

Instruction level automatic differentiation on a reversible Turing machine

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This paper considers the instruction level adjoint mode differential programming, i.e. knowing only the backward rules of basic instructions like +, -, * and /, obtain the gradient of parameters in an arbitrary differentiable program with proper performance. In this paper, we review briefly why instruction level automatic differentiation is hard for current machine learning frameworks and propose an implementation of reversible Turing machine as a solution. We show how reversible programming can differentiate a general program to an arbitrary order automatically by viewing basic instructions as the computational graph.

I. INTRODUCTION

[JG: TODOs: show benchmark, quantum example? recursive gradient approach to obtain hessian] There are two modes of automatic differentiation (AD) [1], the tangent mode [2] and the adjoint mode. Consider a multi-in multi-out function $\vec{y} = f(\vec{x})$, the tangent mode computes a column of its Jacobian $\frac{\partial \vec{y}}{\partial x_i}$ efficiently, where x_i is one of the input variables. Whereas the adjoint mode computes a row of Jacobian $\frac{\partial y_i}{\partial \vec{x}}$ efficiently. Most popular automatic differentiation package implements the adjoint mode differentiation, since the adjoint mode is computational more efficient in variational applications, where the output loss is always a scalar. However, implementing adjoint mode AD requires a program's intermediate state for back propagation, including

1. computation graph,
2. and input variables of nodes in computation graph.

A computational graph is a directed acyclic graph (DAG) that records the relation between data (edges) and functions (nodes). In Pytorch [3] and Flux [4], every variable has a tracker field that stores its parent information, i.e. the input data and function that generate this variable. TensorFlow [5] implements a static computational graph as a description of the program before actual computation happens. Source to source automatic differentiation package Zygote [4, 6] use a intermediate representation of a program the static single assignment (SSA) form as the computation graph in order to propagate a native julia code. Its intermediate stage is cached in a global storage.

Several limitations are observed in these AD implementations due to the recording and caching. First of all, these package requires a lot primitive functions with programmer defined backward rules. This is not necessary given the fact that, at the lowest level, these primitive functions are compiled to instructions, and these instructions are from a finite set including '+', '-', '*', '/' and conditional jump statements. By defining backward rules for these basic instructions and

the automatic differentiation should just work. These machine learning packages can not use instructions as the computational graph for practical reasons. The cost of memorizing the computational graph and intermediate caching kills the performance for more than two orders in simple loops (as we will show latter). Even more, the memory consumption for caching intermediate results increases linearly as time. In many deep learning models like recurrent neural network and residual neural networks, the depth can reach several thousand, the memory wall [7] can be big problem. Secondly, inplace functions are not handled properly in the diagram of computation graph. Even in source to source AD engine Zygote, it is not trivial to handle inplace functions. Most functions in BLAS and LAPACK are implemented as inplace functions. The lack of automatic differentiation support to inplace functions make the memory wall problem even more severe. It is also harmful to code reusing since all packages using BLAS functions should define their own backward rules for their non-inplace wrappers. Thirdly, obtaining higher order gradients are not efficient in these packages. For example, in most machine learning packages, people back propagate the whole program of obtaining first order gradient to obtain the second order gradients. The repeated use of back propagation cause exponential overhead with respect to the order of gradients. A better approach to obtain higher order gradients is through Taylor propagation like in JAX [8]. However Taylor propagation requires writing rules for all primitives. Besides the exponential overhead, the source to source AD engine Zygote suffers from the significant overhead of just in time compiling in Julia language [9].

Our solution to these issues is make a program time reversible. Making use of reversibility has been used in machine learning as a promising approach to save memory. People use information buffer [10] and reversible activation functions to reduce the memory allocations in recurrent neural network [11] and residual neural networks [12]. However, the use of reversibility in these cases are not general purposed.

Hence we develop a embeded domain specific language (eDSL) in Julia language that implements reversible Turing machine. [13, 14]. The gradient of any program writing in this eDSL can be obtained in comparable time to the forward function. The implementation of AD is similar to ForwardDiff [2] but runs backward. There has been

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some prototypes of reversible languages like Janus [15], R (not the popular one), Erlang [16] and object oriented ROOPL []. These languages have reversible control flow that allows user input additional information, the postcondition in control flows to help programs run backward. In the past, the main motivation to make a program reversible is to support reversible devices. Reversible devices do not have a lower bound of energy consumption as indicated by Landauer principle [17]. However CMOS devices still has two orders [14] space to optimize regarding this lower bound. The main contribution of our work is breaking the information barrier between machine learning community and reversible programming community, providing yet another strong motivating to develop a reversible programming. Our eDSL borrows the design of reversible control flow in the Janus, meanwhile provides multiple dispatch based abstraction. With these additional features, the AD engine differentiating a general program could be implemented in less than 100 lines. Our eDSL generates native julia code, and is completely compatible with Julia language. Potential applications includes

1. generate AD rules for primitive functions like `exp`,
2. control problem in robotics [18] where tensors are not welcomed,
3. differentiating over reversible integrators [19] without intermediate state caching,
4. Stabilize linear algebras functions backward rules. Current backward rules for singular value decomposition (SVD) and eigenvalue decomposition (ED) [20–22] are vulnerable to spectrum degeneracy. The development of backward rules for these linear algebra functions can greatly change the research code in physics [23, 24].

In this paper, we first introduce the design of this eDSL in Sec. II and the back propagation of Jacobians and Hessians on this DSL in Sec. III. Then we propose a different training strategy in Sec. IV by making use of reversibility, rather than gradients. In Sec. V, we introduce several examples. In Sec. VI, we discuss on several important issues, how time space tradeoff works, reversible instructions and hardwares and finally an outlook to some open problems to be solved.

II. LANGUAGE DESIGN

In a modern programming language, functions are pushed to a global stack for scheduling. The memory layout of a function is consisted of input arguments, a function frame with informations like return address and saved memory segments, local variables and working stack. After each call, the function clears the input arguments, function frame, local variables and working stack and only stores the return value. In the invertible programming style, this kind of design pattern is no longer the best practise, input variables can not be easily discarded after a function call, since discarding information may ruin reversibility. Hence, a reversible instruction/function call in NiLang changes inputs "inplace".

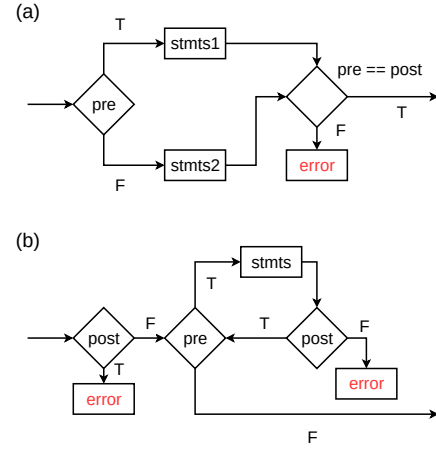


Figure 1. Flow chart for reversible (a) if statement and (b) while statement. “stmts”, “stmts1” and “stmts2” are statements, statements in true branch and statements in false branch respectively. “pre” and “post” are precondition and postconditions respectively. “error” refers to `InvertibilityError`.

NiLang is a reversible eDSL in Julia that simulates reversible Turing machine. The grammar is shown in Appendix A. Its main feature is contained in a single macro `@i`. It interprets a reversible function, and compile this function, as well as its inverse to a finite set of “instructions” written in julia language. These instructions are closed under the inverse operation “`~`”, hence all functions defined in NiLang are also closed under “`~`” operations.

The interpretation of a reversible function consists three stages. The first stage preprocess human input to a reversible IR. It checks human input and removes redundancy in grammar. To be specific, It

- adds missing `@deanc` to make sure `@anc` and `@deanc` statements appear in pairs,
- expands `@routine` macro,
- and expands the symbol `~` in postcondition field as precondition.

Here, the macro `@anc <a> = <expr>` binds variable `<a>` to an initial value specified by `<expr>`, while `@deanc <a> = <expr>` deallocates the variable `<a>`. Before deallocating a variable, the program checks that the variable is restored to its initial value, otherwise an `InvertibilityError` will be thrown. `@anc` and `@deanc` must appear in pairs inside a function call, a while statement or a for statement, otherwise `@deanc` will be added automatically. Similar designs in Janus and R are `local/delocal` statement and `let` statement. The additional check underlines the difference between the irreversible assign statement and reversible ancilla statement. `@routine <name> Stmt` is a statements recorder, it records a statement to symbol `<name>`. When `@routine <name>` or `~@routine <name>` is called, the statement or inverse statement is inserted to that position. A condition expression that appear in the if statement is consist of two boolean

expressions, the precondition and postcondition as shown in Fig. 1 (a). If the precondition is unchanged after the execution of body statements, we can omit the postcondition by inserting \sim in the postcondition field. This shorthand is expanded in this stage.

The second stage generates the inverse function.

statement	inverse
$\langle f \rangle(\langle \text{args} \rangle)$	$(\sim \langle f \rangle)(\langle \text{args} \rangle)$
$\langle \text{out}! \rangle += \langle f \rangle(\langle \text{args} \rangle)$	$\langle \text{out}! \rangle -= \langle f \rangle(\langle \text{args} \rangle)$
$\langle \text{out}! \rangle .+= \langle f \rangle.(\langle \text{args} \rangle)$	$\langle \text{out}! \rangle .-= \langle f \rangle.(\langle \text{args} \rangle)$
$\langle \text{out}! \rangle \forall = \langle f \rangle(\langle \text{args} \rangle)$	$\langle \text{out}! \rangle \forall = \langle f \rangle(\langle \text{args} \rangle)$
$\langle \text{out}! \rangle .\forall = \langle f \rangle(\langle \text{args} \rangle)$	$\langle \text{out}! \rangle .\forall = \langle f \rangle(\langle \text{args} \rangle)$
$\text{@anc } \langle a \rangle = \langle \text{expr} \rangle$	$\text{@deanc } \langle a \rangle = \langle \text{expr} \rangle$
begin $\langle \text{stmts} \rangle$ end	begin $\sim(\langle \text{stmts} \rangle)$ end
if $\langle \text{pre} \rangle, \langle \text{post} \rangle$ $\langle \text{stmts1} \rangle$ else $\langle \text{stmts2} \rangle$ end	if $\langle \text{post} \rangle, \langle \text{pre} \rangle$ $\sim(\langle \text{stmts} \rangle)$ else $\sim(\langle \text{stmts} \rangle)$ end
while $\langle \text{pre} \rangle, \langle \text{post} \rangle$ $\langle \text{stmts} \rangle$ end	while $\langle \text{post} \rangle, \langle \text{pre} \rangle$ $\sim(\langle \text{stmts} \rangle)$ end
for $\langle i \rangle = \langle m \rangle : \langle s \rangle : \langle n \rangle$ $\langle \text{stmts} \rangle$ end	for $\langle i \rangle = \langle m \rangle : \sim \langle s \rangle : \langle n \rangle$ $\sim(\langle \text{stmts} \rangle)$ end
$\text{@safe } \langle \text{expr} \rangle$	$\text{@safe } \langle \text{expr} \rangle$

Table I. A collection of reversible statements.

A condition expression is a two-element tuple, it also allows user putting additional postcondition in control flows to help reverse the program. A postcondition is a boolean expression that evaluated after the controlled body being executed. The @safe macro can be followed by an arbitrary statement, it allows user to use external statements that does not break reversibility. $\text{@safe } \text{@show } \text{var}$ is often used for debugging.

The third stage is translating this reversible IR to native Julia code. It

- adds @instr before each instruction and function call statement,
- attach a return statement after the function definition which returns the modified input variables as the output,
- adds statements to check the consistency between preconditions and postconditions to ensure reversibility,
- compile the inverse function at the same time.

The macro @instr assign the output of a function to the argument list of a function. Hence, the values are changed while the symbol table is not changed. Here, the statement $\text{out}! += x * y$ calls instruction $\oplus(*)$ ($\text{out}!, x, y$), which means accumulate a product of two variables to

target symbol. Combine it with @instr that assigns each output to each input, we simulate a mutable operations.

A. Types and dataviews

A constructor is also a reversible function, it changes the behavior of data or derive a new field from a data. Its reverse function is a “destructor”, a destructor does not deallocate memory directly but unpacks data.

Before introducing dataviews, let's first consider the following example

```
grad(arr[3].value) += x * y
```

In Julia, this statement will raise a syntax error, since a function call can not be assigned. Meanwhile $\text{arr}[3]$ might be a immutable type. In our eDSL, assigning a single argument function call or a immutable type is allowed.

In our interpreter, $\text{grad}(\text{arr}[3].\text{value}) += x * y$ is translated to $\text{@instr } \text{grad}(\text{arr}[3].\text{value}) += x * y$ at the third stage. To execute the instruction, @instr translate the statement to

```
res = (*) (grad(arr[3].value), x, y)
arr[3] = chfield(arr[1], Val(:value),
  chfield(arr[3].value, grad, res[1]))
x = res[2]
y = res[3]
```

$\oplus(*)$ ($\text{grad}(\text{arr}[3].\text{value}), x, y$) computes the output, which is a tuple of length 3. chfield is used to infer the new data by modifying a field or a bijective mapping of a field, it returns a new object. The second and third arguments can be assigned back directly. A dataview of a data can be data itself, a field of its view, an array element of its view, or a bijective mapping of its view. If the default constructor of a type is not overwritten by user, NiLang can modify a field of that type automatically. For a bijective mapping of a field, user need to specify the behavior of a dataview by overloading chfield function.

B. Traditional Invertible Computing Devices

It is possible to design and fabricate a fully reversible processor using resources which are comparable to a conventional microprocessor. Existing CAD tools and silicon technology are sufficient for reversible computer design.

Like quantum computer, it should be able to reset to qubits 0. The reset operation, sometimes can be expensive. In a quantum device, this reset operation can be done by dissipation and decoherence (i.e. interact with environment and get thermalized). Alternatively, a immediate feedback

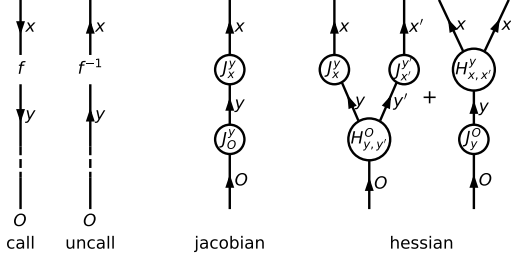


Figure 2. Adjoint rules for Jacobians and Hessians in tensor network language.

loop can be introduced to a quantum device, where a classical computer is regarded as the dissipation source.

III. TAYLOR PROPAGATION ON A REVERSIBLE TURING MACHINE

Taylor propagation is exponentially (as the order) more efficient in obtaining higher order gradients than differentiating lower order gradients recursively. The later requires traversing the computational graph repeatedly. In JAX, in order to support Taylor propagation, the propagation rules for part of primitives manually defined. The exhausted support requires much more effort than the first order gradient propagation. Instruction level automatic differentiation is more flexible in obtaining higher order gradients like Hessian.

A. First order gradient

Given a node $\vec{y} = f(\vec{x})$ in a computational graph, we can propagate the Jacobians in tangent mode like

$$J_{x_i}^O = J_{y_j}^{O y_j} J_{x_i}^{y_j} \quad (1)$$

and the adjoint mode

$$J_I^{y_j} = J_{x_i}^{y_j} J_I^{x_i} \quad (2)$$

Here, I is the inputs and O is the outputs. Einstein's notation is used so that duplicated indices are summed over. Tagent mode instruction level automatic differentiation can be implemented easily in a irreversible language with dual numbers, here we focus on the adjoint mode. The backward rule can be described in tensor network [] language as shown in Fig. 2.

In reversible programming, we have the following implementation

Algorithm 1: Reversible programming AD

```

grad.( $\vec{x}_g$ ) let  $i_{loss}$  be the index of loss variable
 $\vec{y} = f(\vec{x})$ 
 $\vec{y}_g = \text{GVar.}(\vec{y})$ 
 $\vec{x}_g = f^{-1}(\vec{y}_g)$ 
grad( $\vec{y}_g[i_{loss}]$ ) += 1.0

```

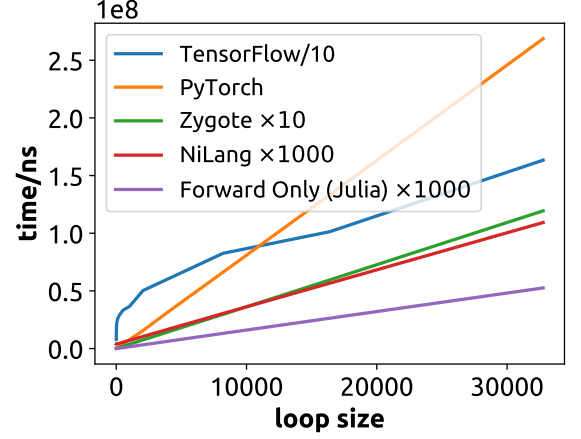


Figure 3. The time for obtaining gradient as function of loop size. $\times n$ in legend represents a rescaling of time.

Here, “.” is the broadcast operations in Julia. GVar is a “reversible type”. GVar(x) attaches a zero gradient field to a variable, which is similar to the dual number in tangent mode automatic differentiation. The gradient can be accessed by grad function. Its inverse ~GVar deallocates the gradient field safely and returns its value field. Here, “safely” means it will check the gradient field to make sure it is in 0 state. When a instruct meets a GVar, besides computing its value field value(\vec{x}) = $f^{-1}(\text{value}(\vec{y}))$, it also updates the gradient field grad(\vec{x}) = $J_{\vec{y}}^{\vec{x}} \text{grad}(\vec{y})$. Since f^{-1} is bijective, $J_{\vec{y}}^{\vec{x}}$ can be easily obtained by inspecting its inverse function f . The final output is stored in the gradient field, when then gradient is not used anymore, the faithful reversible programming style to compute gradients would be uncomputing the whole process to obtain gradient, which increases the hyrarchy by 1. Whenever the hyrarchy increase by 1, the computational overhead doubles comparing with its irreversible counter part.

Due to the multiple dispatch and just in time compiling, most runtime overhead can be removed. Let's consider a simple example that accumulate 1.0 to a target variable x for n times

```

@i function prog(x, one, n::Int)
  for i=1:n
    x += identity(one)
  end
end

```

From the benchmark result shown in Fig. 3. One can see that the NiLang implementation is unreasonably fast, even faster than two times the forward pass written in Julia. The code for benchmark is open for review in our paper github repository [25]. This benchmark does show the actual performance in real applications. In real application, the reversible program can have memory or computing time overhead. We will discuss the details of time and space tradeoff in Sec. VI A.

B. Second order gradient

The second order gradient can also be back propagated

$$\begin{aligned} H_{y_L, y'_L}^f &= 0 \\ H_{y_{i-1}, y'_{i-1}}^f &= J_{y_{i-1}}^{y_i} H_{y_i, y'_i}^f J_{y'_i}^{y'_{i-1}} + J_{y_i}^f H_{y_{i-1}, y'_{i-1}}^{y_i} \end{aligned} \quad (3)$$

In tensor network language, it can be represented as in Fig. 2. This approach can be easily extended to higher orders, or taylor propagation. However, this is not the widely adopted approach to compute higher order gradients. Although backpropagating higher order gradients directly is exponentially faster than back propagating the computational graph for computing lower order gradients for computing higher order gradients, one has to extending the backward rules for each primitive rather than reusing existing ones. Here, we emphasis that with instruction level AD, rewriting backward rules for primitives turns out to be not so difficult. An example is provided in Sec. VB.

C. Gradient on ancilla problem

Ancilla can also carry gradients during computation, sometimes these gradients can not be uncomputed even if their parents can be uncomputed regoriously. In these case, we simply “drop” the gradient field instead of raising an error. In this subsection, we prove doing this is safe, i.e. does not have effect on rest parts of program.

Ancilla is the fixed point of a function, which means

$$\begin{aligned} b, y &\leftarrow f(x, a), \text{ where } b == a \\ \frac{\partial b}{\partial x} &= 0 \end{aligned} \quad (4)$$

During the computation, the gradient field does not have any effect to the value field of variables. The key question is will the loss of gradient part in ancilla affect the reversibility of the gradient part of argument variables. The gradient of argument variable is defined as $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial x} + \frac{\partial L}{\partial b} \frac{\partial b}{\partial x}$, where the second term vanish naturally.

D. Implementation

The automatic differentiation engine is so short that we present the function defintion as follows

```
@i function (g::Grad)(args...; kwargs...)
    @safe @assert count(x -> x isa Loss, args) == 1
    @anc iloss = 0
    @routine getiloss begin
        for i=1:length(args)
            if (tget(args,i) isa Loss, iloss==i)
                iloss += identity(i)
                (~Loss)(tget(args,i))
            end
        end
    end

    g.f(args...; kwargs...)
    GVar.(args)
    grad(tget(args,iloss)) += identity(1.0)
    (~g.f)(args...; kwargs...)

    ~@routine getiloss
end
```

The program first checks the input parameters and locate the loss variable. Then Loss unwraps the loss variable, the location of loss variable is transferred to the ancilla iloss of integer type.

GVar

```
julia> using NiLang, NiLang.AD

julia> x, y = GVar(0.5), GVar(0.6)
(GVar{0.5, 0.0}, GVar{0.6, 0.0})

julia> @instr grad(x) += identity(1.0)

julia> @instr x += identity(y)

julia> y
GVar{0.6, -1.0}

julia> @instr grad(x) -= identity(1.0)

julia> @instr (~GVar)(x)

julia> x
1.1
```

Broadcasting is supported. To avoid possible confusing, tuple indexing is forbidden delebrately, one can use `tget(tuple, 2)` to get the second element of a tuple.

IV. LEARN BY CONSISTENCY

Consider training data consist of input \vec{x}^* and output \vec{y}^* . The goal is to find a set of parameters \vec{p}_x that satisfy $\vec{y}^* = f(\vec{x}^*, \vec{p}_x)$. In traditional machine learning, we define a loss $\mathcal{L} = \text{dist}(\vec{y}^*, f(\vec{x}^*, \vec{p}_x))$ and minimize it with gradient $\frac{\partial \mathcal{L}}{\partial \vec{p}_x}$. This is viable only when the target function is locally differentiable.

Here we provide an alternative by making use of reversibility. We construct a reversible program $\vec{y}, \vec{p}_y = f_r(\vec{x}, \vec{p}_x)$, where

\vec{p}_x and \vec{p}_y are “garbage” spaces which include parameters. The algorithm can be summarized as

Algorithm 2: Learn by consistency

Result: \vec{g}_x

Initialize \vec{x} to \vec{x}^* , garbage space \vec{g}_x to random.

if \vec{g}_y is null **then**

$\vec{x}, \vec{g}_x = f_r^{-1}(\vec{y}^*)$

else

$\vec{y}, \vec{g}_y = f_r(\vec{x}, \vec{g}_x)$

while $\vec{y} \neq \vec{y}^*$ **do**

$\vec{y} = \vec{y}^*$

$\vec{x}, \vec{g}_x = f_r^{-1}(\vec{y}, \vec{g}_y)$

$\vec{x} = \vec{x}^*$

$\vec{y}, \vec{g}_y = f_r(\vec{x}, \vec{g}_x)$

Here, **garbage**(\cdot) is a function for taking the garbage space. This algorithm utilizes the self-consistency relation

$$\vec{g}_x^* = \text{garbage}(f_r^{-1}(\vec{y}^*, \text{garbage}(f_r(\vec{x}^*, \vec{g}_x^*)))), \quad (5)$$

Similar idea of training by consistency is used in self-consistent meanfield theory [] in physics. The difficult part of self-consistent training is to find a self-consistency relation, here the reversibility provides a natural self-consistency relation. Learn by consistency can be used to handle discrete optimization. However, it is not a silver bullet, and should be used with caution. Let’s consider the following example

```
@i function f1(out!, x, y!)
    y! += identity(x)
    out! -= exp(x)
    out! += exp(y!)
end

@i function f2(out!, x!, y!)
    y! += identity(x!)
    out! -= exp(x!)
    x! -= log(-out!)
    out! += exp(y!)
end

function train(f)
    loss = Float64[]
    y = 1.6
    for i=1:100
        out!, x = 0.0, 0.3
        @instr f(out!, x, y)
        push!(loss, out!)
        out! = 1.0
        @instr (~f)(out!, x, y)
    end
    loss
end
```

Functions **f1** and **f2** computes $f(x, y) = e^{(y+x)} - e^x$ and stores the output in a new memory **out!**. The only difference is **f2** “uncompute” x arithmetically. The task of training is to

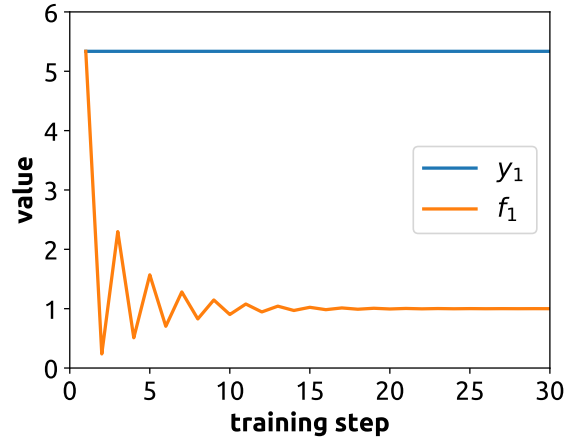


Figure 4. The value of x as a function of self-consistent training step.

find a y that make the output value equal to target value 1. After 200 steps, f_2 runs into the fixed point with x equal to 1 upto machine precision. However, f_1 does not do any training. The training of f_2 fails because this function actually computes $f_1(out!, x, y!) = out! + e^{(y!+x)} - e^x, x, x + y!$, where the training parameter y is completely determined by the garbage space on output side x and $x + y!$. As a result, shifting **out!** directly is the only approach to satisfy the consistency relation. On the other side, $f_2(out!, x, y!) = out! + e^{(y!+x)} - e^x, (x - \log(e^x)), x + y!$, parameters y is not completely determined by the garbage space $(x - \log(e^x)), x + y!$.

By viewing \vec{x} and parameters in \vec{p}_x as variables, we can study the trainability from the information perspective.

Theorem 1. Only if the the conditional entropy $S(\vec{y}|\vec{p}_y)$ is nonzero, algorithm 2 is trainable.

Proof. The above discussion reveals a fact that the training can not work when the output \vec{p}_y completely determines \vec{p}_x , that is

$$\begin{aligned} S(\vec{p}_x|\vec{p}_y) &= S(\vec{p}_x \cup \vec{p}_y) - S(\vec{p}_y) \\ &\leq S((\vec{p}_x \cup \vec{x}) \cup \vec{p}_y) - S(\vec{p}_y), \\ &\leq S((\vec{p}_y \cup \vec{y}) \cup \vec{p}_y) - S(\vec{p}_y), \\ &\leq S(\vec{y}|\vec{p}_y). \end{aligned} \quad (6)$$

The third line uses the bijectivity $S(\vec{x} \cup \vec{p}_x) = S(\vec{y} \cup \vec{p}_y)$. \square

This inequality shows that when the garbage space on the output side satisfies $S(\vec{y}|\vec{p}_y) = 0$, i.e. contains all information to determine the output field, the input parameters are also completely determined by this garbage space. In the above examples, it corresponds to the case $S(e^{(x+y)} - e^x | x \cup x + y) = 0$ in f_1 . One should remove the redundancy of information by uncomputing to make training by consistency work properly.

V. EXAMPLES

A. Computing Fibonacci Numbers

An example that everyone likes

```
@i function rfib(out, n::T) where T
  @anc n1 = zero(T)
  @anc n2 = zero(T)
  @routine init begin
    n1 += identity(n)
    n1 -= identity(1.0)
    n2 += identity(n)
    n2 -= identity(2.0)
  end
  if (value(n) <= 2, ~)
    out += identity(1.0)
  else
    rfib(out, n1)
    rfib(out, n2)
  end
  ~@routine init
end
```

To compute the first Fibonacci number that is greater or equal to 100

```
@i function rfib100(n)
  @safe @assert n == 0
  while (fib(n) < 100, n != 0)
    n += identity(1.0)
  end
end
```

Here, `fib` and `rfib` are defined in Appendix V A. The reversible `while` statement contains two statements, the precondition and postcondition. Before entering the while statement, the program check the postcondition to make sure it is false. After each iteration, postcondition returns true. The inverse function exchanges the precondition and postcondition so that the repetition of loop body is not changed.

B. exp function

An exp function can be computed using Taylor expansion

$$\text{out!} += \sum_n \frac{x^n}{\text{factorial}(n)} \quad (7)$$

Here, the “!” after a variable is used to indicate that a variable is changed after the call of an instruction or function. This is a recursive algorithm that mimics pebble game. Define the term for accumulation $s_n \equiv \frac{x^n}{\text{factorial}(n)}$, the recursion relation is written as $s_n = \frac{x s_{n-1}}{n}$. There is no known constant memory and polynomial time algorithm to pebble game. Here the case is different. Notice $*$ and $/$ are arithmetically reversible

to each other, we can uncompute $s_{n-1} = \frac{n s_n}{x}$ to deallocate memory. By allowing loss of several digit precision of result, implementing the constant memory reversible exp function is possible

```
using NiLang, NiLang.AD

@i function iexp(out!, x::T; atol::Float64=1e-14)
  where T
    @anc anc1 = zero(T)
    @anc anc2 = zero(T)
    @anc anc3 = zero(T)
    @anc iplus = 0
    @anc expout = zero(T)

    out! += identity(1.0)
    @routine r1 begin
      anc1 += identity(1.0)
      while (value(anc1) > atol, iplus != 0)
        iplus += identity(1)
        anc2 += anc1 * x
        anc3 += anc2 / iplus
        expout += identity(anc3)
        # arithmetic uncompute
        anc1 -= anc2 / x
        anc2 -= anc3 * iplus
        SWAP(anc1, anc3)
      end
    end

    out! += identity(expout)

    ~@routine r1
end
```

The definition of SWAP instruction can be found in Appendix B. The two lines bellow the comment “# arithmetic uncompute” “uncomputes” variables `anc1` and `anc2`, this uncomputation is only true arithmetically, but not for floating point number due to the rounding error. As a result, the final output is not exact due to the rounding error. On the other side, the reversibility is not harmed since the inverse call at the last line of function uncomputes all ancilla bits rigorously. The `while` statement takes two conditions, the precondition and postcondition. Precondition `val(anc1) > atol` indicates when to break the forward pass and post condition `!isapprox(iplus, 0.0)` indicates when to break the backward pass.

To obtain the gradient, one can wrap the loss with `Loss` type and feed it into `iexp` function

```

julia> out!, x = 0.0, 1.6
(0.0, 1.6)

julia> @instr iexp'(Loss(out!), x)

julia> grad(x)
4.9530324244260555

julia> out!, x = 0.0, 1.6
(0.0, 1.6)

julia> simple_hessian(iexp, (Loss(out!), x))
2×2 Array{Float64,2}:
 0.0  0.0
 0.0  4.95303

```

`iexp'` returns an object of type `Grad{typeof(exp)}`, it returns input variables with updated gradient field. The loss variable is specified by a wrapper `Loss`, notice we don't distinguish input and output in reversible programming. The gradient functions are implemented reversibly so that the gradients can be differentiated again to obtain Hessians as shown in Fig. 5.

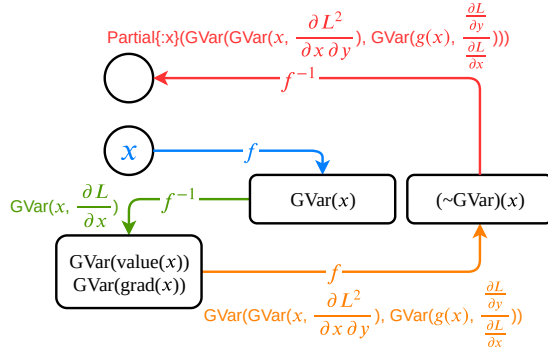


Figure 5. Obtaining the second order gradient with the reversible differentiation approach. Colors blue, green, orange and red indicate the four stages, data types and fields used for computation are marked in the same color.

There are four stages in computing Hessian in the naive approach, the first two stages are obtaining gradients, the third stage is wrapping each field in `GVar` with `GVar` and compute forward function. Then we pick a variable `y` to compute a row of Hessian by adding 1 to `grad(y)`. At the final stage, the `~GVar` operation does not unwrap `GVar` directly because the gradient field of gradients may be non-zeros. Instead, we use `Partial{:,FIELD}(\cdot)` to safely invert `GVar` on data type `GVar{<:GVar, <:GVar}`. It takes a field without discarding information. In `NiLang`, `simple_hessian` obtains the Hessian matrix in this way by iterating over different `ys`.

The back propagation approach can be more efficient in obtaining higher order gradients.

```

julia> out!, x = 0.0, 1.6
(0.0, 1.6)

julia> @instr iexp''(Loss(out!), x)

julia> collect_hessian()
2×2 Array{Float64,2}:
 0.0  0.0
 0.0  4.95303

```

`iexp''` computes the second order derivative by wrapping the variable into type `BeijingRing`. This is a special data structure to store Hessians. Whenever an n -th variable is created, we push a ring of size $2n - 1$ in to a global tape. Whenever an ancilla is deallocated, we pop a ring from the top. The n -th ring stores $H_{i \leq n, n}$ and $H_{n, i < n}$. We didn't use the symmetry relation $H_{i,j} = H_{j,i}$ here to simplify the implementation of backward rules described in the right most panel of Fig. 2. The final result can be collected by calling a global function `collect_hessian`.

C. QR decomposition

Not only simple functions, linear algebra functions

tation of QR decomposition is correct

```
@i function iqr(Q, R, A::AbstractMatrix{T}) where T
  @anc anc_norm = zero(T)
  @anc anc_dot = zeros(T, size(A,2))
  @anc ri = zeros(T, size(A,1))
  for col = 1:size(A, 1)
    ri .+= identity.(A[:,col])
    for precol = 1:col-1
      idot(anc_dot[precol], Q[:,precol], ri)

      R[precol,col] += identity(anc_dot[precol])
      for row = 1:size(Q,1)
        ri[row] -= anc_dot[precol] * Q[row, precol]
      end
      inorm2(anc_norm, ri)

      R[col, col] += anc_norm^0.5
      for row = 1:size(Q,1)
        Q[row,col] += ri[row] / R[col, col]
      end

      ~(ri .+= identity.(A[:,col]));
      for precol = 1:col-1
        idot(anc_dot[precol], Q[:,precol], ri)
        for row = 1:size(Q,1)
          ri[row] -= anc_dot[precol] * Q[row, precol]
        end
        inorm2(anc_norm, ri)
      end
    end
  end
end
```

where idot and inorm2 are implemented as

```
@i function idot(out, v1::AbstractVector{T}, v2)
  where T
  @anc anc1 = zero(T)
  for i = 1:length(v1)
    anc1 += identity(v1[i])
    CONJ(anc1)
    out += v1[i]*v2[i]
    CONJ(anc1)
    anc1 -= identity(v1[i])
  end
end

@i function inorm2(out, vec::AbstractVector{T})
  where T
  @anc anc1 = zero(T)
  for i = 1:length(vec)
    anc1 += identity(vec[i])
    CONJ(anc1)
    out += anc1*vec[i]
    CONJ(anc1)
    anc1 -= identity(vec[i])
  end
end
```

One can easily check the gradient of this naive implemen-

```
using Test
A = randn(4,4)
q = zero(A)
r = zero(A)

@i function test1(out, q, r, A)
  iqr(q, r, A)
  out += identity(q[1,2])
end

@i function test2(out, q, r, A)
  iqr(q, r, A)
  out += identity(r[1,2])
end

@test check_grad(test1, (Loss(0.0), q, r, A);
  atol=0.05, verbose=true)
@test check_grad(test2, (Loss(0.0), q, r, A);
  atol=0.05, verbose=true)
```

Here, the check_grad function is a gradient checker function defined in NiLangCore.ADCore.

D. Unitary Matrices

Recurrent networks with a unitary parametrized network ease the gradient exploding and vanishing problem [26–28]. One of the simplest way to parametrize a unitary matrix is representing a unitary matrix as a product of two-level unitary operations [28]. A unitary matrix of size $N \times N$ can be parametrized by $k = N(N - 1)/2$ two level unitary matrices [29]. A two-level unitary matrices can be applied in $O(1)$ time. A real unitary matrix can be parametrized compactly by k rotation operations $\text{ROT}(a!, b!, \theta)$, where θ is the rotation angle, $a!$ and $b!$ are target registers.

$$\text{ROT}(a!, b!, \theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} a! \\ b! \end{bmatrix} \quad (8)$$

```

@i function umm!(x, )
  @anc k = 0
  @anc Nin = size(x, 2)
  @anc Nout = size(x, 1)
  for j=1:Nout
    for i=Nin-1:-1:j
      k += identity(1)
      ROT(x[i], x[i+1], [k])
    end
  end

  # uncompute k
  for j=1:Nout
    for i=Nin-1:-1:j
      k -= identity(1)
    end
  end
end

```

Its backward rule of a ROT instruction is

$$\begin{aligned}
\bar{\theta} &= \sum \frac{\partial R(\theta)}{\partial \theta} \odot (\bar{y}x^T) \\
&= \text{Tr} \left[\frac{\partial R(\theta)}{\partial \theta}^T \bar{y}x^T \right] \\
&= \text{Tr} \left[R \left(\frac{\pi}{2} - \theta \right) \bar{y}x^T \right]
\end{aligned} \tag{9}$$

We bind the adjoint function of ROT to its reverse IROT, and define a new function that dispatch to GVar variables

```

@i function IROT(a!::GVar, b!::GVar, ::GVar)
  IROT(value(a!), value(b!), value())
  NEG(value())
  value() -= identity(/2)
  ROT(grad(a!), grad(b!), value())
  grad() += value(a!) * grad(a!)
  grad() += value(b!) * grad(b!)
  value() += identity(/2)
  NEG(value())
  ROT(grad(a!), grad(b!), /2)
end

```

VI. DISCUSSION AND OUTLOOK

In this paper, we introduce differential programming on a reversible Turing machine implemented as a Julia eDSL. It is able to differentiate over any program consisting of instructions and control flows to any order reliably without sophisticated design of computational graph and intermediate state caching. Besides automatic differentiation, we introduce a new training strategy learn by consistency that does not rely on gradients.

In the following, we discussed the practical side of writing reversible programs, and several future directions to go. Notably, we introduce the concept of “arithmetic

uncomputing” to reduce the overhead of recursive reversible algorithms.

A. Time Space Tradeoff

So far, we have introduced the eDSL. There are many other designs of reversible language and instruction set. The reversible Turing machine may have either a space overhead proportional to computing time T or a computational overhead that sometimes can be even exponential given limited space. In the simplest g -segment trade off scheme [30, 31], it takes $\text{Time}(T) = T^{\log_g(4g-2)}$ and $\text{Space}(T) = (g-1)S \log_g T$. This section, we try to convince the reader that the overhead of reversible computing is not as terrible as people thought.

First, one should notice that even in the worst case, the overhead of a reversible program is not more than a traditional machine learning package. In pytorch, a tensor memorize every input of a primitive. The program is apparently reversible since it does not discard any information. For deep neural networks, people used checkpointing trick to trade time with space [32], which is also a widely used trick in reversible programming [13]. Reversible programming AD is sometimes more memory efficient. Comparing with logging computational graph, reversible programming has the advantage of supporting inplace functions, which is difficult in both traditional and source to source AD framework. The example of parametrizing unitary matrices costs zero memory allocation.

Second, some computational overhead of running recursive algorithms with limited space resources can be mitigated by “pseudo uncomputing” without sacrificing reversibility like in the `iexp` example.

Third, making reversible programming an eDSL rather than an independent language allows flexible choices between reversibility and computational overhead. For example, in order to deallocate the gradient memory in a reversible language one has to uncompute the whole process of obtaining this gradient. In this eDSL, we can just deallocate the memory irreversibly, i.e. trade energy with time. This underlines the fact that a reversible program is more suited in a program with small granularity. We can quantify it by introducing

Definition 1 (program granularity). The logarithm of the ratio between the execution time of a reversible program and its irreversible counter part.

$$\log_2 \frac{\text{Time}(T)}{T} \tag{10}$$

In the lowest granularity, instruction design, we need ancilla bits. Defining primitive functions like `iexp` requires uncomputing ancillas. Deallocating the gradient further increase the granularity by ~ 1 . After the training, the inverse training of whole programs should be done to deallocate all the memory used for training. As a result, the program complexity increase exponentially as the granularity increase. The granularity can be decreased by flattening the functions, since the uncomputing of ancillas can be executed at any level of granularity.

One should notice the memory advantage of reversible programming to machine learning does come from reversibility itself, but from a better data tracking strategy inspired from invertible programming. Normally, a reversible program is not as memory efficient as its irreversible counterpart due to the additional requirement of no information loss. A naive approach that keeping track of all informations will cost an additional space $O(T)$, where T stands for the execution time in a irreversible TM, the longer the program runs, the larger the memory usage is. This is exactly the approach to keeping reversibility in most machine learning packages in the market. The point is, an reversible Turing Machine is able to trade space with time. In some cases, it may cause polynomial overhead than its irreversible counterpart.

B. Instructions and Hardware

So far, our eDSL is not really compiled to instructions, instead it runs on a irreversible host Julia. In the future, it can be compiled to low level instructions and is executable on a reversible devices. For example, the control flow defined in this NiLang can be compiled to reversible instructions like conditioned goto statement. It is designed in such a way that the target instruction is a come from statement which specifies the postcondition. [33]

Arithmetic instructions should be redesigned to support better reversible programs. The major obstacle to exact reversibility programming is current floating point adders used in our computing devices are not exactly reversible. There are proposals of reversible floating point adders [34, 35] that introduces garbage bits to ensure reversibility. In other words, to represent a 64 bit floating point number requires more than 64 bits in storage. Reversible multiplier is also possible in similar approach. [36] With these infrastructure, a reversible program can be executed without suffering from the irreversibility from rounding error. In machine learning field, people using information buffer in multiplication operations [10] in an approach to enforce invertibility in a memory efficient way.

Reversible programming is not necessarily related to reversible hardware, reversible programs is a subset of irreversible programs hence can be simulated efficiently with CMOS technologies [33]. However, only using reversible hardware [] can break the energy efficiency barrier by Landauer principle. Reversible hardware are not necessarily related to reversible gates such as Toffoli gate and Fredkin gate. Devices with the ability of recovering signal energy is able to save energy, which is known as generalized reversible computing. [37, 38] In the following, we comment briefly on a special type of reversible device Quantum computer.

C. Quantum Computers

One of the fundamental difficulty of building a quantum computer is, unlike a classical state, an unknown quantum state can not be copied. Quantum random access memory [39]

is very hard to design and implement, it is known to have many caveats [40]. A quantum state in a environment will decoherence and can not be recovered, this underlines the simulation nature of quantum devices. Reversible computing does not enjoy the quantum advantage from entanglement, nor the quantum disadvantages from non-cloning and decoherence. Only the limitation of reversibility is retained, reversibility comes from the fact that microscopic processes are all unitary. In microscopic world, irreversibility is rare, it can come from the interaction with classical devices, like environment induces decaying, qubit state resetting, measurements and classical feedbacks to quantum devices. These are typically harder to implement on a quantum device.

Given the fundamental limitations of quantum decoherence and non-cloning and the microscopic reversible nature. It is reasonable to have a reversible computing device to bridge the gap between classical and universal quantum computing. By introducing entanglement little by little, we can accelerate some basic components like a reversible adder. The quantum fourier transformation provides a shortcut to the adder by introducing only one additional gate, the CPHASE gate even though it is a classical in classical out algorithm. [] Interestingly, by introducing rotation gates $R_y(\theta)$ and $R_z(\theta)$ in the reversible programming, we make NiLang a path integral based universal quantum simulator as shown in Appendix ???. The compiling theory developed for reversible programming will have profounding effect to quantum computers.

D. Outlook

So far NiLang is not full ready for productivity. It can be improved from multiple perspectives, compiling support to merge the uncomputing can decrease granularity and hence reduce overhead. Additional instructions like stack operations and logical operations are under consideration. It is also interesting to see how it can be combined with a high performance quantum simulator like Yao. It is able to provide control flow to Yao's QBIR. By porting a quantum simulator, it is interesting to see how quantum simulator can improve the instruction design. Notice a quantum fourier transformation (QFT) based quantum adder and multiplier is sometimes more efficient than a classical adder [41] [JG: Is this true?]. Reversible programming is known to have the advantage in parallel computing [42] and debugging [43], it is interesting to see how it combines with other parts of Julia packages like CUDAnative [44] and Debugger, it would be interesting to see our eDSL running on a GPU with little synchronization overhead [JG: Is this even possible?] and using an interactive debugging with bidirectional move. This could be used to reduce the memory cost in normalizing flow, time reversible integrator, recurrent neural network and residual neural network.

VII. ACKNOWLEDGMENTS

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Appendix A: NiLang Grammar

Terminologies

- *ident*, symbols
- *num*, numbers
- ϵ , empty statement
- *JuliaExpr*, native julia expression
- $[]$, zero or one repetitions.

```

⟨Stmts⟩ ::=  $\epsilon$ 
           | ⟨Stmt⟩
           | ⟨Stmts⟩ ⟨Stmt⟩
⟨Stmt⟩ ::= ⟨BlockStmt⟩
           | ⟨IfStmt⟩
           | ⟨WhileStmt⟩
           | ⟨ForStmt⟩
           | ⟨InstrStmt⟩
           | ⟨RevStmt⟩
           | ⟨@anc⟩ ⟨Stmt⟩
           | ⟨@routine⟩ ⟨Stmt⟩
           | ⟨@safe⟩ JuliaExpr
           | ⟨CallStmt⟩
⟨BlockStmt⟩ ::= begin ⟨Stmts⟩ end
⟨RevCond⟩ ::= ( JuliaExpr , JuliaExpr )
⟨IfStmt⟩ ::= if ⟨RevCond⟩ ⟨Stmts⟩ [else ⟨Stmts⟩] end
⟨WhileStmt⟩ ::= while ⟨RevCond⟩ ⟨Stmts⟩ end
⟨Range⟩ ::= JuliaExpr : JuliaExpr [: JuliaExpr]
⟨ForStmt⟩ ::= for ident = ⟨Range⟩ ⟨Stmts⟩ end
⟨CallStmt⟩ ::= JuliaExpr ( [⟨DataViews⟩] )
⟨Constant⟩ ::= num |  $\pi$ 
⟨InstrBinOp⟩ ::= += | -= |  $\forall$  =
⟨InstrTrailer⟩ ::= [.] ( [⟨DataViews⟩] )
⟨InstrStmt⟩ ::= ⟨DataView⟩ ⟨InstrBinOp⟩ ident [⟨InstrTrailer⟩]
⟨RevStmt⟩ ::=  $\sim$  ⟨Stmt⟩
⟨@routine⟩ ::= @routine ident ⟨Stmt⟩
⟨AncArg⟩ ::= ident = JuliaExpr
⟨@anc⟩ ::= @anc ⟨AncArg⟩
           | @deanc ⟨AncArg⟩
⟨@safe⟩ ::= @safe JuliaExpr
⟨DataViews⟩ ::=  $\epsilon$ 
               | ⟨DataView⟩
               | ⟨DataViews⟩ , ⟨DataView⟩
⟨DataView⟩ ::= ⟨DataView⟩ [ JuliaExpr ]
               | ⟨DataView⟩ . ident
               | JuliaExpr ( ⟨DataView⟩ )
               | ⟨Constant⟩
               | ident

```


One can use `@i function` $\langle Stmts \rangle$ `end` to define a function as well as its inverse. All *JuliaExpr* is should be pure, otherwise the reversibility is not guranted.

Dataview is a bijective mapping of an object or a field (or item) of an object. When modifying the dataview of an object, it changes the object directly with the `chfield` method.

Appendix B: Instruction Table

Even though $\oplus(\text{identity})$, $\oplus(*)$, $\oplus(/)$ and their reverse together with control flows are sufficient to write an arbitrary differentiable program. For convinience we provide more,

instruction	output
SWAP(a, b)	b, a
ROT(a, b, θ)	$a \cos \theta - b \sin \theta, b \cos \theta + a \sin \theta, \theta$
IROT(a, b, θ)	$a \cos \theta + b \sin \theta, b \cos \theta - a \sin \theta, \theta$
$y += a^b$	$y + a^b, a, b$
$y += \exp(x)$	$y + e^x, x$
$y += \log(x)$	$y + \log x, x$
$y += \sin(x)$	$y + \sin x, x$
$y += \cos(x)$	$y + \cos x, x$
$y += \text{abs}(x)$	$y + x , x$
NEG(y)	$-y$
CONJ(y)	y'

Table II. A collection of reversible instructions.