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Citation for published version:

Link:
Link to publication record in Edinburgh Research Explorer

Document Version:
Peer reviewed version

Published In:
The 34th International Conference on Machine Learning (ICML 2017)

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Learning Continuous Semantic Representations of Symbolic Expressions

Miltiadis Allamanis ¹  Pankajan Chanthirasegaran ²  Pushmeet Kohli ³  Charles Sutton ² ⁴

Abstract

Combining abstract, symbolic reasoning with continuous neural reasoning is a grand challenge of representation learning. As a step in this direction, we propose a new architecture, called neural equivalence networks, for the problem of learning continuous semantic representations of algebraic and logical expressions. These networks are trained to represent semantic equivalence, even of expressions that are syntactically very different. The challenge is that semantic representations must be computed in a syntax-directed manner, because semantics is compositional, but at the same time, small changes in syntax can lead to very large changes in semantics, which can be difficult for continuous neural architectures. We perform an exhaustive evaluation on the task of checking equivalence on a highly diverse class of symbolic algebraic and boolean expression types, showing that our model significantly outperforms existing architectures.

1. Introduction

Combining abstract, symbolic reasoning with continuous neural reasoning is a grand challenge of representation learning. This is particularly important while dealing with exponentially large domains such as source code and logical expressions. Symbolic notation allows us to abstractly represent a large set of states that may be perceptually very different. Although symbolic reasoning is very powerful, it also tends to be hard. For example, problems such as the satisfiability of boolean expressions and automated formal proofs tend to be NP-hard or worse. This raises the exciting opportunity of using pattern recognition within symbolic reasoning, that is, to learn patterns from datasets of symbolic expressions that approximately represent semantic relationships. However, apart from some notable exceptions (Alemi et al., 2016; Loos et al., 2017; Zaremba et al., 2014), this area has received relatively little attention in machine learning. In this work, we explore the direction of learning continuous semantic representations of symbolic expressions. The goal is for expressions with similar semantics to have similar continuous representations, even if their syntactic representation is very different. Such representations have the potential to allow a new class of symbolic reasoning methods based on heuristics that depend on the continuous representations, for example, by guiding a search procedure in a symbolic solver based on a distance metric in the continuous space. In this paper, we make a first essential step of addressing the problem of learning continuous semantic representations (SEMVECs) for symbolic expressions. Our aim is, given access to a training set of pairs of expressions for which semantic equivalence is known, to assign continuous vectors to symbolic expressions in such a way that semantically equivalent, but syntactically diverse expressions are assigned to identical (or highly similar) continuous vectors. This is an important but hard problem; learning composable SEMVECs of symbolic expressions requires that we learn about the semantics of symbolic elements and operators and how they map to the continuous representation space, thus encapsulating implicit knowledge about symbolic semantics and its recursive abstractive nature. As we show in our evaluation, relatively simple logical and polynomial expressions present significant challenges and their semantics cannot be sufficiently represented by existing neural network architectures.

Our work in similar in spirit to the work of Zaremba et al. (2014), who focus on learning expression representations to aid the search for computationally efficient identities. They use recursive neural networks (TREENN)¹ (Socher et al., 2012) for modeling homogenous, single-variable polynomial expressions. While they present impressive results, we find that the TREENN model fails when applied to more complex symbolic polynomial and boolean expressions. In particular, in our experiments we find that TREENNs tend to assign similar representations to syntactically similar expressions, even when they are semantically very different. The underlying conceptual problem is how to develop a continuous representation that follows syntax but not too much, ²

¹To avoid confusion, we use TREENN for recursive neural networks and RNN for recurrent neural networks.

Work started when M. Allamanis was at Edinburgh. This work was done while P. Kohli was at Microsoft. ¹ Microsoft Research, Cambridge, UK ² University of Edinburgh, UK ³ DeepMind, London, UK ⁴ The Alan Turing Institute, London, UK. Correspondence to: Miltiadis Allamanis <t-mialla@microsoft.com>.

Proceedings of the 34th Annual Conference on Machine Learning, Sydney, Australia, PMLR 70, 2017. Copyright 2017 by the author(s).
that respects compositionality while also representing the fact that a small syntactic change can be a large semantic one.

To tackle this problem, we propose a new architecture, called neural equivalence networks (EqNET). EqNETs learn how syntactic composition recursively composes SEMVECs, like a TREEENN, but are also designed to model large changes in semantics as the network progresses up the syntax tree. As equivalence is transitive, we formulate an objective function for training based on equivalence classes rather than pairwise decisions. The network architecture is based on composing residual-like multi-layer networks, which allows more flexibility in modeling the semantic mapping up the syntax tree. To encourage representations within an equivalence class to be tightly clustered, we also introduce a training method that we call subexpression autoencoding, which uses an autoencoder to force the representation of each subexpression to be predictable and reversible from its syntactic neighbors. Experimental evaluation on a highly diverse class of symbolic algebraic and boolean expression types shows that EqNETs dramatically outperform existing architectures like TREEENN and RNNs.

To summarize, the main contributions of our work are: (a) We formulate the problem of learning continuous semantic representations (SEMVECS) of symbolic expressions and develop benchmarks for this task. (b) We present neural equivalence networks (EqNETs), a neural network architecture that learns to represent expression semantics onto a continuous semantic representation space and how to perform symbolic operations in this space. (c) We provide an extensive evaluation on boolean and polynomial expressions, showing that EqNETs perform dramatically better than state-of-the-art alternatives. Code and data are available at groups.inf.ed.ac.uk/cup/semvec.

2. Model

In this work, we are interested in learning semantic, compositional representations of mathematical expressions, which we call SEMVECS, and in learning to generate identical representations for expressions that are semantically equivalent, i.e. they belong to the same equivalence class. Equivalence is a stronger property than similarity, which has been the focus of previous work in neural network learning (Chopra et al., 2005), since equivalence is additionally a transitive relationship.

Problem Hardness. Finding the equivalence of arbitrary symbolic expressions is a NP-hard problem or worse. For example, if we focus on boolean expressions, reducing an expression to the representation of the false equivalence class amounts to proving its non-satisfiability — an NP-complete problem. Of course, we do not expect to circumvent an NP-complete problem with neural networks. A network for solving boolean equivalence would require an exponential number of nodes in the size of the expression if \( P \neq NP \). Instead, our goal is to develop architectures that efficiently learn to solve the equivalence problems for expressions that are similar to a smaller number of expressions in a given training set. The supplementary material shows a sample of such expressions that illustrate the hardness of this problem.

Notation and Framework. To allow our representations to be compositional, we employ the general framework of recursive neural networks (TREEENN) (Socher et al., 2012, 2013), in our case operating on tree structures of the syntactic parse of a formula. Given a tree \( T \), TREEENN learn distributed representations for each node in the tree by recursively combining the representations of its subtrees using a neural network. We denote the children of a node \( n \) as \( \text{ch}(n) \) which is a (possibly empty) ordered tuple of nodes. We also use \( \text{par}(n) \) to refer to the parent node of \( n \). Each node in our tree has a type, e.g. a terminal node could be of type “a” referring to the variable \( a \) or of type “\&\&” referring to a node of the logical \&\& (\&\&) operation. We refer to the type of a node \( n \) as \( \tau_n \). In pseudocode, TREEENN retrieve the representation of a tree \( T \) rooted at node \( \rho \) by invoking the function \( \text{TREEENN}(\rho) \) that returns a vector representation \( r_\rho \in \mathbb{R}^P \), i.e., a SEMVEC. The function is defined as

\[
\begin{align*}
\text{TREEENN} \text{ (current node } n) & \\
\text{if } n \text{ is not a leaf then} & \\
& r_n \leftarrow \text{COMBINE} (\text{TREEENN}(c_0), \ldots, \text{TREEENN}(c_k), \tau_n), \\
\text{where } (c_0, \ldots, c_k) &= \text{ch}(n) \\
\text{else} & \\
& r_n \leftarrow \text{LOOKUPLEAFEMBEDDING}(\tau_n) \\
& \text{return } r_n
\end{align*}
\]

The general framework of TREEENN allows two points of variation, the implementation of LOOKUPLEAFEMBEDDING and COMBINE. Traditional TREEENN (Socher et al., 2013) define LOOKUPLEAFEMBEDDING as a simple lookup operation within a matrix of embeddings and COMBINE as a single-layer neural network. As discussed next, these will both prove to be serious limitations in our setting. To train these networks to learn SEMVECS, we will use a supervised objective based on a set of known equivalence relations (see Section 2.2).

2.1. Neural Equivalence Networks

Our domain requires that the network learns to abstract away syntax, assigning identical representations to expressions that may be syntactically different but semantically equivalent, and also assigning different representations to expressions that may be syntactically very similar but non-equivalent. In this work, we find that standard neural architectures do not handle well this challenge. To represent semantics from syntax, we need to learn to recursively compose and decompose semantic representations and re-
move syntactic “noise”. Any syntactic operation may signif-
ificantly change semantics (e.g. negation, or appending
∧FALSE) while we may reach the same semantic state
through many possible operations. This necessitates us-
ning high-curvature operations over the semantic repre-
sentation space. Furthermore, some operations are semantically
reversible and thus we need to learn reversible semantic
representations (e.g. ¬¬A and A should have an identical
SEMVECs). Based on these, we define neural equivalence
networks (EQNET), which learn to compose represen-
tations of equivalence classes into new equivalence classes (Fig-
ure 1a). Our network follows the TREEENN architecture,
i.e. is implemented using TREEENN to model the composi-
tional nature of symbolic expressions but is adapted based
on the domain requirements. The extensions we introduce
have two aims: first, to improve the network training; and
second, and more interestingly, to encourage the learned
representations to abstract away surface level information
while retaining semantic content.

The first extension that we introduce is to the network struc-
ture at each layer in the tree. Traditional TREEENN (Socher
et al., 2013) use a single-layer neural network at each tree
node. During our preliminary investigations and in Sec-
tion 3, we found that single layer networks are not ade-
quately expressive to capture all operations that transform
the input SEMVECs to the output SEMVEC and maintain
semantic equivalences, requiring high-curvature operations.
Part of the problem stems from the fact that within the
Euclidean space of SEMVECs some operations need to be
non-linear. For example a simple XOR boolean operator re-
quires high-curvature operations in the continuous semantic
representation space. Instead, we turn to multi-layer neural
networks. In particular, we define the network as shown
in the function COMBINE in Figure 1b. This uses a two-
layer MLP with a residual-like connection to compute the
SEMVEC of each parent node in that syntax tree given that
of its children. Each node type \( \tau_n \), e.g., each logical oper-
ator, has a different set of weights. We experimented with
deeper networks but this did not yield any improvements.

However, as TREEENN becomes deeper, they suffer from
optimization issues, such as diminishing and exploding gra-
dients. This is essentially because of the highly composi-
tional nature of tree structures, where the same network
(i.e. the COMBINE non-linear function) is used recursively,
causing it to “echo” its own errors and producing unstable
feedback loops. We observe this problem even with only two-
layer MLPs, as the overall network can become quite deep
when using two layers for each node in the syntax
tree. We resolve this issue in the training procedure by con-
straining each SEMVEC to have unit norm. That is, we
set \( \text{LOOKUPLEAFEMBEDDING}(\tau_n) = (C_{\tau_n} - C_{\tau_n} \|_{2} / \|C_{\tau_n}\|_{2}) \), and
we normalize the output of the final layer of COMBINE in
Figure 1b. The normalization step of \( l_{out} \) and \( C_{\tau_n} \) is some-
what similar to weight normalization (Salimans & Kingma,
2016) and vaguely resembles layer normalization (Ba et al.,
2016). Normalizing the SEMVECs partially resolves issues
with diminishing and exploding gradients, and removes a
spurious degree of freedom in the semantic representation.
As simple as this modification may seem, we found it vital
for obtaining good performance, and all of our multi-layer
TREEENN converged to low-performing settings without it.

Although these modifications seem to improve the represen-
tation capacity of the network and its ability to be trained,
we found that they were not on their own sufficient for good
performance. In our early experiments, we noticed that the
networks were primarily focusing on syntax instead of semantics, \textit{i.e.}, expressions that were nearby in the continuous space were primarily ones that were syntactically similar. At the same time, we observed that the networks did not learn to unify representations of the same equivalence class, observing multiple syntactically distinct but semantically equivalent expressions to have distant SEMVECS.

Therefore we modify the training objective in order to encourage the representations to become more abstract, reducing their dependence on surface-level syntactic information. We add a regularization term on the SEMVECS that we call a subexpression autoencoder (SUBEXPÆ). We design this regularization to encourage the SEMVECS to have two properties: abstraction and reversibility. Because abstraction arguably means removing irrelevant information, a network with a bottleneck layer seems natural, but we want the training objective to encourage the bottleneck to discard syntactic information rather than semantic information. To achieve this, we introduce a component that aims to encourage reversibility, which we explain by an example. Observe that given the semantic representation of any two of the three nodes of a subexpression (by which we mean the parent, left child, right child of an expression tree) it is often possible to completely determine or at least place strong constraints on the semantics of the third. For example, consider a boolean formula \( F(a, b) = F_1(a, b) \lor F_2(a, b) \) where \( F_1 \) and \( F_2 \) are arbitrary propositional formulae over the variables \( a, b \). Then clearly if we know that \( F \) implies that \( a \) is true but \( F_1 \) does not, then \( F_2 \) must imply that \( a \) is true. More generally, if \( F \) belongs to some equivalence class \( e_0 \) and \( F_1 \) belongs to a different class \( e_1 \), we want the continuous representation of \( F_2 \) to reflect that there are strong constraints on the equivalence class of \( F_2 \).

Subexpression autoencoding encourages abstraction by employing an autoencoder with a bottleneck, thereby removing irrelevant information from the representations, and encourages reversibility by autoencoding the parent and child representations together, to encourage dependence in the representations of parent and children. More specifically, given any node \( p \) in the tree with children \( c_0 \ldots c_k \), we can define a parent-children tuple \([r_{c_0}, \ldots, r_{c_k}, r_p]\) containing the (computed) SEMVECS of the children and parent nodes. What SUBEXPÆ does is to autoencode this representation tuple into a low-dimensional space with a denoising autoencoder. We then seek to minimize the reconstruction error of the child representations \([\hat{r}_{c_0}, \ldots, \hat{r}_{c_k}]\) as well as the reconstructed parent representation \( \hat{r}_p \), that can be computed from the reconstructed children. More formally, we minimize the return value of SUBEXPÆ in Figure 1c where \( \mathbf{n} \) is a binary noise vector with \( \kappa \) percent of its elements set to zero. Note that the encoder is specific to the parent node type \( r_p \). Although our SUBEXPÆ may seem similar to the recursive autoencoders of \cite{socher2011natural}, it differs in two major ways. First, SUBEXPÆ autoencodes on the entire parent-children representation tuple, rather than the child representations alone. Second, the encoding is not used to compute the parent representation, but only serves as a regularizer.

Subexpression autoencoding has several desirable effects. First, it forces each parent-children tuple to lie in a low-dimensional space, requiring the network to compress information from the individual subexpressions. Second, because the denoising autoencoder is reconstructing parent and child representations together, this encourages child representations to be predictable from parents and siblings. Putting these two together, the goal is that the information discarded by the autoencoder bottleneck will be more syntactic than semantic, assuming that the semantics of child node is more predictable from its parent and sibling than its syntactic realization. The goal is to nudge the network to learn consistent, reversible semantics. Additionally, subexpression autoencoding has the potential to gradually unify distant representations that belong to the same equivalence class.

To illustrate this point, imagine two semantically equivalent \( e_0 \) and \( e_0' \) child nodes of different expressions that have distant SEMVECS, \textit{i.e.}, \( \|r_{e_0} - r_{e_0'}\|_2 \gg \epsilon \) although \texttt{COMBINE}(\( r_{e_0'}, \ldots \)) \( \approx \texttt{COMBINE}(r_{e_0}, \ldots) \). In some cases due to the autoencoder noise, the differences between the input tuple \( x', x'' \) that contain \( r_{e_0} \) and \( r_{e_0'} \) will be non-existent and the decoder will predict a single location \( \hat{r}_{e_0} \) (possibly different from \( r_{e_0} \) and \( r_{e_0'} \)). Then, when minimizing the reconstruction error, both \( r_{e_0} \) and \( r_{e_0'} \) will be attracted to \( \hat{r}_{e_0} \) and eventually should merge.

### 2.2. Training

We train EQNETs from a dataset of expressions whose semantic equivalence is known. Given a training set \( T = \{T_1 \ldots T_N\} \) of parse trees of expressions, we assume that the training set is partitioned into equivalence classes \( \mathcal{E} = \{e_1 \ldots e_j\} \). We use a supervised objective similar to classification; the difference between classification and our setting is that whereas standard classification problems consider a fixed set of class labels, in our setting the number of equivalence classes in the training set will vary with \( N \).

Given an expression tree \( T \) that belongs to the equivalence class \( e_i \in \mathcal{E} \), we compute the probability

\[
P(e_i|T) = \frac{\exp \left( \text{TreeNN}(T)^\top q_{e_i} + b_i \right)}{\sum_j \exp \left( \text{TreeNN}(T)^\top q_{e_j} + b_j \right)}
\]  

(1)

where \( q_{e_i} \) are model parameters that we can interpret as representations of each equivalence class that appears in the training class, and \( b_i \) are scalar bias terms. Note that in this work, we only use information about the equivalence class of the whole expression \( T \), ignoring available information about subexpressions. This is without loss of generality, because if we do know the equivalence class of a subexpression of \( T \), we can simply add that subexpression to the training set. To train the model, we use a max-margin
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objective that maximizes classification accuracy, i.e.

$$\mathcal{L}_{\text{ACC}}(T, e_i) = \max \left( 0, \arg \max_{e_j \neq e_i, e_j \in \mathcal{E}} \log \frac{P(e_j|T)}{P(e_i|T)} + m \right)$$

(2)

where $m > 0$ is a scalar margin. And therefore the optimized loss function for a single expression tree $T$ that belongs to equivalence class $e_i \in \mathcal{E}$ is

$$\mathcal{L}(T, e_i) = \mathcal{L}_{\text{ACC}}(T, e_i) + \frac{\mu}{|Q|} \sum_{n \in Q} \text{SUBEXP} \text{AE}(\text{ch}(n), n)$$

(3)

where $Q = \{ n \in T : |\text{ch}(n)| > 0 \}$, i.e. contains the non-leaf nodes of $T$ and $\mu \in (0, 1]$ a scalar weight. We found that subexpression autoencoding is counterproductive early in training, before the SEMVECs begin to represent aspects of semantics. So, for each epoch $t$, we set $\mu = 1 - 10^{-\nu t}$ with $\nu \geq 0$. Instead of the supervised objective that we propose, an alternative option for training EqNet would be a Siamese objective (Chopra et al., 2005) that learns about similarities (rather than equivalence) between expressions. In practice, we found the optimization to be very unstable, yielding suboptimal performance. We believe that this has to do with the compositional and recursive nature of the task that creates unstable dynamics and the fact that equivalence is a stronger property than similarity.

3. Evaluation

Datasets. We generate datasets of expressions grouped into equivalence classes from two domains. The datasets from the BOOL domain contain boolean expressions and the POLY datasets contain polynomial expressions. In both domains, an expression is either a variable, a binary operator that combines two expressions, or a unary operator applied to a single expression. When defining equivalence, we interpret distinct variables as referring to different entities in the domain, so that, e.g., the polynomials $c \cdot (a \cdot a + b)$ and $f \cdot (d \cdot d + e)$ are not equivalent. For each domain, we generate “simple” datasets which use a smaller set of possible operators and “standard” datasets which use a larger set of more complex operators. We generate each dataset by exhaustively generating all parse trees up to a maximum tree size. All expressions are symbolically simplified into a canonical form in order to determine their equivalence class and are grouped accordingly. Table 1 shows the datasets we generated. In the supplementary material we present some sample expressions. For the polynomial domain, we also generated ONEV-POLY datasets, which are polynomials over a single variable, since they are similar to the setting considered by Zaremba et al. (2014) — although ONEV-POLY is still a little more general because it is not restricted to homogeneous polynomials. Learning SEMVECs for boolean expressions is already a hard problem; with $n$ boolean variables, there are $2^{2^n}$ equivalence classes (i.e. one for each possible truth table). We split the datasets into training, validation and test sets. We create two test sets, one to measure generalization performance on equivalence classes that were seen in the training data (SEENEQCLASS), and one to measure generalization to unseen equivalence classes (UNSEENEQCLASS). It is easiest to describe UNSEENEQCLASS first. To create the UNSEENEQCLASS, we randomly select 20% of all the equivalence classes, and place all of their expressions in the test set. We select equivalence classes only if they contain at least two expressions but less than three times the average number of expressions per equivalence class. We thus avoid selecting very common (and hence trivial to learn) equivalence classes in the test set. Then, to create SEENEQCLASS, we take the remaining 80% of the equivalence classes, and randomly split the expressions in each class into training, validation, SEENEQCLASS test in the proportions 60%–15%–25%. We provide the datasets online at groups.inf.ed.ac.uk/cup/semvec.

Baselines. To compare the performance of our model, we train the following baselines. TF-IDF: learns a representation given the expression tokens (variables, operators and parentheses). This captures topical/declarative knowledge but is unable to capture procedural knowledge. GRU refers to the token-level gated recurrent unit encoder of Bahdanau et al. (2015) that encodes the token-sequence of an expression into a distributed representation. Stack-augmented RNN refers to the work of Joulin & Mikolov (2015) which was used to learn algorithmic patterns and uses a stack as a memory and operates on the expression tokens. We also include two recursive neural networks (TREENN). The 1-layer TREENN which is the original TREENN also used by Zaremba et al. (2014). We also include a 2-layer TREENN, where COMBINE is a classic two-layer MLP without residual connections. This shows the effect of SEMVEC normalization and subexpression autoencoder.

Hyperparameters. We tune the hyperparameters of all models using Bayesian optimization (Snoek et al., 2012) on a boolean dataset with 5 variables and maximum tree size of 7 (not shown in Table 1) using the average $k$-NN ($k = 1, \ldots, 15$) statistics (described next). The selected hyperparameters are detailed in the supplementary material.

3.1. Quantitative Evaluation

Metrics. To evaluate the quality of the learned representations we count the proportion of $k$ nearest neighbors of each expression (using cosine similarity) that belong to the same equivalence class. More formally, given a test query expression $q$ in an equivalence class $c$ we find the $k$ nearest neighbors $\mathbb{N}_k(q)$ of $q$ across all expressions, and define the
Table 1. Dataset statistics and results. SIMP datasets contain simple operators (“∧, ∨, ¬” for BOOL and “+, −” for POLY) while the rest contain all operators (i.e. “∧, ∨, ¬, ⊕, ⇒” for BOOL and “+, −, ∨, ¬” for POLY). ⊕ is the XOR operator. The number in the dataset name indicates its expressions’ maximum tree size. L refers to a “larger” number of 10 variables. H is the entropy of equivalence classes.

<table>
<thead>
<tr>
<th>Dataset</th>
<th># Vars</th>
<th># Classes</th>
<th># Exprs</th>
<th># H</th>
<th>score5 (%) in</th>
<th>EqNet</th>
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</table>

\[ score_k(q) = \frac{|N_k(q) \cap c|}{\min(k, |c|)}. \]  

To report results for a given testset, we simply average \( score_k(q) \) for all expressions \( q \) in the testset. We also report the precision-recall curves for the problem of clustering the SEMVECS into their appropriate equivalence classes.

**Evaluation.** Figure 2 presents the average per-model precision-recall curves across the datasets. Table 1 shows \( score_5 \) of UNSEENQCLASS. Detailed plots are found in the supplementary material. EqNET performs better for all datasets, by a large margin. The only exception is POLY5, where the 2-L TREEENN performs better. However, this may have to do with the small size of the dataset. The reader may observe that the simple datasets (containing fewer operations and variables) are easier to learn. Understandably, introducing more variables increases the size of the represented space reducing performance. The tf-idf method performs better in settings with more variables, because it captures well the variables and operations used. Similar observations can be made for sequence models. The one and two layer TREEENN have mixed performance; we believe that this has to do with exploding and diminishing gradients due to the deep and highly compositional nature of TREEENN. Although Zaremba et al. (2014) consider a different problem to us, they use data similar to the ONEW-POLY datasets with a traditional TREEENN architecture. Our evaluation suggests that EqNETs perform much better within the ONEW-POLY setting.

**Evaluation of Compositionality.** We evaluate whether EqNETs successfully learn to compute compositional representations, rather than overfitting to expression trees of a small size. To do this we consider a type of transfer setting, in which we train on simpler datasets, but test on more complex ones; for example, training on the training set of BOOL5 but testing on the testset of BOOL8. We average over 11 different train-test pairs (full list in supplementary material) and show the results in Figure 3a and Figure 3b. These graphs again show that EqNETs are better than any of the other methods, and indeed, performance is only a bit worse than in the non-transfer setting.

**Impact of EqNET Components** EqNETs differ from traditional TREEENN in two major ways, which we analyze here. First, SUBEXP&E decreases performance. When training the network with and without SUBEXP&E, on average, the area under the curve (AUC) of \( score_k \) decreases by 16.8\% on the SEENQCLASS and 19.7\% on the UNSEENQCLASS. This difference is smaller in the transfer setting, where AUC decreases by 8.8\% on average. However, even in this setting we observe that SUBEXP&E helps more in large and diverse datasets. The second key difference to traditional TREEENN is the output normalization and the residual connections. Comparing our model to the one-layer and two-layer TREEENN again, we find that output normalization results in important improvements (the two-layer TREEENN have on average 60.9\% smaller AUC). We note that only the combination of the residual connections and the output normalization improve the performance, whereas when used separately, there are no significant improvements over the two-layer TREEENN.

3.2. Qualitative Evaluation

Table 2 shows expressions whose SEMVEC nearest neighbor is of an expression of another equivalence class. Manually inspecting boolean expressions, we find that EqNET confusions happen more when a XOR or implication operator is
Learning Continuous Semantic Representations of Symbolic Expressions

Figure 2. Precision-Recall Curves averaged across datasets.

Table 2. Non semantically equivalent first nearest-neighbors from BOOL8 and POLY8. A checkmark indicates that the method correctly results in the nearest neighbor being from the same equivalence class.

<table>
<thead>
<tr>
<th>Expresion</th>
<th>tf-idf</th>
<th>GRU</th>
<th>StackRNN</th>
<th>TreeNN-1Layer</th>
<th>TreeNN-2Layer</th>
<th>EqNet</th>
</tr>
</thead>
<tbody>
<tr>
<td>a \land (a \land (\neg a))</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>a \land (\neg a) \Rightarrow a</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>a \land (a \land (\neg a))</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>a \land (\neg a) \Rightarrow a</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>(a \land (a \land (\neg a))) \Rightarrow a</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>(a \land (\neg a)) \Rightarrow a</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>a \land (a \land (\neg a))</td>
<td>✓</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>a \land (\neg a) \Rightarrow a</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

Figure 3. Evaluation of compositionality: training set simpler than test set. Average \textit{score}_k (y-axis in log-scale). Markers are shown every three ticks for clarity. TREEENN refers to Socher et al. (2012).

Figure 4. Visualization of \textit{score}_k for all expression nodes for three BOOL10 and four POLY8 test sample expressions using EQNET. The darker the color, the lower the score, i.e. white implies a score of 1 and dark red a score of 0.

to compose expressions that achieve good score, even if the subexpressions achieve a worse score. This suggests that for common expressions, (e.g. single variables and monomials) the network tends to select a unique location, without merging the equivalence classes or affecting the upstream performance of the network. Larger scale interactive t-SNE visualizations can be found at online.

Figure 5 presents two PCA visualizations of the \textsc{SemVecs} of simple expressions and their negations/negatives. It can be discerned that the black dots and their negations (in red) are discriminated in the semantic representation space. Figure 5b shows this property in a clear manner: left-right discriminates between polynomials with 1 and \neg a, top-bottom between polynomials with \neg b and b and the diagonal parallel to \textit{y} = \neg \textit{x} between \neg a and \neg c. We observe a similar behavior in Figure 5a for boolean expressions.

4. Related Work

Researchers have proposed compilation schemes that can transform any given program or expression to an equivalent neural network (Gruau et al., 1995; Neto et al., 2003; Siegel-
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Figure 5. A PCA visualization of some simple non-equivalent boolean and polynomial expressions (black-square) and their negations (red-circle). The lines connect the negated expressions.

One can consider a serialized version of the resulting neural network as a representation of the expression. However, it is not clear how we could compare the serialized representations corresponding to two expressions and whether this mapping preserves semantic distances.

Recursive neural networks (TREENN) (Socher et al., 2012; 2013) have been successfully used in NLP with multiple applications. Socher et al. (2012) show that TREENNs can learn to compute the values of some simple propositional statements. EQNET’s SUBEXPAE may resemble recursive autoencoders (Socher et al., 2011) but differs in form and function, encoding the whole parent-children tuple to force a clustering behavior. In addition, when encoding each expression our architecture does not use a pooling layer but directly produces a single representation for the expression.

Mou et al. (2016) design tree convolutional networks to classify code into student submission tasks. Although they learn representations of the student tasks, these representations capture task-specific syntactic features rather than code semantics. Piech et al. (2015) also learn distributed matrix representations of student code submissions. However, to learn the representations, they use input and output program states and do not test for program equivalence. Additionally, these representations do not necessarily represent program equivalence, since they do not learn the representations over all possible input-outputs. Allamanis et al. (2016) learn variable-sized representations of source code snippets to summarize them with a short function-like name but aim learn summarization features in code rather than representations of symbolic expression equivalence.

More closely related is the work of Zaremba et al. (2014) who use a TREENN to guide the search for more efficient mathematical identities, limited to homogeneous single-variable polynomial expressions. In contrast, EQNETs consider at a much wider set of expressions, employ subexpression autoencoding to guide the learned SEMVECS to better represent equivalence, and do not use search when looking for equivalent expressions. Alemi et al. (2016) use RNNs and convolutional neural networks to detect features within mathematical expressions to speed the search for premise selection in automated theorem proving but do not explicitly account for semantic equivalence. In the future, SEMVECS may be useful within this area.

Our work is also related to recent work on neural network architectures that learn controllers/programs (Gruau et al., 1995; Graves et al., 2014; Joulin & Mikolov, 2015; Grefenstette et al., 2015; Dyer et al., 2015; Reed & de Freitas, 2016; Neelakantan et al., 2015; Kaiser & Sutskever, 2016). In contrast to this work, we do not aim to learn how to evaluate expressions or execute programs with neural network architectures but to learn continuous semantic representations (SEMVECS) of expression semantics irrespectively of how they are syntactically expressed or evaluated.

5. Discussion & Conclusions

In this work, we presented EQNETs, a first step in learning continuous semantic representations (SEMVECS) of procedural knowledge. SEMVECS have the potential of bridging continuous representations with symbolic representations, useful in multiple applications in artificial intelligence, machine learning and programming languages.

We show that EQNETs perform significantly better than state-of-the-art alternatives. But further improvements are needed, especially for more robust training of compositional models. In addition, even for relatively small symbolic expressions, we have an exponential explosion of the semantic space to be represented. Fixed-sized SEMVECS, like the ones used in EQNET, eventually limit the capacity that is available to represent procedural knowledge. In the future, to represent more complex procedures, variable-sized representations would seem to be required.
Acknowledgments

This work was supported by Microsoft Research through its PhD Scholarship Programme and the Engineering and Physical Sciences Research Council [grant number EP/K024043/1]. We thank the University of Edinburgh Data Science EPSRC Centre for Doctoral Training for providing additional computational resources.

References


Socher, Richard, Pennington, Jeffrey, Huang, Eric H, Ng, Andrew Y, and Manning, Christopher D. Semi-supervised recursive autoencoders for predicting sentiment distributions. In EMNLP, 2011.


A. Synthetic Expression Datasets

Table 3 and Table 4 are sample expressions within an equivalence class for the two types of datasets we consider.

B. Detailed Evaluation

Figure 6 presents the detailed evaluation for our \( k \)-NN metric for each dataset. Figure 7 shows the detailed evaluation when using models trained on simpler datasets but tested
All hyperparameters were optimized using the Spearmint \( \text{Figure 9b} \). The results for \( \text{Unerparameters} \) similar and are not plotted here. More complex operators tend to have worse performance (\( \text{Figure 9a} \)) and expressions with characteristics. As expected as the number of variables increase, the performance worsens (\( \text{Figure 9a} \)) and expressions with more complex ones, essentially evaluating the learned compositionality of the models. \( \text{Figure 9} \) shows how the performance varies across the datasets based on their characteristics. As expected as the number of variables increase, the performance worsens (\( \text{Figure 9a} \)) and expressions with more complex operators tend to have worse performance (\( \text{Figure 9b} \)). The results for \text{UNSEENEQCLASS} look very similar and are not plotted here.

### C. Model Hyperparameters

The optimized hyperparameters are detailed in \text{Table 5}. All hyperparameters were optimized using the Spearmint (\text{Snoek et al., 2012}) Bayesian optimization package. The same range of values was used for all common model hyperparameters.

\[
\text{Table 3. Sample of BOOL8 data.}
\]

\[
\begin{array}{cccc}
\text{BOOL8} & (\neg a) \land (\neg b) & (\neg a \land \neg c) \lor (\neg b \land a \land c) \lor (c \land b) & (\neg a) \land b \land c \\
\text{a}\neg(\neg a) \Rightarrow ((\neg a \land b)) & c \oplus (((\neg a) \Rightarrow a) \Rightarrow b) & \neg(\neg b) \lor ((\neg c) \lor a)) \\
\neg((b \lor (\neg (\neg a))) \lor b) & \neg((b \oplus (b \lor a)) \oplus c) & (a \lor b) \land c \land (\neg a) \\
(\neg a) \oplus ((a \lor b) \oplus a) & \neg((\neg (b \lor (\neg a))) \lor c) & (\neg((\neg (\neg b) \Rightarrow a)) \land c \\
(b \Rightarrow (b \Rightarrow a)) \land (\neg a) & ((b \lor a) \oplus (\neg b)) \oplus c & (c \land (c \Rightarrow (\neg a))) \land b \\
((\neg a) \Rightarrow b) \Rightarrow (a \oplus a) & (\neg((b \oplus a) \land a)) \lor c & b \land (\neg(b \land (c \Rightarrow a))) \\
\end{array}
\]

\[
\text{Table 4. Sample of POLY8 data.}
\]

\[
\begin{array}{cccc}
\text{POLY8} & \neg a - c & c^2 & b^2c^2 \\
(b - a) - (c + b) & (c \cdot c) + (b - b) & (b \cdot b) \cdot (c \cdot c) \\
(b - c + (b + a)) & ((c \cdot c) - c) + c & c \cdot (c \cdot (b \cdot b)) \\
a - ((a + a) + c) & ((b + c) - c) \cdot c & c \cdot (b \cdot c) \cdot (b \cdot c) \\
(a - (a + a)) - c & c \cdot (c - (a - a)) & ((c \cdot b) \cdot c) \cdot b \\
(b - b) - (a + c) & c \cdot c & ((c \cdot c) \cdot b) \cdot b \\
\end{array}
\]
Figure 6. Evaluation of $score_x$ (y axis) for $x = 1, \ldots, 15$, on the respective SEENeqCLASS and UNSEENeqCLASS where each model has been trained on. The markers are shown every five ticks of the x-axis to make the graph more clear. TREEENN refers to the model of Socher et al. (2012).

Table 5. Hyperparameters used in this work.

<table>
<thead>
<tr>
<th>Model</th>
<th>Hyperparameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>EQNET</td>
<td>learning rate $10^{-2.1}$, rmsprop $\rho = 0.88$, momentum 0.88, minibatch size 900, representation size $D = 64$, autoencoder size $M = 8$, autoencoder noise $\kappa = 0.61$, gradient clipping 1.82, initial parameter standard deviation $10^{-2.05}$, dropout rate .11, hidden layer size 8, $\nu = 4$, curriculum initial tree size 6.96, curriculum step per epoch 2.72, objective margin $m = 0.5$</td>
</tr>
<tr>
<td>1-layer-TREEENN</td>
<td>learning rate $10^{-3.5}$, rmsprop $\rho = 0.6$, momentum 0.01, minibatch size 650, representation size $D = 64$, gradient clipping 3.6, initial parameter standard deviation $10^{-1.28}$, dropout 0.0, curriculum initial tree size 2.8, curriculum step per epoch 2.4, objective margin $m = 2.41$</td>
</tr>
<tr>
<td>2-layer-TREEENN</td>
<td>learning rate $10^{-3.5}$, rmsprop $\rho = 0.9$, momentum 0.95, minibatch size 1000, representation size $D = 64$, gradient clipping 5, initial parameter standard deviation $10^{-4}$, dropout 0.0, hidden layer size 16, curriculum initial tree size 6.5, curriculum step per epoch 2.25, objective margin $m = 0.62$</td>
</tr>
<tr>
<td>GRU</td>
<td>learning rate $10^{-2.31}$, rmsprop $\rho = 0.90$, momentum 0.66, minibatch size 100, representation size $D = 64$, gradient clipping 0.87, token embedding size 128, initial parameter standard deviation $10^{-1}$, dropout rate 0.26</td>
</tr>
<tr>
<td>StackRNN</td>
<td>learning rate $10^{-2.9}$, rmsprop $\rho = 0.99$, momentum 0.85, minibatch size 500, representation size $D = 64$, gradient clipping 0.70, token embedding size 64, RNN parameter weights initialization standard deviation $10^{-4}$, embedding weight initialization standard deviation $10^{-3}$, dropout 0.0, stack count 40</td>
</tr>
</tbody>
</table>
Figure 7. Evaluation of compositionality. Evaluation of $score_x$ (y axis) for $x = 1, \ldots, 15$. The markers are shown every five ticks of the x-axis to make the graph more clear. TREENN refers to the model of Socher et al. (2012).

Figure 8. Receiver operating characteristic (ROC) curves averaged across datasets.
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Figure 9. EqNet performance on SeenEqClass for various dataset characteristics.

(a) Performance vs. Number of Variables

(b) Performance vs. Operator Complexity