miniKanren as a Tool for Symbolic Computation in Python

BRANDON T. WILLARD, University of Chicago

In this article, we give a brief overview of the current state and future potential of symbolic computation within the Python statistical modeling and machine learning community. We detail the use of miniKanren (Byrd 2009) as an underlying framework for term rewriting and symbolic mathematics, as well as its ability to orchestrate the use of existing Python libraries per Rocklin (2013). We also discuss the relevance and potential of relational programming for implementing more robust, portable, domain-specific "math-level" optimizations—with a slight focus on Bayesian modeling. Finally, we describe the work going forward and raise some questions regarding potential cross-overs between statistical modeling and programming language theory.

ACM Reference format:
Brandon T. Willard. 2016. miniKanren as a Tool for Symbolic Computation in Python. 1, 1, Article 1 (January 2016), 21 pages. DOI: 10.1145/nnnnnn.nnnnnnn

1 INTRODUCTION

Throughout, we will focus on two categories of tools within the modern machine learning, statistics, and data science world: Tensor Libraries and Probabilistic Programming Languages (PPLs).

For our purposes, it’s sufficient to say that tensor libraries are the modern wrappers for standard linear algebra operations—traditionally offered by BLAS (BLA 2020) and LAPACK (LAP 2020)—with extensions to handle general arrays, perform tensor operations, and efficiently compute gradients—usually via automatic differentiation (AD). These libraries are the main workhorses of deep learning (DL) libraries, and, because of this strong association, tensor libraries often provide deep learning-specific functionality (e.g. tools for constructing DL models, common activation functions, etc.)

Probabilistic programming languages are domain-specific languages that aid in the specification of statistical models and the application of estimation methods on said models. Often, PPLs will reflect the formal, probability theory-based language used to specify statistical models, but that connection with probability theory tends to serve primarily in an interface role. PPLs also implement related elements—like random variables and statistical distributions—and, in some cases, they provide limited support for the laws and identities of probability theory (e.g. addition and multiplication of random variables).

Nowadays, PPLs are increasingly backed by tensor libraries, so the two subjects are connected in this way. There is an appreciable amount of symbolic computation behind the standard Deep Learning libraries of today, like Theano (Bergstra et al. 2010), TensorFlow (Ten 2020), and PyTorch (PyT 2020).

At the very least, these libraries provide classes that represent tensor algebra in graphical form and functions that manipulate graphs. Furthermore, these graphs are used to compute derivatives—via Automatic Differentiation (AD), parallelize or vectorize operations, and, in limited cases, explicitly perform algebraic simplifications.

Regardless of whether or not you’re in a camp that says AD falls well within standard symbolic mathematics, these libraries are undoubtedly performing symbolic calculations, and most of them are on a path toward even more symbolic computation and outright symbolic mathematics.

Theano’s optimizations are perhaps the best example of more open-ended symbolic computation within modern tensor libraries. It provides an entire subsystem for incorporating custom "graph optimizations" that
implements pattern matching, term substitution, utilizes common sub-expression elimination (CSE), offers multiple graph traversal strategies and fixed-point operators, etc. The optimization system is used to perform graph canonicalization and specialization through a number of standard matrix algebra identities, and, with these, it is able to avoid numerous unnecessary numeric calculations and increase the overall “flexibility” of function/model specification.

Unfortunately, most other tensor libraries do not offer as much in the way of user-level Python manipulation of graphs. In the case of TensorFlow, an internal graph canonicalization and optimization library Grappler (Larsen and Shpeisman 2019) is being actively developed. At the moment—its core work is done exclusively in C++ and the potential for robust user-defined optimizations isn’t clear.

Outside of the aforementioned tensor libraries, other projects approach similar symbolic-oriented operations—like AD—through function tracing (JAX 2020) and Python AST parsing (tan 2020). As with most tensor libraries, these projects aren’t particularly focused on supporting generic graph manipulation or symbolic mathematics. Nevertheless, they demonstrate another burgeoning entry-point to general symbolic computation.

At this point in time, there is a fairly well established set of modern machine learning and statistical modeling libraries that are all fundamentally built upon the basics of symbolic graphs representing tensor algebra operations. They all vary in the degree to which they implement symbolic mathematics or programmatically encode the underlying high-level math. Regardless, the case for more advanced symbolic computation and mathematics is slowly being made by multiple influential projects, and there’s already enough reason and prior work to start assessing the directions this could go, and how we might get the most out of it.

Ideally, symbolic work within the machine learning and statistical modeling community would progress by developing constructively on top of well established projects, so that quality code can be reused, existing expertise can be leveraged, and community involvement from domain experts is easily incorporated.

Within the Python community, Rocklin (2013) states the same sentiments with regards to the intelligent use of optimized linear algebra functions and the basics of term rewriting. This work follows the same principles, but focuses on the areas of statistical modeling and, more specifically, Bayesian modeling. That is to say, we seek flexible, compartmentalized and open systems that are easily integrated with established libraries and map well to their high-level abstractions. Ideally, we could have all this without much context switching—in other words, the need to operate in more than one programming languages or between programming languages.

2 WHAT WE WANT TO DO IN STATISTICAL MODELING

We believe that the statistical modeling and machine learning communities need a framework within which they can develop their own high-level, symbolic “optimizations” specific to the domains of statistical modeling and machine learning. Ideally, such a framework would have the properties outlined in Section 1 and build upon the already well established Python machine learning and statistics ecosystem, instead of attempting to outright reinvent it or rewrite its staple offerings.

These symbolic optimizations should be usable internally by new and existing libraries to drive advanced automations. As well, they should be usable in an interactive way by researchers, where the researchers themselves can dynamically add new theorems and immediately use the resulting automations for high-level testing, experimentation, and concrete applications.

Statistical modeling is surprisingly amenable to symbolic methods (Carette and Shan 2016; Carette et al. 2008)—and especially when one restricts the context to specific practices like Bayesian modeling (Shan and Ramsey 2017), where there exist fundamental relations such as “conjugacy” (Robert 2007, Chapter 3.3)—that are easily automated with simple pattern matching.

Another example is Rao-Blackwellization. Rao-Blackwellization is derived from the Rao-Blackwell Theorem (Casella and Robert 1996), which states—roughly—that analytically computed conditional expectations outperform
their un-integrated counterparts. In other words, if you can get a closed-form answer to an integral, instead of estimating the integral with samples, you should use the closed-form answer.

It applies in a rather general sense to numerous Markov Chain Monte Carlo methods, but its automation is something that falls well outside of most libraries, arguably due to its symbolic computation requirements.

The Rao-Blackwellizations appearing in published material are often driven by simple high-level identities–identities which we can alternatively classify as relations. Some of those relations reflect basic theorems in probability theory and statistics, like the following normal (or Gaussian) random variable identity–expressed as a rule:

\[
\begin{align*}
\text{(sum-of-normals)} & \quad X \sim N(\mu_x, \sigma_x^2), \quad Y \sim N(\mu_y, \sigma_y^2), \quad X + Y = Z \\
\quad & \quad Z \sim N(\mu_x + \mu_y, \sigma_x^2 + \sigma_y^2)
\end{align*}
\]  

(1)

There are numerous examples like (1), and they all take the form of relations. Hiding behind these relations are the closed-form integrals that would otherwise be painstaking to compute directly with symbolic algebra.

As a matter of fact, there are at least two ways to frame identities like these: in terms of random variables, and in terms of their corresponding distribution functions. This means that one can turn theorems like Rao-Blackwellization into an integration problem. Unfortunately, term graphs produced by the distribution-based approach can be much more complex than the corresponding random variable graphs. Our focus will be on the latter approach, since it offers more opportunities to solve equivalent integration problems using only collections of simple random variable identities.

This general idea has analogs in the approaches used by modern symbolic integration systems themselves. When such systems employ Fox H and Meijer G functions (Peasgood 2009; Roach 1997), they are effectively using only a few simple algebraic convolution identities applied to broad classes of hypergeometric functions–many of which can be encoded by simple look-up tables.

Since those systems are intended to reach a much greater number of functions and constraints, they are necessarily more complex; however, a majority of the work being done by statistical modeling deals with a comparatively smaller set of standard distributions, so major improvements can be made without invoking the complexity of symbolic integration systems.

Currently, statistical modeling systems do not directly support these types of “knowledge” additions, nor do they attempt to systematically employ these well-known and far-reaching theorems–like Rao-Blackwellization. Instead, this kind of work is still restricted to the user-level, where it is performed by hand and used as input to such systems. At the present, the best systems simply provide broadly useful identities and theorems as advice in their manuals and message boards.

In particular, Stan (Stan Development Team 2014) is known for having a well written manual that details user-level manipulations to account for common sampling issues arising due to poorly specified models (Gelman 2019). Note that the description "poorly specified" is conditional on the given estimation approach.

Among the advice given in Stan’s manual is the classic pathological "funnel" model of Neal (2003). This model can be reparameterized using the following rule between a standard Gaussian random variable and its affine transform:

\[
\begin{align*}
\text{(normal-affine-transform)} & \quad Y \sim N(0, 1), \quad X = \mu + \sigma Y \\
\quad & \quad X \sim N(\mu, \sigma^2)
\end{align*}
\]  

(2)

Under (2), terms in the funnel model can be expanded resulting in an equivalent model that exhibits much better sampling properties.

The work we detail here is motivated by the desire to see relations like these used within statistical modeling systems, so that model specification is more flexible and less brittle with respect to the exact specification of a model.
Systems like Stan and the Python-based PyMC (Salvatier et al. 2016) are PPLs, so their role as programming languages is clear, and—in line with most programming languages—compiler optimizations can be used to improve performance and expand the expressive potential of a language’s syntax.

Projects like Stan and PyMC rely almost exclusively on AD and have more or less superseded older projects based on different, non-gradient-based generalized methodologies, like BUGS (Lunn et al. 2009). BUGS used some of the domain-specific identities implied here to construct a surprisingly robust expert system that could automatically construct a sampler for a given model. We would like to make such systems easier to produce and extend, and we would like to see them built on top of tensor libraries, so that the AD-driven methods of modern PPLs can be used in tandem.

One noteworthy example is PyMC’s internal logic for determining an appropriate sampler. This logic could benefit from an easily extensible, expert-like system that matches models to samplers. Just like the optimization system in Theano, the graph of a PyMC model can be manipulated to produce a more suitable, yet equivalent, model for a given sampler, or—conversely—produce a customized sampler for a given model. In extreme cases, the posterior distribution ultimately estimated by PyMC could be returned in closed-form. A small example of this is given in Section 4.6.

Otherwise, there are entire classes of efficient, model-specific samplers that are currently out of these PPLs’ reach, and the addition of some straightforward and flexible term rewriting capabilities would make them immediately available. Some examples involve Gibbs samplers, scale mixture representations for sparsity priors (Bhadra et al. 2016), non-Gaussian models (Polson et al. 2013), and parameter expansions (Scott 2010).

As a proof of concept using Theano’s existing optimization system, automatic simplification of random variables was demonstrated in Willard (2017). While it is more than possible to extend the same approach into auto-conjugation and related statistical optimizations, the scalability and means of specifying new optimizations within Theano wasn’t promising.

One important concern involves the need to use identities in more than one direction. For instance, one direction of the identity underlying (2) is useful for computational reasons (e.g. the funnel problems) and the other direction helps one determine the distribution type of sub-term (i.e. given \(Y \sim N(0, 1)\) we can derive distribution of \(X\)) in a larger model. The latter information might be needed by a system that constructs custom samplers, or to reformulate a model so that it can be used by a given sampling routine.

This otherwise natural use of identities isn’t covered well by modern programming frameworks, and that’s where logic and relational programming becomes a real consideration.

Considerations like these also lead quickly into the domain of term rewriting (Baader and Nipkow 1999). Graph normalization/canonicalization, rewrite rule completion (Huet 1981), and general equational reasoning are all ground-level subjects in the features we’ve described.

With this in mind, it’s likely that our objectives won’t often lead to the classical term rewriting niceties, like easily determined normal forms and term orderings with strong guarantees. Given our desire for an interactive system in which to perform ad hoc additions and experimentation, it seems even less likely. Even so, when such niceties are available, we would at least like a suitable framework in which to derive and apply them. Furthermore, if it’s ever possible to produce any results from a less-than-perfect set of identities, then we would like a framework that facilitates that, too.

Overall, we seek a middle ground that provides an approachable, powerful, yet light-weight framework for creating and orchestrating domain-specific relations.

As well, we would like this framework to promote joint development between experts in statistics, machine learning, term rewriting, type theory, code synthesis, and related areas. We believe miniKanren could serve an important role within this intersection of requirements.
3 WHERE MINIKANREN FITS IN

Computer science researchers have been—and continue to—actively pursue topics in symbolic computation specifically within the area of statistical modeling (Sato et al. 2018; Shan and Ramsey 2017; Walia et al. 2018). While very in-line with the automations described here, much of this work takes the form of entirely new languages or very broad theoretical work that doesn’t always lend itself to more immediate input from experts in the areas of statistical modeling methods.

In other cases, the limitations involve the degree of specialization, where exclusive focus is often on neural network-specific DSLs and frameworks, or only certain types of optimizations (Vasilache et al. 2018; Wei et al. 2017).

Regarding Python and statistical modeling, the recent automatic conjugation and rescaling examples of Gorinova et al. (2018); Hoffman (2018) are perhaps the most germane; however, their approach relies entirely on an existing pattern-matching and rewrite system (Radul 2020) that is non-relational and uses the Python stack for backtracking. As we’ve stated earlier, the use of relations has important conceptual and implementation advantages (e.g. the concepts being implemented are fundamentally relational, and the inherent code reuse arising from “bidirectional” applications of identities).

As well, use of the Python stack for backtracking puts severe limitations on the size of graphs manageable by such a system. Python throws `RecursionErrors` when the stack reaches a fixed size, and term graphs representing real models are by no means small, so unification alone is liable to cause irreconcilable errors. Our implementation of unification in Python (Willard 2020c) demonstrates this exact problem in its unit tests, and, as a result, the library uses a coroutine-based trampoline to avoid excessive use of the Python stack.

Simply increasing the recursion limit (e.g. via `sys.setrecursionlimit`) is—at best—a single-case solution, and it’s often safer to pursue a more “pythonic” rewrite (i.e. loop or list comprehension-based approach). Also, Python currently lacks even the most basic forms of tail recursion elimination—and it’s very unlikely to appear in later versions (Rossum 2009).

Furthermore, Hoffman (2018) doesn’t provide clear examples of how rewrite rules are specified in their proposed system, so it’s difficult to assess exactly how expressive their DSL is, or even how well it works within Python and its standard collection types.

This is where miniKanren comes in. It serves as a minimal, lightweight relational DSL that orchestrates unification and reification and operates exclusively within an existing host language. Furthermore, its core functionality is succinctly described in a single page of code, which helps make its inner workings very transparent to the interested developer (Hemann and Friedman 2013).

In contrast with other unification-driven systems, its “internal” mechanics maintain direct connections with multiple high-level theoretical concepts (e.g. unification, complete search, relational programming, CPS, etc.), so, for instance—its use as a type theory prototyping language automatically provides exciting connections to both basic and cutting-edge symbolic computation (e.g. automatic theorem proving (Near et al. 2008)). As a matter of fact, the use of typing rules to describe the automation of high-level inference algorithms in Walia et al. (2018) is a direct example of how elements of type theory can be used in high-level statistical model optimization, and miniKanren can serve as a bridge to fast implementations.

miniKanren inherently provides a degree of high-level portability and low-level flexibility. Relations can be built on top of other relations, and, in these cases, the goals that implement such composite relations in miniKanren are often easily ported to miniKanrens in other host languages. miniKanren doesn’t enforce a formal, host-language independent semantics, yet it still lends well to this kind of portability. This lack of formal semantics also makes it easier to address performance and domain specific issues in multiple ways—like the `RecursionErrors` described above. With these properties, miniKanren has exactly the type of generality and flexibility to serve as a basis for
more fluid collaboration—in symbolic computation—between independent communities of computer scientists and statisticians.

In the following section, we will illustrate many of these points using our Python implementation of miniKanren.

4 SYMBOLIC COMPUTATION IN PYTHON DRIVEN BY MINIKANREN

In the following sections we detail our implementation of miniKanren (Willard 2020d), operating under the PyPi name miniKanren and Python package name kanren. We also describe its ecosystem of complementary packages etuples, cons, and symbolic-pymc.

kanren is a fork that tries to maintain syntactic parity with its predecessor logpy (Rocklin 2018), but now deviates significantly in terms of core mechanics and offerings. The most important difference is in the relational status of logpy’s goals; most were not truly relational. This was largely due to the use of an exception-based goal reordering system, which served as the exclusive means of handling missing cons-based capabilities and minimalistic constraints. Basically, one could attempt to develop entirely in standard Python at the goal constructor level, and throw special EarlyGoalError exceptions when goal constructor arguments were not sufficiently ground for a given task. The exception would cause the goals to be reordered until an ordering satisfied these goals’ groundedness requirements.

This exception-based approach was combined with a lightweight tuple-based, Lisp-like expression evaluator that operated in tandem with the goal reordering. Both of these components were built directly into the core stream processing functions and introduced additional complexity and challenges, but, most of all, they made it much easier to construct non-relational goals and imposed new, non-miniKanren semantics that increased the barrier to entry beyond a simple understanding of core Python and miniKanren.

Our implementation of miniKanren’s core mechanics does not operate on Lisp-like idioms, yet it maintains an operational similarity to the Scheme implementations. Additionally, it provides a straightforward object-oriented framework for implementing truly relational constraints. These points will be covered in more detail in the following sub-sections.

First, we must note that both Python implementations share the same small, but noteworthy, deviations from the standard Scheme-based miniKanrens. Specifically, the basic miniKanren states are implemented using Python’s built-in dict type, the \equiv goal is represented by the function eq, there is no fresh—instead, fresh logic variables are constructed explicitly using the function var—and the functionality of bind and mplus are represented by the logical “and” and “or” functions lall and lany and are essentially the conj and disj stream functions of Hemann and Friedman (2013).

4.1 Goals as Generators

Our implementation of miniKanren represents goals using Python’s built-in generators (Gen 2020; Foundation 2020).

Listing 4.1 illustrates the general form of a miniKanren goal and some of the idioms available to them.

Listing 4.1: Example idioms for generator-based goals in Python.

```python
1 def relationo(*args):
2     """Construct a goal for this relation."""
3
4 def relationo_goal(S):
5     """Generate states for the relation `relationo`.
```
I.e. this is the goal that's generated.

Parameters
---------
S: Mapping
   The miniKanren state (e.g. unification mappings/dict).

Yields
------
miniKanren states.

nonlocal args

args_rf = reify(args, S)

x = 1
for a in args_rf:
    S_new = S.copy()
    if isvar(a) or x > 3:
        S_new[a] = x
        z = yield S_new #
    if not z:
        x += 1
if some_condition:
    yield S #
else:
    return

a_lv = var()
    yield from lall(conso(1, a_lv, args), eq(a_lv, [2, 3])) #
    yield from relationo(*new_args) #
return relationo_goal

Simply put, a goal is responsible for either explicitly generating its goal stream (e.g. Line 30 and 36) or deferring to other goals and/or goal combinations via the stream manipulation functions lall and lany (e.g. Line 41).
The idioms described in Listing 4.1 are realized in a number of low-level goal implementations within kanren. One good example is the permuteo goal, which relates an ordered collection to its permutations. Within permuteo, low-level Python steps are taken in order to efficiently compute differences of hashable collections when the arguments are ground, and, when one argument is unground, Python’s built-in permutation generator itertools.permutations is used to efficiently generate unification arguments for the unground term. This strictly Python-based low-level implementation of a goal is both completely relational and considerably more scalable than an implementation built on the basic miniKanren relations and amounting to Bogosort (Kiselyov et al. 2005).

Within ordinary goals like relationo_goal one is able to leverage the naturally delayed nature of Python’s generators and seamlessly define recursive goals (e.g. Line 43) by calls to the outer goal constructor relationo, and, in the case of goal constructors that do not define their own low-level goals, recursion is facilitated by the η-delay function, Zzz, of Hemann and Friedman (2013).

This approach also makes it possible for goals to more easily control the type and order of the results it streams. The loop around Line 30 in Listing 4.1, demonstrates how a goal can easily keep and manage its state—e.g. the variable x—and use it to affect the goal stream it produces.

Also, using Python’s coroutine capabilities, Line 30 shows how it’s possible to send results back to a goal when the process evaluating the stream uses generator.send (PEP 2020a). In this case, a goal could be given “upstream” information.

Also, using Python’s __length_hint__ (PEP 2020b) spec, goals and stream manipulation functions could be told when a stream is empty or simply make decisions based on partial information about a stream’s size. Such information could help determine efficient orderings within lall conjunctions and between conde branches, by—say—allowing these operators to choose finite streams over potentially infinite ones in certain cases.

Overall, the resulting simplicity of this approach is an example of how well miniKanren’s underlying mechanics can be adapted to host languages in which the standard list-based approach isn’t as natural or efficient as it is in Scheme.

4.2 Constraints

Our Python implementation follows the approach of Hemann and Friedman (2017) to implement a minimal constraint system in miniKanren. Listing 4.2 provides some simple illustrations of the standard disequality (named neq here) and type constraints—the latter using Python’s isinstance naming scheme.

```
>>> from kanren.constraints import neq, isinstanceo

>>> run(0, x,
...    neq(x, 1), # Not "equal" to 1
...    neq(x, 3), # Not "equal" to 3
...    membero(x, (1, 2, 3)))
(2,)

>>> from numbers import Integral

>>> run(0, x,
...    isinstanceo(x, Integral), # 'x' must be of type 'Integral'
...    membero(x, (1.1, 2, 3.2, 4)))
```

Vol. 1, No. 1, Article 1. Publication date: January 2016.
When constraints are used, the state type—normally an ordinary Python `dict`—is replaced with a new type: `ConstrainedState`. This type is a subclass of the interface `Mapping`, so it behaves effectively the same as a standard `dict`. The main functionality provided by `ConstrainedState` is constraint store tracking and validation. Constraint store validation occurs after each successful unification involving a `ConstrainedState`. Adding new constraints involves constructing a custom constraint store class and a goal that assigns the constraint and adds or updates the associated store in a miniKanren state. For convenience, there is an abstract `PredicateStore` type that simplifies the construction of predicate-based constraints.

Given that constraint checking is tied directly to the `Mapping` interface, one can dispatch on key addition, deletion, and updating in order to implement more efficient constraint store management and validation.

4.3 cons

One of the main challenges involved in implementing miniKanren in some host languages is the lack of immediate support for important Scheme/Lisp-like elements. The most notable for Python being `cons`.

`cons` support is important for maintaining certain forms of simplicity and expressiveness in term rewriting. For instance, while "pattern matching"—or unification—alone can be rather straightforward to implement, and more than a couple of the software systems mentioned here have introduced basic pattern matching, they all tend to lack the expressive simplicity afforded by list-based terms and proper `cons` semantics.

A good example is Theano’s unification system (Gra 2020); although it does provide a tuple-based interface for defining forms to match and replace, and it supports logic variables within said forms, it doesn’t provide a means of expressing a `cons` pair. As a result, attempting to construct a pattern that matches a specific operator (or `car`) and an unspecified number/type of arguments (or `cdr`)—or vice versa—falls outside of the system’s reach.

Our Python implementation of miniKanren preserves nearly all the same algebraic datatype semantics of Lisp’s `cons` by way of our `cons` package (Willard 2020e). The `cons` package provides a minimal `ConsType` class, along with a set of easily extensible generic functions for `car` and `cdr`.

As Listing 4.3 demonstrates, with `cons` we’re able to succinctly express the aforementioned "pattern" for all the built-in ordered collection types, and reify accordingly.

Listing 4.3: `cons` pair unification and reification using Python’s built-in lists.
Later, in Listing 4.12, we provide another example of how a cons-compliant unification system makes non-trivial patterns easier to express.

4.4 S-Expressions
Since Python doesn’t already provide a programmatically convenient form of expressions or terms, we’ve constructed a simple ExpressionTuple class—or etuple for short—that extends the built-in tuple with the ability to evaluate itself, cache the results, and maintain the cached results between non-modifying reconstructions and re-evaluations of the same etuple.

Python does provide AST objects that fully represent its built-in expressions, but they are cumbersome to work with and do not provide much of the desired functionality for term rewriting (e.g. access to nested elements is too indirect, their construction and use involves irrelevant meta information, etc.) See Willard (2018) for examples of term rewriting using Python AST objects and miniKanren.

As we demonstrate in a later example (i.e. Listing 4.9), etuples are an extremely convenient way to leverage a target library’s user-level functions (e.g. TensorFlow’s matrix multiplication function) without having to manually construct fully reifiable term graphs—many of which require detailed information that may not be available at the time of a goal’s evaluation.

Listing 4.4: Constructing a simple etuple.

```python
>>> from operator import add
>>> from etuples import etuple, etuplize

>>> et = etuple(add, 1, 2)
>>> et
ExpressionTuple((<built-in function add>, 1, 2))
```

etuples can be indexed—and generally treated—like immutable tuples:

Listing 4.5: etuple indexing example.

```python
>>> et[0:2]
ExpressionTuple((<built-in function add>, 1))
```

Evaluation is available through a simple cached property:
Furthermore, it is easy to specify conversions to and from `etuple`s for arbitrary types. Listing 4.7 constructs two custom classes, `Node` and `Operator`, and specifies the `car` and `cdr` for the `Node` type via the generic functions (Rocklin 2019) `rands rator`, respectively. An `apply` dispatch is also specified, which represents a combination of `cons` (via the aforementioned `cons` library) and an S-expression evaluation.

```
from collections.abc import Sequence
from etuples import rator, rands, apply
from etuples.core import ExpressionTuple

class Node:
    def __init__(self, rator, rands):
        self.rator, self.rands = rator, rands

    def __eq__(self, other):
        return self.rator == other.rator and self.rands == other.rands

class Operator:
    def __init__(self, op_name):
        self.op_name = op_name

    def __call__(self, *args):
        return Node(Operator(self.op_name), args)

    def __repr__(self):
        return self.op_name

    def __eq__(self, other):
        return self.op_name == other.op_name

rands.add((Node,), lambda x: x.rands)
rator.add((Node,), lambda x: x.rator)

@apply.register(Operator, (Sequence, ExpressionTuple))
```

Listing 4.7: Adding `etuple` support to a standard Python class.
def apply_Operator(rator, rands):
    return Node(rator, rands)

With the specification of rands, rator, and apply for Node types, it is now possible to convert Node objects to etuples using the etuplize function. Listing 4.8 demonstrates this process and shows how the underlying object is preserved through conversion and evaluation.

Listing 4.8: Converting a supported class instance into an etuple.

```python
>>> mul_op, add_op = Operator("*"), Operator("+")
>>> mul_node = Node(mul_op, [1, 2])
>>> add_node = Node(add_op, [mul_node, 3])
>>> et = etuplize(add_node)

>>> pprint(et)
e(+, e(*, 1, 2), 3)

>>> et.eval_obj is add_node
True
```

4.5 Relations for Term Rewriting

Our Python implementation of miniKanren is motivated by the need to cover some of the symbolic computation objectives laid out here, so, in response, it provides relations that are specific to those needs.

The most important set of relations involve graph traversal and manipulation. symbolic-pymc provides “meta” relations for applying goals to arbitrary “walkable” structures (i.e. collections that fully support cons semantics via car and cdr).

Listing 4.9 constructs an example goal that represents two simple mathematical identities: i.e. \(x + x = 2x\) and \(\log \exp x = x\).

Listing 4.9: An example goal that implements some basic mathematical relations.

```python
def single_math_reduceo(expanded_term, reduced_term):
    """Construct a goal for some simple math reductions."""
    x_lv = var()
    return lall(
        # Create a logic variable to represent our variable term "x"
        x_lv = var(),
        # Apply an 'isinstance' constraint on the logic variable
        isinstance(x_lv, Real),
        isinstance(x_lv, ExpressionTuple),
        conde(
            # add(x, x) == mul(2, x)
```
We can combine the goal in Listing 4.9 with the “meta” goal, reduceo, which applies a goal recursively until a fixed-point is reached—assuming the relevant goal is a reduction, of course. (The meta goal should really be named fixedpointo.) Additionally, we create another partial function that sets some default arguments for the walko meta goal.

Listing 4.10: Partial functions for a fixed-point calculation and graph walking.

```python
math_reduceo = partial(reduceo, single_math_reduceo)
term_walko = partial(walko, rator_goal=eq, null_type=ExpressionTuple)
```

Listing 4.11 applies the goals to two unground logic variables, demonstrating how miniKanren nicely covers both term expansion and reduction, as well as graph traversal and fixed-point calculations, in a single concise framework. (The symbols prefixed by ~ in the output are unground logic variables.)

Listing 4.11: Simultaneous mathematical term “expansion” and “reduction”.

```python
>>> expanded_term = var()
>>> reduced_term = var()
>>> res = run(10, [expanded_term, reduced_term],
            term_walko(math_reduceo, expanded_term, reduced_term))

>>> rjust = max(map(lambda x: len(str(x[0])), res))
>>> print('\n'.join((f'{str(e):>{rjust}} == {str(r)}' for e, r in res)))

add(~2291, ~2291) == mul(2, ~2291)
~2288(~2288) == ~2288()
log(exp(add(~2297, ~2297))) == mul(2, ~2297)
~2288(add(~2303, ~2303)) == ~2288(mul(2, ~2303))
log(exp(log(exp(add(~2309, ~2309))))) == mul(2, ~2309)
~2288(~2294) == ~2288(~2294)
log(exp(log(exp(log(exp(add(~2315, ~2315))))))) == mul(2, ~2315)
~2288(~2300()) == ~2288(~2300())
log(exp(log(exp(log(exp(log(exp(add(~2325, ~2325))))))))) == mul(2, ~2325)
~2288(~2294, add(~2331, ~2331)) == ~2288(~2294, mul(2, ~2331))
```
To further demonstrate the expressive power of miniKanren in this context, in Listing 4.12 we show how easy it is to perform term reduction, expansion, or both under structural constraints on the desired terms. Specifically, we ask for the first ten expanded/reduced term pairs where the expanded term is a logarithm with at least one argument.

In Listing 4.12, we use `cons` three times to constrain the logic variable `expanded_term` to only `log` terms with an `add` term as the first argument, and we’ll further restrict the `add` term to one not containing another `add` as its first argument.

### Listing 4.12: Constrained term “expansion” and “reduction”.

```python
>>> from kanren.constraints import neq

>>> log_arg = var()
>>> first_arg = var()
>>> first_arg_car, first_arg_cdr = var(), var()

>>> res = run(10, [expanded_term, reduced_term],
            eq(etuple(log, log_arg), expanded_term),
            eq(etuple(add, first_arg, var()), log_arg),
            conso(first_arg_car, first_arg_cdr, first_arg),
            neq(first_arg_car, add),
            term_walko(math_reduction, expanded_term, reduced_term))

>>> rjust = max(map(lambda x: len(str(x[0])), res))
>>> print('\n'.join((f'{str(e)} == {str(r)}' for e, r in res)))

 >>> log(add((0.771, 0.772)) == log(mul(2, (0.771, 0.772)))
 >>> log(add(log(exp(add(0.815, 0.815))), add(0.829, 0.829))) ==
   log(add(mul(2, 0.815), mul(2, 0.829)))
 >>> log(add((0.771, 0.772), add(0.851, 0.851))) ==
   log(add((0.771, 0.772), mul(2, 0.851)))
 >>> log(add(0.806(add(0.869, 0.869)), add(0.887, 0.887))) ==
   log(add(0.806(mul(2, 0.869)), mul(2, 0.887)))
 >>> log(add((0.771, 0.772), 0.844(mul(2, 0.909)))) ==
   log(add((0.771, 0.772), 0.844(mul(2, 0.909))))
 >>> log(add(log(exp(0.788)), add(0.935, 0.935))) ==
   log(add(log(add(0.788, mul(2, 0.935))),
   log(exp(add(0.945, 0.945)))))) ==
   log(add((0.771, 0.772), log(exp(add(0.945, 0.945))))))
 >>> log(add(0.806(add(0.808, 0.967), add(0.985, 0.985))) ==
   log(add(0.806(add(0.808, add(0.967, 0.967)), add(0.985, 0.985)))
 >>> log(add((0.771, 0.772), 0.844(add(0.846, add(0.1007, 0.1007)))) ==
   log(add((0.771, 0.772), 0.844(add(0.846, add(0.1007, 0.1007)))))
```
Listing 4.12 – continued

>>> log(add(log(exp(log(exp(add(~_1021, ~_1021))))), add(~_1035, ~_1035))) ==

\[ \log(\exp(\log(\exp(\log(\exp(\beta_1 + \beta_1))))), \exp(\beta_3 + \beta_3)) \]

By properly supporting cons semantics, we were able to constructively express a non-trivial term constraint with only four simple goals.

4.6 The symbolic-pymc Package

In order to bring together miniKanren and the popular tensor libraries Theano and TensorFlow, our project symbolic-pymc provides “meta” type analogs for the essential tensor graph types of each “backend” tensor library. These meta types allow for more graph mutability than the “base” libraries themselves tend to provide. They also allow one to use logic variables where the base libraries wouldn’t.

Basic use of symbolic-pymc involves either conversion of an existing base–i.e. Theano or TensorFlow–graph into a corresponding meta graph, or direct construction of meta graphs that are later converted (or “reified”) to one of the base graph types. miniKanren goals generally work at the meta graph level, where—for instance—one would apply goals that unify a converted base graph with a pure meta graph containing logic variables.

While it is possible to achieve the same results with only etuples, meta graphs are a convenient form that allow developers to think and operate at the standard Python object level. They also provide a more direct means of graph validation and setup, since checks can–and are–performed during meta graph construction, whereas standard etuples would not be able to perform such operations until the resulting etuple is fully constructed and evaluated. Likewise, meta graphs are more appropriate for specifying and obtaining derived information, like shapes and data types, for a (sub)graph instead of miniKanren.

To demonstrate the use of symbolic-pymc, we consider a simple conjugate model constructed using PyMC3 in Listing 4.13.

Listing 4.13: A beta-binomial conjugate model in PyMC3.

```python
import pymc3 as pm
with pm.Model() as model:
    p = pm.Beta("p", alpha=2, beta=2)
    y = pm.Binomial("y", n=totals, p=p, observed=obs_counts)
```

A user will generally have some data specifying the values for totals and obs_counts and will want to estimate the posterior distribution of p. In the Bayesian world, posterior distributions are generally the object of interest and estimation.

More specifically, we want to estimate the distribution for a rate of success, p, given a total number of events, totals, and observed successes, obs_counts, under the assumption that the events are binomially distributed with rate p. We let p take a beta distribution prior, and that completes our Bayesian specification of a model.

Mathematically, this simple model is stated as follows:

\[ Y \sim \text{Binom}(N, p) \]
\[ p \sim \text{Beta}(2, 2) \]

(3)
and it has a well known closed-form posterior distribution given by

\[
(p \mid Y = y) \sim \text{Beta}(2 + y, 2 + N - y)
\]

(4)

Instead of wasting resources estimating the posterior numerically (e.g., using `pm.sample(model)` to run a Markov Chain Monte Carlo sampler), we can simply extract the underlying Theano graph from `model` and apply a relation that represents the underlying conjugacy and use the resulting posterior.

The general rule implied by this situation is

\[
\text{(beta-binomial-conjugate)} \quad Y \sim \text{Binom}(N, p), \quad p \sim \text{Beta}(\alpha, \beta)
\]

\[
(p \mid Y = y) \sim \text{Beta}(\alpha + y, \beta + N - y)
\]

(5)

Listing 4.14 converts the PyMC3 model object, `model`, into a standard Theano graph that represents the relationship between random variables in the model.

Listing 4.14: Converting a PyMC3 model into a Theano graph of the model’s sample-space.

```python
from symbolic_pymc.theano.pymc3 import model_graph
from symbolic_pymc.theano.utils import canonicalize

# Convert the PyMC3 graph into a symbolic-pymc graph
fgraph = model_graph(model)

# Perform a set of standard algebraic simplifications using Theano
fgraph = canonicalize(fgraph, in_place=False)
```

Listing 4.15 uses miniKanren to construct a goal, `betabin_conjugateo`, that matches terms taking the form of Equation (3) in the first argument and the resulting posterior of Equation (4) in the second argument. It makes use of both meta objects and `etuple`s.

Listing 4.15: A miniKanren goal that implements the beta-binomial conjugate rule in (5).

```python
def betabin_conjugateo(x, y):
    """Replace an observed Beta-Binomial model with an unobserved posterior
    \sim \text{Beta-Binomial model}.""
    obs_lv = var()

    beta_size, beta_rng, beta_name_lv = var(), var(), var()
    alpha_lv, beta_lv = var(), var()
    # We use meta objects directly to construct the "pattern" we want to match
    beta_rv_lv = mt.BetaRV(alpha_lv, beta_lv, size=beta_size, rng=beta_rng,
                           name=beta_name_lv)

    binom_size, binom_rng, binom_name_lv = var(), var(), var()
    N_lv = var()
    binom_lv = mt.BinomialRV(N_lv, beta_rv_lv, size=binom_size, rng=binom_rng,
                             name=binom_name_lv)
```
Listing 4.15 – continued

```python
# Here we use etuples for the output terms
obs_sum = etuple(mt.sum, obs_lv)
alpha_new = etuple(mt.add, alpha_lv, obs_sum)
beta_new = etuple(mt.add, beta_lv, etuple(mt.sub, etuple(mt.sum, N_lv), obs_sum))

beta_post_rv_lv = etuple(
    mt.BetaRV, alpha_new, beta_new, beta_size, beta_rng, name=etuple(add, beta_name_lv, "_post")
)
binom_new_lv = etuple(
    mt.BinomialRV,
    N_lv, beta_post_rv_lv, binom_size, binom_rng,
    name=etuple(add, binom_name_lv, "_post"),
)

return lall(eq(x, mt.observed(obs_lv, binom_lv)), eq(y, binom_new_lv))
```

Finally, Listing 4.16 shows how the goal can be applied to the model’s graph and how a new Theano graph and PyMC3 model is constructed from the output.

Listing 4.16: Running the beta-binomial conjugate goal and creating a PyMC3 model for the results.

```python
from symbolic_pymc.theano.pymc3 import graph_model

q = var()
res = run(1, q, betabin_conjugateo(fgraph.outputs[0], q))
expr_graph = res[0].eval_obj
fgraph_conj = expr_graph.reify()

# Convert the Theano graph into a PyMC3 model
model_conjugated = graph_model(fgraph_conj)
```

Willard (2020b) gives a more thorough walk-through of symbolic-pymc and miniKanren–using TensorFlow graphs.
5 DISCUSSION

Looking forward, the “functions grimoire” project of Johansson (2020), Fungrim, is a great example of community-sourced and programmatically encoded domain knowledge in mathematics. It serves as a prime example of an independently developed, high-level knowledge encoding effort from which relations could be sourced and used by miniKanren in Python. In Byrd (2020) miniKanren is used to reason over an external database of medical knowledge, so the a precedent for this type of work has already been set.

One currently unexplored area involves interactions between miniKanren and symbolic algebra libraries. Although a lot of symbolic algebra is possible using miniKanren alone, we don’t necessarily expect it to replace symbolic algebra libraries any time soon. Luckily, when our statistical modeling goals require advanced symbolic algebra functionality provided by existing libraries, like SymPy (SymPy Development Team 2014), they can be used directly from within miniKanren. For example, one could use SymPy to perform a Laplace transform— or its inverse— within an implementation of a normal scale mixture (Bhadra et al. 2020) relation between random variables, since the underlying mathematical relation is functionally described by Laplace transforms in both directions.

A combination of miniKanren and computer algebra could also be used to realize elements of the computer algebra and interactive theorem proving synthesis described in Kaliszyk and Wiedijk (2007).

Perhaps another concrete example of how a symbolic algebra library could be leveraged by miniKanren is given by the system described in Walia et al. (2018). Here, miniKanren could be used to implement the typing rules, and the integrate steps could be outsourced to SymPy. By targeting standard NumPy (Numpy Developers 2017) output, the results could be used by any number of systems, like JAX, that provide vectorization, JIT compilation, etc.

Ultimately, we’ve described the construction of a strictly Python version of the system in Walia et al. (2018) that makes use of multiple popular, actively developed projects specializing in their respective domains (e.g. symbolic integration, vectorization, JIT compilation). The original implementation uses a complex pipeline (Walia et al. 2018, Figure 1) that operates across multiple independent systems, one of which is Hakaru (Narayanan et al. 2016). Hakaru is an entirely independent system and programming language for probabilistic programming. In contrast, the system we describe is simply an orchestration of existing Python libraries driven by miniKanren, and it can make use of whichever tensor libraries, compilation frameworks, and PPLs are most suitable.

Regarding miniKanren itself, consider the following idiom:

```python
(conde ((== lhs match-form-1)
       (== rhs replace-form-1))
      ((== lhs match-form-2)
       (== rhs replace-form-2))
      ...)
```

condes like this are natural for encoding identities of the form match-form-1 = replace-form-1 that are applied to the terms lhs and rhs. They also appear in implementations of relational interpreters where they encode the supported forms of a target language (e.g. variable assignment, conditionals, etc.)

These conde idioms comprise a large portion of the miniKanren work implied here, and their size could grow very quickly over time. This leads to performance questions that are possibly answered by work on guided search (Swords and Friedman; Zhang et al. 2018) and discerning conde branch selection (Boskin et al. 2018).

, Vol. 1, No. 1, Article 1. Publication date: January 2016.
There is also little reason to think that a single conde will—or even should—encode most of a system’s implemented identities, so a means of compiling goals—say—for the purposes of merging branches might be worth considering, as well.

With equational identities nicely encoded by conde forms, there’s also the possibility that the rewrite-completion algorithms mentioned in Section 2 could be applied automatically. When a complete and reduced rewrite system can be generated from a conde, it would be interesting to know whether or not the resulting system improves the general performance of miniKanren.

Also, is it possible that some cases of non-terminating goal orderings could be avoided by completion? Likewise, could the results of completion be used to produce a new, equivalent conde that results in fewer goal evaluations and/or failed branches?

Alternatively, is it possible that miniKanren could be utilized by a completion algorithm itself so that it produces potentially relevant results when it otherwise wouldn’t terminate (e.g. via infinite goal streams)? What are the advantages of performing completion in a relational fashion, and what unique elements can miniKanren provide to that situation (e.g. easier implementation of experimental completion algorithms)?

Proving rewrite termination and completion itself can involve SAT problems (Endrullis et al. 2008; Klein and Hirokawa 2011); can miniKanren’s constraint capabilities—among other things—be applied in this area?

Our Python implementation of miniKanren comes with experimental support for associative and commutative (AC) relations. We’ve found utility in assigning these two properties to existing operators from other libraries (e.g. addition operators in Theano and TensorFlow) as a means of adding flexibility to the exact representation of graphs. This is especially important in instances where graph normalization isn’t entirely consistent or available via the targeted graph backend (e.g. TensorFlow).

The process of implementing these AC relations has opened a few questions that cannot be properly treated here. Questions such as "How can operators with arbitrary—but known and fixed—arities be efficiently supported?" and "How can we overcome some of the goal ordering issues that arise due to commutativity?".

In (Willard 2020a), we address the latter question with a "groundedness"-based term reordering goal. This reordering is performed on the cdr sub-terms as a relation is applied between term graphs, since the order in which a relation is applied to corresponding sub-terms is—generally—immaterial. In other words, when walking a goal relo between the lists '(a b) and '(c 2), for fresh variables a, b, and c, the goal can be applied in any order, e.g. (relo a c) then (relo b 2), or (relo b 2) then (relo a c). When—for instance—(relo a b) diverges because both arguments are fresh, while (relo b 2) fails, a walk that performs the former ordering will diverge, while one that does the latter will fail. The “groundedness” ordering goal simply reorders the corresponding pairs according to how grounded they are to arrive at the non-diverging order of application.

Finally, we would like to point out the potential for an exciting ‘feedback loop’: as statistical modeling improves the processing of miniKanren (Zhang et al. 2018), miniKanren can also improve the process of statistical modeling.

ACKNOWLEDGMENTS
The author would like to thank Jason Hemann and William Byrd for their invaluable input and inspiring work.

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