batch
2	20	20
1	30	30
2	40	10
5	60	10
3	20	8
3	40	5
5	30	3

local network N_2		
mini-batches	minibatch size	descent steps per batch
3	20	20
1	30	15
3	60	4
3	40	10
3	20	3
3	40	2
3	30	1

In all this gives, for each training segment, the following numbers:

- for the global network, 21 minibatches with 780 samples and 194 gradient descent steps
- for the local network, 19 minibatches with 660 samples and 135 gradient descent steps.

All of these choices are arbitrary. The basic ideas are to overtrain at the start of the training segment, doing a high number of gradient descent steps on a small minibatch, then to train more gradually towards the end of the segment. The gradual part at the end is due to the fact that the networks will be used for further proofs (either sampling or doing the

actual proofs) only at the end of the training segment. I couldn't say how good these choices are.

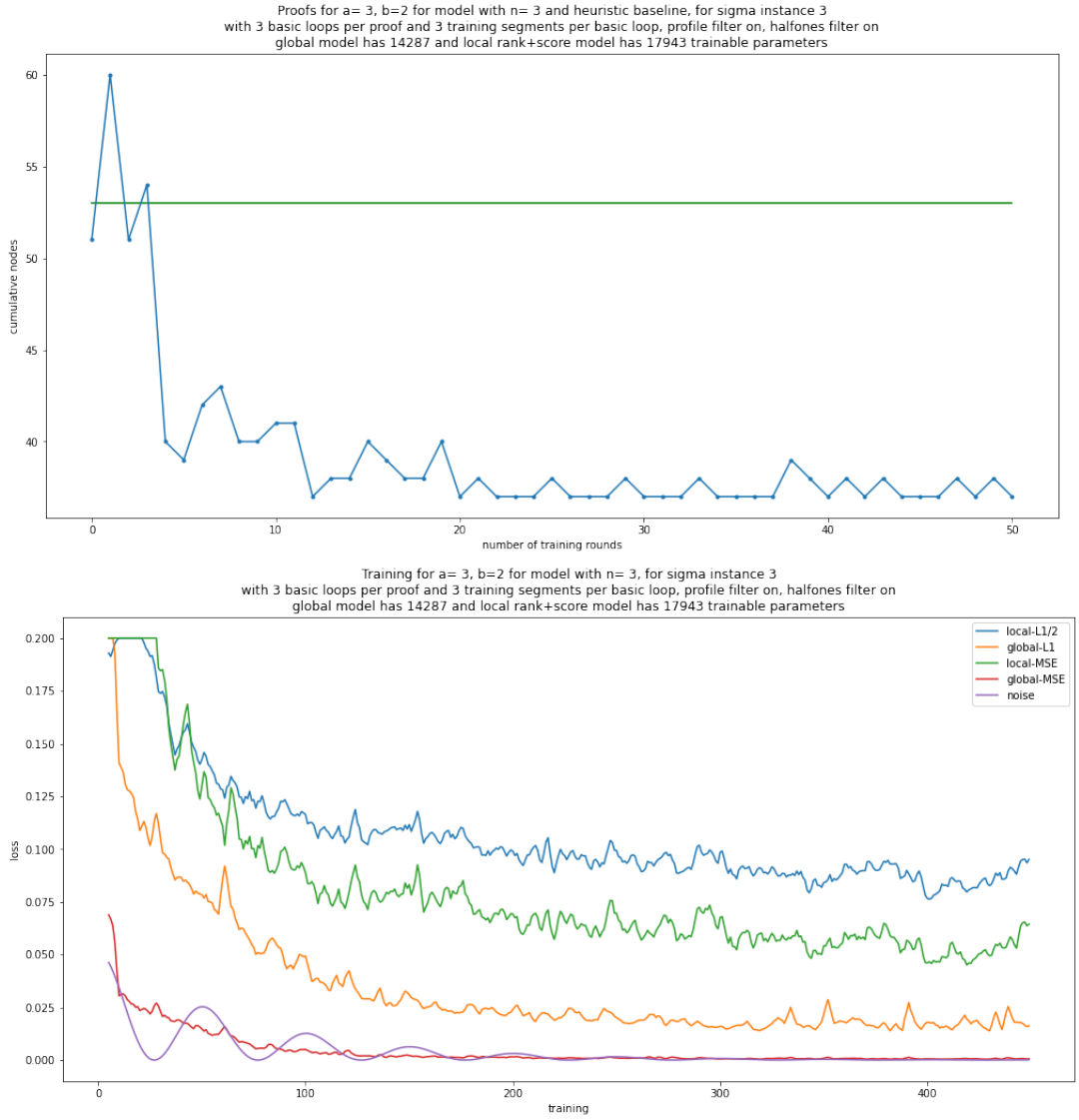
In the diagrams shown below, the caption gives the number of basic loop iterations per proof, and the number of training segments per basic loop. Therefore, the total number of gradient descent steps (resp. samples) in between each pair of proofs will be the product of the above values (194 or 135, resp. 780 or 660) by the number of basic loop iterations and then by the number of training segments per basic loop.

11.2 Heuristic baseline

For comparison, we give the results of an heuristic benchmark strategy (horizontal line on the graphs). This strategy is obtained by choosing an ordering of the locations (x, y) and just following the rule of making a cut at the first available location. It turns out that a pretty good result is obtained by taking the following order: first $(0, 0)$, then $(1, 1)$, then $(1, 0)$, then $(0, 1)$, then continuing with the remaining (x, y) in lexicographic order starting with $(0, 2)$. That strategy was found almost by accident. It seems to give a reasonable baseline number for comparison, which in some cases is the minimum. The learning mechanism is able to do better (or just as well when it is the minimum).

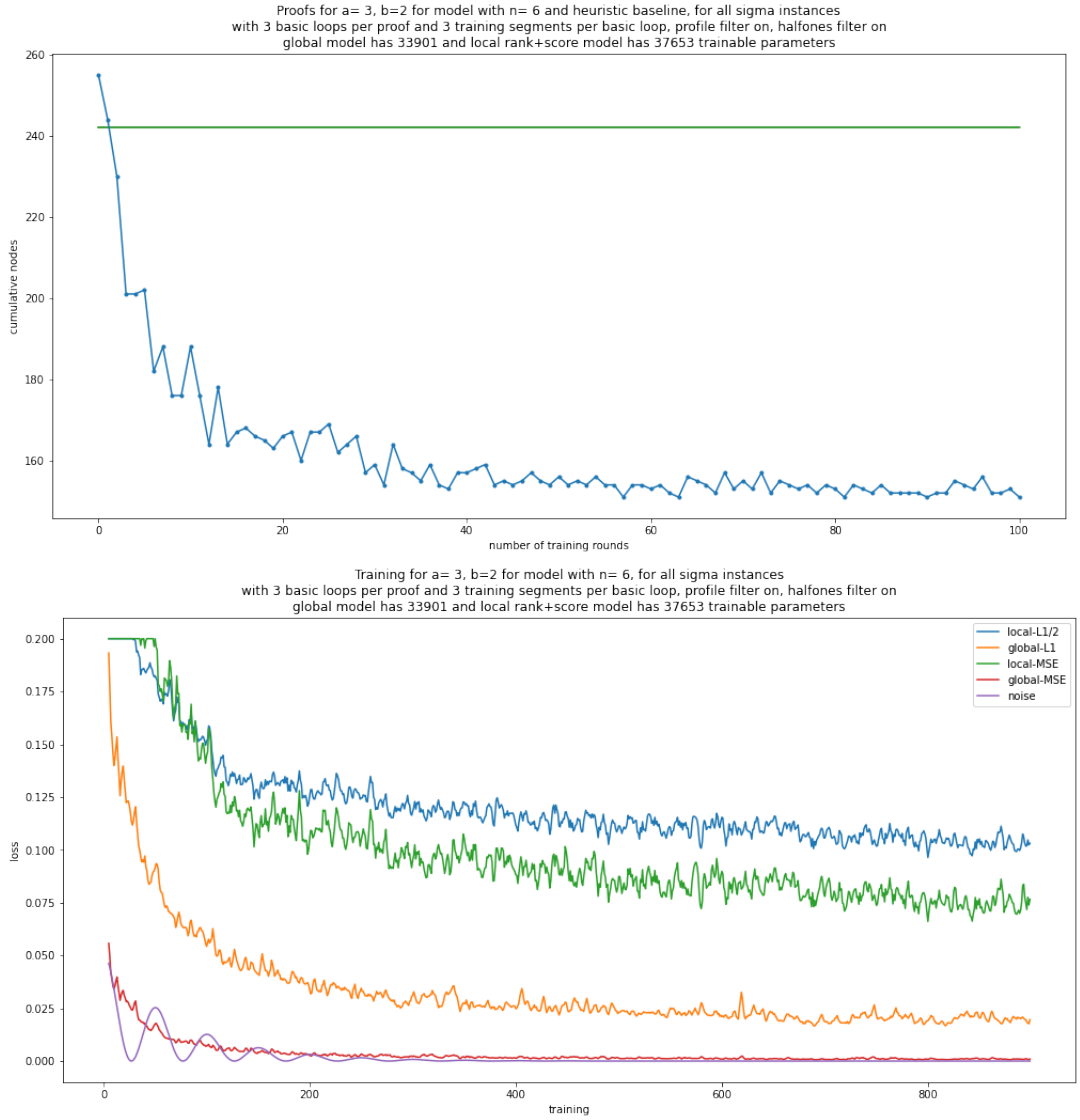
11.3 Size $(3, 2)$

Here is the most difficult case for size $(a, b) = (3, 2)$, namely $\sigma = 3$. See the next section for a discussion of these cases. The first graph is the number of proof nodes in the sequence of proofs, and the second graph gives various loss functions of the training as the machine evolves. These are all from a "cold start", that is to say the neural networks are given their randomized initial state as provided by the standard pytorch layer implementations. Several loss data points (3 per basic loop, the number of basic loops is given in the caption, in this case it is also 3 so we have 9 loss values for each proof value) are taken in between each pair of proofs, so the horizontal labels aren't the same.



We note that it looks like the theoretical minimum is 37, which is indeed the case, see Theorem 12.1 below.

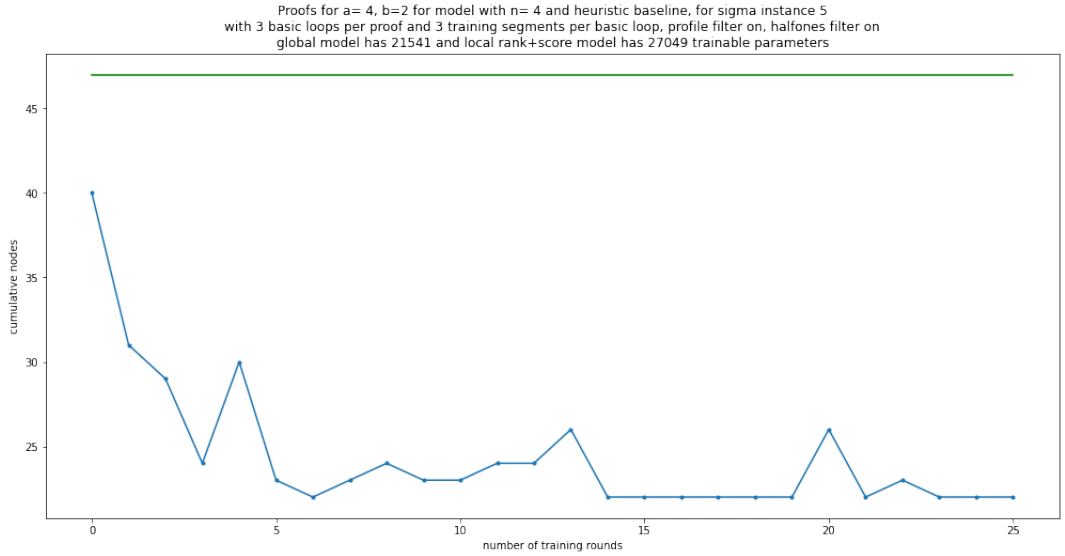
The other values of σ are generally easier to treat individually. We record here the result of looking at the full collection of proofs with the 13 initial values of σ simultaneously.

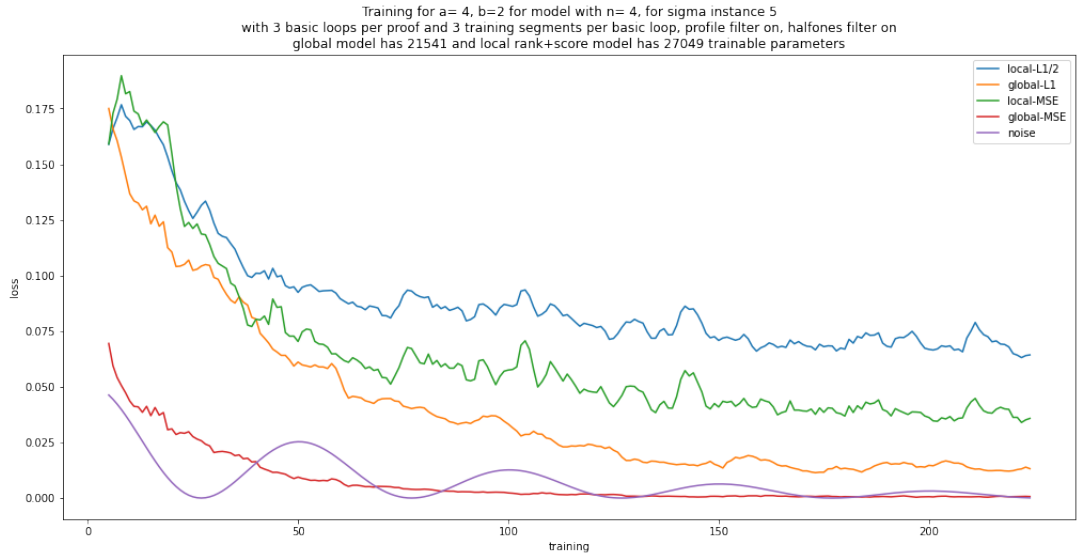


The theoretical minimum value of 151 (see Theorem 12.1) is attained at several proofs (numbers 57, 63, 81, 90, 100), although the model has a tendency to stabilize around a slightly higher value of 152 or 153.

11.4 Size $(4, 2)$

Here is a case for size $(a, b) = (4, 2)$, with $\sigma = 5$.

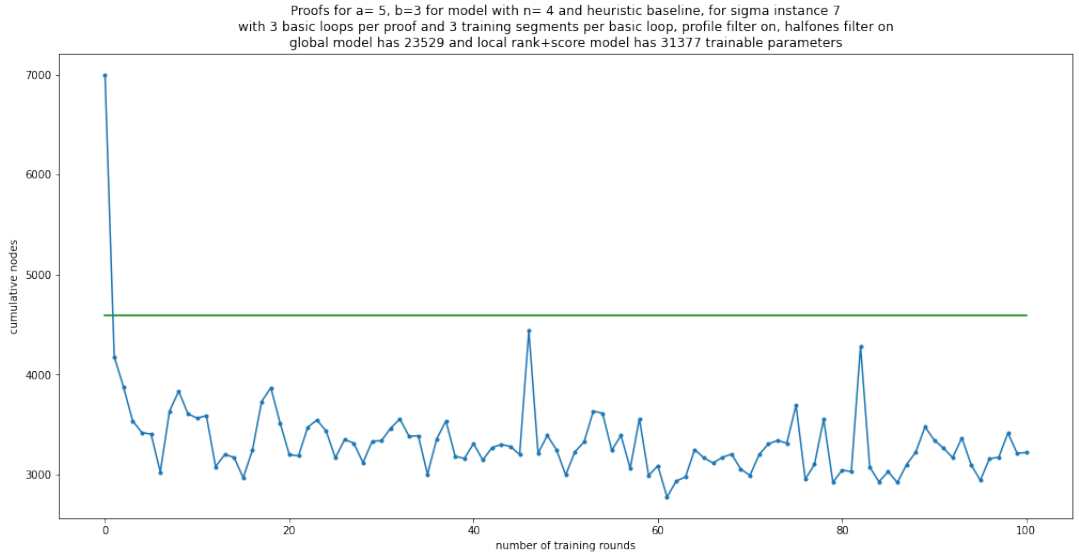


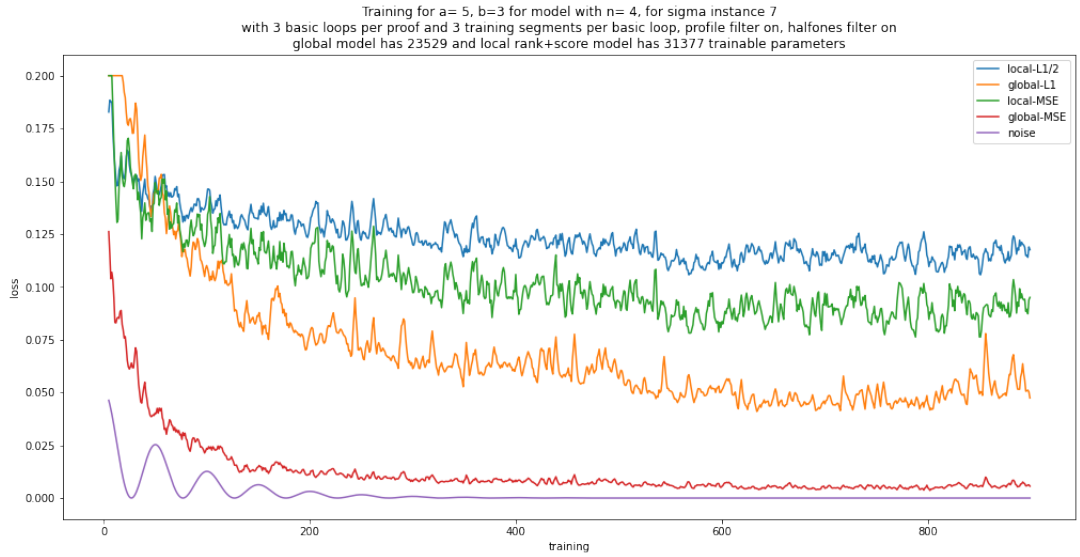


We conjecture that the theoretical minimum in this case is the value 22 that is attained first at proof number 6 and often at the end.

11.5 Size $(5, 3)$

Here is a sample case for size $(a, b) = (5, 3)$, namely $\sigma = 7$. This is the first one in the range of suggested locations.

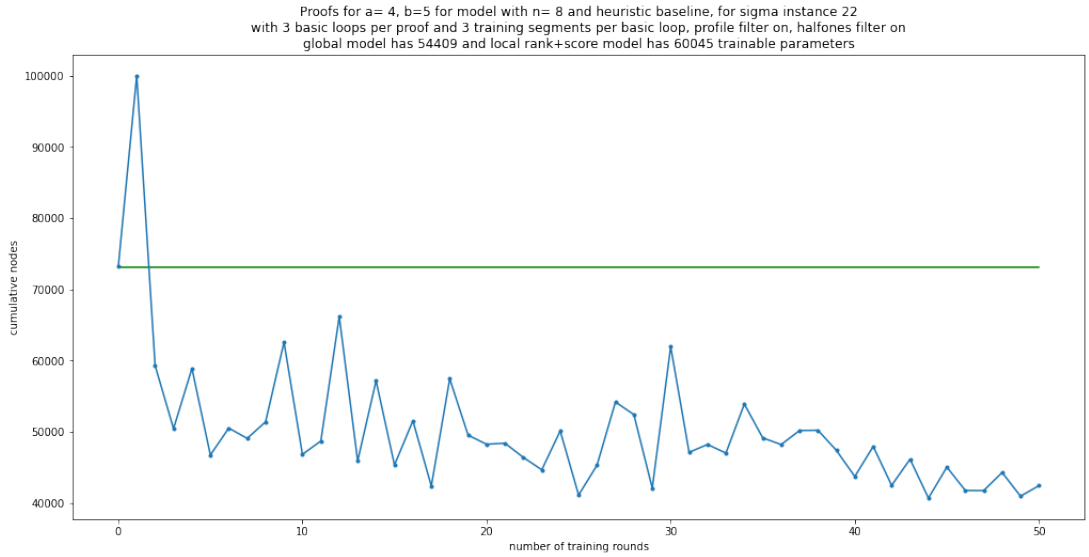


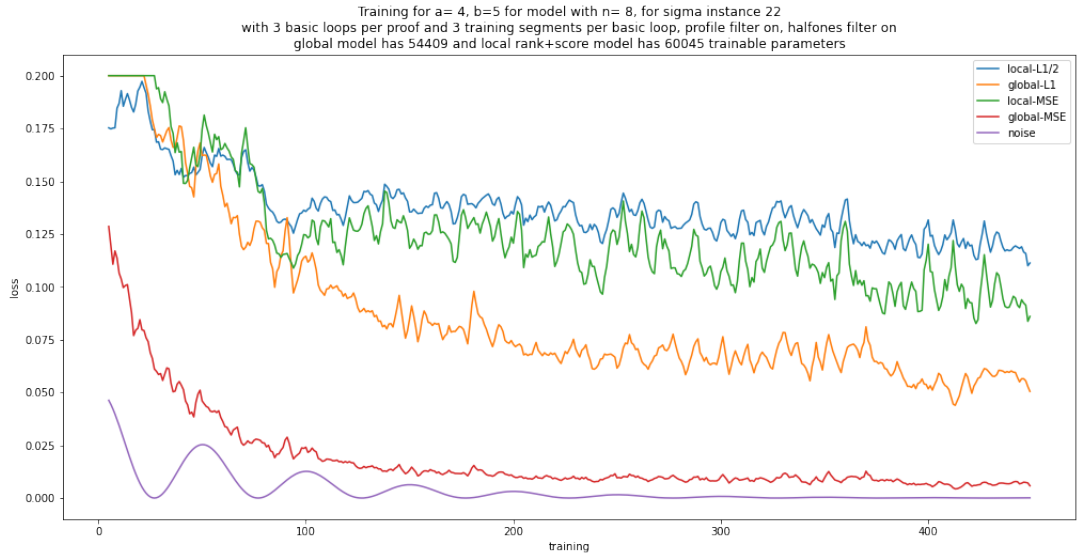


Here the minimal value attained, at around proof number 60, is 2773. We don't know how far that might be from the theoretical minimum.

11.6 Size $(4, 5)$

Here is a sample case for size $(a, b) = (4, 5)$, namely $\sigma = 22$. Again, this is the first in the range of suggested locations. This training and proving process, for a cycle of 50 proofs, took 2 hours 35 minutes on Colab GPU.





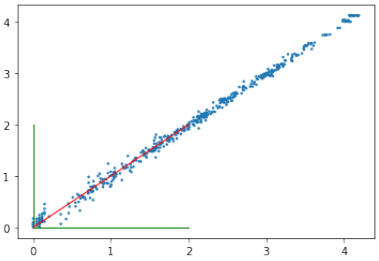
The minimal value attained, at proof number 44, is 40720 (with anew 40984 at proof 49). We don't know how far that might be from the theoretical minimum.

In this case, that the number of nodes in the proof tree is of the same order of magnitude as the number of trainable parameters in the neural network. Here we have chosen a larger value $n = 8$ for the size of the networks in view of the larger size of the problem, leading to 54409 global and 60045 local parameters. The output data for choice of cut at a node involves at least 2 and up to $a^2 = 16$ values, so in all we can say that the number of parameters for network N_2 is significantly smaller than the number of data values required to do a single proof.

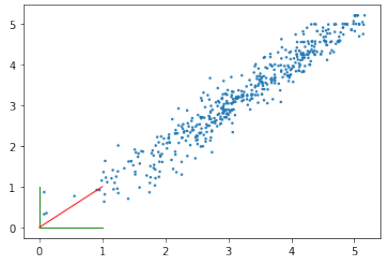
Here are plots of the predictions of the global and local networks N and N_2, after having

trained for the cycle 50 proofs.

global



local



Recall that training data for N_2 includes the rank plus the score, see the modification 7.1, that is why it doesn't appear all that accurate even at this stage.

12 Proof of minimality

We now go back to smaller values of (a, b), namely let's look at the case $a = 3$ and $b = 2$. There are 13 σ-instances initiating the proof. If we choose one of the ones with a larger proof size, namely $\sigma = 3$, the training process seems to lead to a minimum of nodes = 37. It is natural to conjecture that this is in fact the theoretical minimum for the number of nodes in the proof.

In view of the small size of this example it was feasible to find the minimal size and show that it is indeed 37. We calculate the theoretical minima for all cases of size $(a, b) = (3, 2)$. Note that these proofs use the profile filter and half-ones filter (see 4.1). For $\sigma = 3$ it wasn't possible to find the minimum without the filters, since the depth becomes too big (the baseline number of nodes in that case is 537).

Theorem 12.1. *For the case $a = 3$ and $b = 2$, the minimal number of nodes $\nu_{\min}$ in a classification proof according to our scheme is given in the following table:*

σ	0	1	2	3	4	5	6	7	8	9	10	11	12
$\nu_{\min}$	9	21	23	37	11	5	3	5	3	11	3	3	17

Our pair of neural networks configured and trained as described in previous sections is able to find a minimal proof in each case. The minimum for all σ instances together is 151*, and the model is able to find this value, although sparsely (see the graphics above).*

Proof. (Indication) We calculate the minimal size of proof in the following way. We successively create a tree-like object where each vertex corresponds to the result of a succession of cuts with its associated mask. Below a vertex v are vertices corresponding to each of

the locations (x, y, p) that are available in the mask associated to v, and we then place the mask resulting from cutting at (x, y, p) then processing. Vertices corresponding to done or impossible masks are not included. As this object is being created, we also run the proof model on each new set of vertices. This gives an upper bound for the number of nodes below a given one in the proof. The lower bound on new vertices is set to 1. The upper and lower bounds are then propagated upwards in the tree, by the rule that the number of nodes associated to the cut (x, y) at a vertex v, is the sum over p of the number of nodes at each available (x, y, p). Then, the number of nodes associated to v is equal to the minimum of these values over available (x, y), plus 1 for v itself. This propagation is the same for the lower and upper bounds.

The tree is furthermore pruned at each successive step by the following rules: if a vertex gets a lower bound equal to its upper bound then it is removed from play. Also, if a collection of vertices associated to (x, y) yield a lower bound that is greater than the minima of the upper bounds over all (x, y) under a given vertex, then that collection of vertices will not yield anything useful and they are pruned.

We note that the pruning is essential otherwise the size of the tree needed to calculate the minimum would be way too big.

In the pruning process, a very small improvement may be seen by using our proving scheme and trained model, as opposed to using the baseline heuristic strategy, to calculate the upper bounds.

The tree extension, proof computation, propagation and pruning steps are repeated until the lower bound and upper bound at the root vertex coincide, this is then the minimal value. For runtime reasons, we calculated separately the bounds for the 27 vertices obtained after the first cut.

Warning: my implementation of the above strategy of proof is not certified to be correct, so this should only be considered as an indication of proof. These minimal values do agree with the smallest values found by the neural networks, so it seems likely that they are correct.

We record here the matrices giving number of nodes depending on the initial cut location (x, y). The minimal value for the instance σ is then $\nu_{\min} = k + 1$ where k is the minimal value of the entries in the matrix. The $+1$ is for the root node itself.

$$\sigma = 0 \quad \begin{pmatrix} 8 & 8 & 8 \\ 8 & 8 & 8 \\ 8 & 8 & 8 \end{pmatrix} \quad \nu_{\min} = 9 \quad \dots \quad \sigma = 1 \quad \begin{pmatrix} 34 & 26 & 26 \\ 20 & 20 & 20 \\ 20 & 20 & 20 \end{pmatrix} \quad \nu_{\min} = 21$$

$$\sigma = 2 \quad \begin{pmatrix} 30 & 29 & 28 \\ 29 & 30 & 28 \\ 22 & 22 & 22 \end{pmatrix} \quad \nu_{\min} = 23 \quad \ldots \quad \sigma = 3 \quad \begin{pmatrix} 36 & 36 & 36 \\ 36 & 36 & 36 \\ 36 & 36 & 36 \end{pmatrix} \quad \nu_{\min} = 37$$

$$\sigma = 4 \quad \begin{pmatrix} 18 & 13 & 13 \\ 12 & 12 & 10 \\ 12 & 10 & 12 \end{pmatrix} \quad \nu_{\min} = 11 \quad \ldots \quad \sigma = 5 \quad \begin{pmatrix} 4 & 6 & 7 \\ 6 & 4 & 7 \\ 5 & 5 & 5 \end{pmatrix} \quad \nu_{\min} = 5$$

$$\sigma = 6 \quad \begin{pmatrix} 2 & 3 & 5 \\ 3 & 2 & 5 \\ 3 & 3 & 3 \end{pmatrix} \quad \nu_{\min} = 3 \quad \ldots \quad \sigma = 7 \quad \begin{pmatrix} 4 & 6 & 6 \\ 6 & 4 & 5 \\ 6 & 5 & 4 \end{pmatrix} \quad \nu_{\min} = 5$$

$$\sigma = 8 \quad \begin{pmatrix} 2 & 3 & 3 \\ 3 & 2 & 3 \\ 3 & 3 & 2 \end{pmatrix} \quad \nu_{\min} = 3 \quad \ldots \quad \sigma = 9 \quad \begin{pmatrix} 14 & 14 & 13 \\ 14 & 14 & 13 \\ 10 & 10 & 10 \end{pmatrix} \quad \nu_{\min} = 11$$

$$\sigma = 10 \quad \begin{pmatrix} 2 & 3 & 3 \\ 3 & 2 & 4 \\ 3 & 4 & 2 \end{pmatrix} \quad \nu_{\min} = 3 \quad \ldots \quad \sigma = 11 \quad \begin{pmatrix} 2 & 2 & 3 \\ 2 & 2 & 3 \\ 3 & 3 & 2 \end{pmatrix} \quad \nu_{\min} = 3$$

$$\sigma = 12 \quad \begin{pmatrix} 16 & 16 & 16 \\ 16 & 16 & 16 \\ 16 & 16 & 16 \end{pmatrix} \quad \nu_{\min} = 17$$

Note that for σ instances 0, 3 and 12 the number of nodes doesn't depend on the first cut.

Of course it depends on subsequent cuts. Let us consider this question in further detail for the case $\sigma = 3$. Here the minimal value doesn't depend on the first cut location, but it does depend on the second one as we shall see.

	$y = 0$	$y = 1$	$y = 2$
$x = 0$	$13 + 10 + 13$	$14 + 10 + 12$	$14 + 10 + 12$
$x = 1$	$14 + 10 + 12$	$13 + 10 + 13$	$14 + 10 + 12$
$x = 2$	$14 + 10 + 12$	$14 + 10 + 12$	$13 + 10 + 13$

The table entries refer to the number of nodes at the values $p = 0$, $p = 1$ and $p = 2$. Thus, $14 + 10 + 12$ indicates 14 nodes for $p = 0$, 10 nodes for $p = 1$ and 12 nodes for $p = 2$. Thus, for example, the table indicates that the count of nodes at $(x, y, p) = (0, 0, 0)$ is 13, whereas the count for $(x, y, p) = (1, 2, 0)$ is 14.

We observe that the sums are 36 in each location. Adding one for the root node gives the desired value of 37 nodes. The table shows that the first cut may be chosen arbitrarily: all choices of (x, y) can correspond to minimal proofs.

Continue by looking at the node values for the next choice of cuts in a few examples. We'll consider a node v obtained at location (x, y, p) from the first choice of cut. Recall that a choice of cut is a choice of (x, y) yielding in this case three vertices below corresponding to $(x, y, 0)$,$(x, y, 1)$ and $(x, y, 2)$. We give the matrix $(n_{x',y'})$ that gives the number of nodes (but not including 1 for v, that is added into $\nu_{\min}$) corresponding to a second cut (x', y'). The values (x', y') corresponding to the previous cut are unavailable.

- vertex from first cut at $(0, 0, 0)$ lower bounds for next cut $\begin{bmatrix} - & 12 & 12 \\ 12 & 13 & 14 \\ 12 & 14 & 13 \end{bmatrix}$ $\nu_{\min} = 13$
- vertex from first cut at $(0, 0, 1)$ lower bounds for next cut $\begin{bmatrix} - & 9 & 9 \\ 9 & 9 & 9 \\ 9 & 9 & 9 \end{bmatrix}$ $\nu_{\min} = 10$
- vertex from first cut at $(0, 0, 2)$ lower bounds for next cut $\begin{bmatrix} - & 14 & 14 \\ 12 & 13 & 15 \\ 12 & 15 & 13 \end{bmatrix}$ $\nu_{\min} = 13$

These are going to enter into the full minimum value at the cut location $(x, y) = (0, 0)$. In the first and third cases, the neural network has to choose correctly the next cut in order to get a minimal value.

This completes our summary of the computations that go into the proof. □

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