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Syntax-Directed Derivative Code (Part II: Intraprocedural Adjoint Code)

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Abstract. This is the second instance in a series of papers on single-pass generation of derivative codes by syntax-directed translation. We consider the automatic generation of adjoint code by reverse mode automatic differentiation implemented as the bottom-up propagation of synthesized attributes on the abstract syntax tree. A proof-of-concept implementation is presented based on a simple LALR(1) parser generated by the parser generator `bison`. The approach offers all advantages of adjoint codes while exhibiting the highly desirable ease of implementation.

1 Motivation and Summary of Results

In this paper we present a method for generating *adjoint* versions of numerical simulation programs that implement vector functions

$$F : I\!R^n \rightarrow I\!R^m, \quad \mathbf{y} = F(\mathbf{x}), \quad \mathbf{x} = (x_k)_{k=1,\ldots,n}, \; \mathbf{y} = (y_l)_{l=1,\ldots,m}, \tag{1}$$

automatically by syntax-directed translation. The resulting adjoint programs $\bar{F} = \bar{F}(\mathbf{x}, \bar{\mathbf{y}})$ compute adjoints $\bar{\mathbf{x}}$, that is, products of the transposed of the Jacobian matrix

$$F' = (f'_{l,k})_{k=1,\ldots,n}^{l=1,\ldots,m} \equiv \left(\frac{\partial y_l}{\partial x_k}\right)_{k=1,\ldots,n}^{l=1,\ldots,m} \in I\!R^{m\times n} \tag{2}$$

with a direction $\bar{\mathbf{y}}$ in the output space $I\!R^m$. Formally,

$$\bar{\mathbf{x}} = \bar{F}(\mathbf{x}, \bar{\mathbf{y}}) \equiv (F')^T \cdot \bar{\mathbf{y}} \quad . \tag{3}$$

To motivate the requirement for adjoint codes we discuss a simple parameter estimation problem as the solution of a non-linear least-squares optimization problem. Consider a numerical simulation program for a mathematical model $\mathbf{y} = F(\mathbf{x}, \mathbf{p})$ where $\mathbf{x} \in I\!R^{n_1}$, $\mathbf{p} \in I\!R^{n_2}$, and $\mathbf{y} \in I\!R^m$. For given measurements $(\mathbf{x}^j, \mathbf{y}^j), j = 1, \ldots, k$, we define the residual function

$$r_i(\mathbf{p}) \equiv \mathbf{y}^i - F(\mathbf{x}^i, \mathbf{p}), \quad i = 1, \ldots, k \quad .$$

Informally, our objective is to adapt the parameters $\mathbf{p}$ such that the data is represented by the model in the best possible way. This simple kind of parameter estimation can be performed by solving the nonlinear least-squares problem

$$\text{minimize} \quad g(\mathbf{p}) \equiv \frac{1}{2} r^T(\mathbf{p}) r(\mathbf{p}) \quad ,$$

for example, using steepest descent

$$\mathbf{p}^{j+1} = \mathbf{p}^j - \alpha_j \nabla g(\mathbf{p}^j)$$

to minimize some norm of the residual. Note, that

$$\nabla g(\mathbf{p}^j) = (r'(\mathbf{p}^j))^T r(\mathbf{p}^j)$$

can be computed by an adjoint model at a small constant multiple of the cost for evaluating r itself. A line-search for α_j, that is

$$\text{minimize} \quad g(\alpha_j) \quad \big(\text{for given } \mathbf{p}^j \text{ and } \nabla g(\mathbf{p}^j)\big)$$

is performed at each step j by applying Newton's method to $g'(\alpha_j) = 0$ as

$$\alpha_j^{k+1} = \alpha_j^k - \frac{g'(\alpha_j^k)}{g''(\alpha_j^k)} \quad .$$

The scalar first and second derivatives of the univariate scalar function $g(\alpha)$ can be computed via a univariate Taylor model [GUW00]. The latter can be generated easily by making simple modifications to the syntax-directed tangent-linear code generator from part one of this series of papers [Nau05].

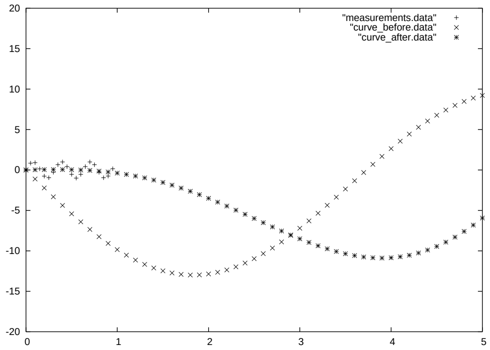
As an example we consider the very simple model[1]

$$y = \sum_{i=0}^{\nu-1} p_i \sin(p_{\nu+i} \cdot x) \tag{4}$$

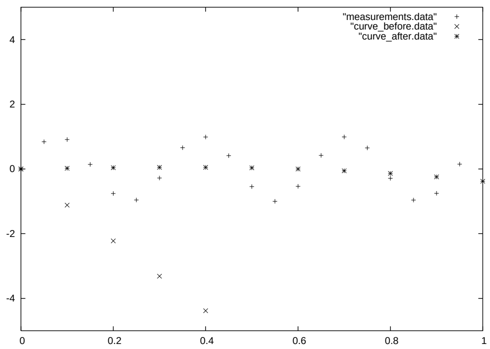
for $\mathbf{p} \in I\!R^n$, $n = 2\nu$, and $x, y \in I\!R$. We set $\nu = 10$, $p_i = i + 1$, and $p_{\nu+i} = \cos(i+1)$. Suppose that we have n measurements available for the interval $[0, 1)$ evenly distributed according to $\mathbf{y}_i = \sin(n \cdot i)$. The graph of the function and the measurements are plotted in Figure 1(a) using $\times$ and $+$, respectively. Running the optimization procedure leads to a new set of parameters resulting in the fitted curve that is shown as a sequence of $*$ symbols in Figure 1(a). Figure 1(b) shows all three curves over the interval of interest.

There are at least three different approaches to computing the gradient of g with respect to $\mathbf{p}$. One can approximate its values by finite difference quotients or use a tangent-linear model that can be generated by syntax-directed translation as described in [Nau05]. In both of these cases, the computational complexity is of the order of n as either each of the inputs needs to be perturbed separately or n directional derivatives need to be computed. Alternatively, an adjoint model can give us ∇g at a computational complexity of order $m = 1$ plus some overhead for reversing the control and data flow that heavily depends on the method used and on the computational platform. We ran a little experiment with $\nu = 10^4$ to test the actual run time differences. The result is summarized in the following table.

[1] We use this function as a model of a person attempting to walk along a "straight line" under the influence of too much alcohol during a motivational lecture on "Adjoints by Source Transformation." The example proved to be useful for getting students interested in the subject...



(a)



(b)

Fig. 1. Curve Fitting through Parameter Estimation

ν	FDC	TLC	ADC
10^4	45 sec	43 sec	$<$ 1 sec
10^5	$>$ 1 h	$>$ 1 h	$<$ 1 sec

The codes can be downloaded for verifying experiments from the project's website. The obvious conclusion from these simple experiments is that adjoint codes must play a crucial role in modern numerical analysis such as in optimization or in the context of numerical inverse problems in general. As numerical simulation programs for real-world applications are not as simple as Equation (4), it is highly desirable to generate adjoint codes automatically. Various tools for *automatic differentiation* (AD; see [Gri00]) including ADIFOR 3 [CF00], ADOL-C [GJU96], the differentiation-enabled NAGWare Fortran 95 compiler [NR05], OpenAD [WHH$^+$05], TAF [GK03], and TAPENADE [HP04] have been developed over the past decades that help scientists and engineers to handle much larger dimensions – both in terms of the code size and of the dimension of the parameter space – as used to be possible with classical numerical differentiation by finite differences or by hand-coding derivative codes.

In this paper we present a single-pass approach to the automatic generation of adjoint code by syntax-directed translation. The method is both elegant and easy to implement. A disadvantage is the inability to perform data flow analysis due to the missing intermediate representation. Nevertheless, a syntax-directed adjoint code generator may serve as a support tool in the context of semi-automatic development of adjoint codes, and may even represent a good starting point for the development of more sophisticated source transformation tools for AD. Moreover, it could represent a useful extension of the first pass of existing tools to generate an intermediate representation of the program that is easier to optimize by state-of-the-art compiler algorithms.

The structure of the paper is as follows. In Section (2) we summarize the theoretical concepts behind reverse mode AD in the context of adjoint code generation by source transformation. The syntax-directed translation algorithm for straight-line programs is introduced in Section (3) and generalized to subroutines with control-flow structures in Section (4). A simple proof-of-concept implementation is discussed in Section (5). We make detailed references to the source code that is appended in Section (A). We draw conclusions in Section (6) together with an outlook to syntax-directed adjoint code generation in the presence of interprocedural flow of control.

2 Fundamentals of Adjoint Codes

Let the subroutine / user-defined function $\mathbf{y} = F(\mathbf{x})$ implement a vector function as defined in Equation (1). The values of the m *dependent* variables y_j, $j = 1, \ldots, m$, are calculated as functions of the n *independent* variables x_i, $i = 1, \ldots, n$. The subroutine F represents an implementation of the mathematical model for some underlying real-world application and it will be referred to as the *forward code.* The forward code is expected to be written in some high-level imperative programming language such as C or Fortran.[2] More general, it should be possible to decompose F into a sequence of scalar assignments of the form

$$v_j = \varphi_j(v_k)_{k \prec j} \ , \quad j = 1, \ldots, q \ , \tag{5}$$

(referred to as the *code list* in [Nau05]) where $q = p + m$ and such that the result of every intrinsic function and elementary arithmetic operation is assigned to a unique intermediate variable v_j, $j = 1, \ldots, q$. Following the notation in [Gri00] we write $k \prec j$ whenever some variable v_j depends directly on another variable v_k. The code list induces a directed acyclic *computational graph* $G = (V, E)$ with integer vertices $V = \{1 - n, \ldots, q\}$ and edges $E = \{(i, j) : i \prec j\}$ as shown, for example, in [GR91]. It is assumed that the local partial derivatives

$$c_{ji} = \frac{\partial \varphi_j}{\partial v_i}(v_k)_{k \prec j} \tag{6}$$

of the *elemental* functions φ_j, $j = 1, \ldots, q$, exist and that they are jointly continuous in some open neighborhood of the current argument $(v_k)_{k \prec j}$. In this case, an augmented version of the forward code can be implemented that computes F itself and the set of all local partial derivatives as defined in Equation (6). As in [Nau05] we refer to this augmented forward code as the *linearized code list.* The *linearized computational graph* is obtained by attaching the local partial derivatives to the corresponding edges.

Example

Consider

$$\begin{aligned} x &= x \cdot \sin(x \cdot y) \\ y &= x \cdot y \\ x &= \sin(x) \end{aligned} \tag{7}$$

The linearized computational graph is shown in Figure 2.

The reverse mode of AD (see [Gri00, Sect. 3.3] for a more complete coverage of the theoretical foundation of this method) uses these local partial derivatives to propagate adjoints $\bar{v}_j$ backwards for $j = q, \ldots, 1 - n$ with respect to the data flow of the forward code from the outputs to the inputs. Products of the

[2] As in [Nau05] and without loss of generality, our proof-of-concept implementation `sdac` (see Section (5)) focuses on a subset of C.

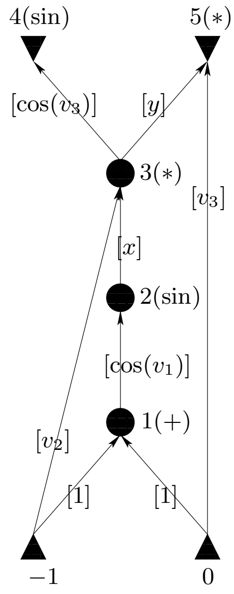


Fig. 2. Linearized Computational Graph: Intermediate and dependent vertices are marked with the corresponding elemental functions (in "(...)"). Expressions for the local partial derivatives are attached to the edges (in "[...]"). Initialization of $v_{-1} \equiv x$ and $v_0 \equiv y$ allows for the computation of all intermediate values $v_1, \ldots, v_5$ and the computation of values for the local partial derivatives.

transposed Jacobian matrix with a vector of adjoints of the outputs are computed by initializing the adjoints of the dependent variables $\bar{y}_j \equiv \bar{v}_{p+j}$, $j = 1, \ldots, m$.

In practical implementations we distinguish between two fundamental approaches to reverse mode. In its non-incremental version the local partial derivatives are computed during the augmented forward evaluation (first line in Equation (8)).

$$\begin{array}{l} v_j = \varphi_j(v_i)_{i \prec j};\ c_{j,i} = \dfrac{\partial \varphi_j}{\partial v_i} \quad \text{for } i \prec j \text{ and } j = 1, \ldots, q \\ \bar{v}_j = \displaystyle\sum_{k: j \prec k} c_{kj} \cdot \bar{v}_k \quad \text{for } j = q, \ldots, 1-n \end{array} . \tag{8}$$

In incremental reverse mode the local partial derivatives are computed during the adjoint evaluation (second line in Equation (9)).

$$\begin{array}{l} v_j = \varphi_j(v_i)_{i \prec j};\ \bar{v}_j = 0 \quad \text{for } j = 1, \ldots, q \\ c_{j,i} = \dfrac{\partial \varphi_j}{\partial v_i};\ \bar{v}_i = \bar{v}_i + c_{j,i} \cdot \bar{v}_j \quad \text{for } i \prec j \text{ and } j = q, \ldots, 1 \end{array} . \tag{9}$$

One can think of various combinations of both methods. The Jacobian $F'(\mathbf{x})$ is accumulated by reverse propagation of the Cartesian basis vectors in $I\!R^m$ at a complexity of $O(m)$. In particular, gradients of single dependent variables with respect to all independent variables can be obtained at a computational cost that is a small multiple of the cost of running the forward code.

In practice (from the viewpoint of a source transformation AD tool developer) the incremental form of reverse mode AD is preferred as it is better suited for state-of-the-art parsing algorithms and traversals of the abstract syntax tree (see Section (3) and established compiler literature such as [ASU86]). Moreover, the explicit construction of the code list is impossible because of control flow statements in the forward code. The theoretical concepts can be applied without change only to parts of the code whose data flow structure is statically known at compile time such as single assignments or sequences thereof (also known as *basic blocks*). In Section (3) we build code lists of single assignments to propagate adjoints. However, first a few general remarks should be made to facilitate a better understanding of the source transformation approach.

Consider an arbitrary assignment of the form

$$u_j = \varphi(u_i)_{i \prec j} \tag{10}$$

where, possibly, $\&u_j \in \{\&u_i : i \prec j\}$ as well as $\&u_{i_1} = \&u_{i_2}$ for $i_1 \prec j$ and $i_2 \prec j$. We use $\&u$ to denote the memory address referred to by a variable u. The first assignment in Equation (7) is a good example.

In general, it is undecidable at compile time if $\&u_{i_1} = \&u_{i_2}$ as this may depend on parameters that are only available at run time. Alias analysis [Muc97] may help. Lacking any program analysis one needs to assume conservatively that $\&u_j = \&u_i$ for all $i \prec j$ to ensure the correctness of the adjoint code.

As a consequence of overwriting a given location in memory may represent different code list variables. For example, x corresponds to v_{-1}, v_3, and v_4 in Equation (7) and Figure 2. Note that the adjoints of all code list variables need to be initialized with zero to ensure the correctness of the incremental reverse mode. The adjoint of u_j in Equation (10) dies (its value is no longer used) once it has been used to increment the adjoints of all arguments of φ. Referring to Figure 2 the value of $\bar{v}_3$ is dead once it has been used to increment $\bar{v}_2$ and $\bar{v}_{-1}$. However, the memory location $\&u_j$ may well be incremented by some succeeding adjoint statement for the reasons stated above. Hence, adjoint variables need to be reset to zero immediately after their death.

If we can prove that some $\&u_j$ is always read only once after its initialization and before getting overwritten, then its adjoint does not need to be initialized with zero and all adjoint statements that have $\bar{u}_j$ on the left-hand side simply overwrite its value. The restriction to code lists of single assignments ensures that the above requirement is satisfied. Hence, no assignment to an adjoint code list variable is in incremental form nor does an adjoint code list variable need to be reset to zero after its death.

Example

The simple syntax-directed adjoint code compiler `sdac` (see Section (5)) takes this approach. Listing 1.1 shows the adjoint code that is generated for the forward code in Equation (7). For example, the first statement is decomposed into a code list in lines 7 – 13. The code list variables are stored on a stack as they may potentially be overwritten by the code lists of succeeding assignment and at the same time they may be required to compute the partial derivatives of some preceding assignment. Only v1, v2, and v3 are overwritten and none of them is ever used by a preceding assignment. However, the data flow analysis that could detect such situations in general [HNP05] is not part of `sdac`. In any case the conservative approach ensures correctness.

In the adjoint section of the code (lines 21 – 34) all assignments to the adjoint code list variables (lines 21, 22, 24, 25, and 28–31) are non-incremental. The adjoint program variables x_ and y_ are always incremented when they occur on the left-hand side (lines 23, 26, 27, and 32 – 34). They are set to zero right after their values got assigned to an adjoint code list variable (lines 21, 24, 28). For example, setting x_=0 in line 21 ensures that the result of the incrementation in line 23 is numerically correct. The overall correctness of the code generated by `sdac` is verified against results obtained by running the tangent-linear code generated by `sdtlc` as described in Section (5).

Listing 1.1. Adjoint Code for Equation (7)

```
1  double v1, v1_;
2  double v2, v2_;
3  double v3, v3_;
4  double v4, v4_;
5  double v5, v5_;
6  double v6, v6_;
7  push(v1); v1=x;
8  push(v2); v2=x;
9  push(v3); v3=y;
10 push(v4); v4=v2*v3;
11 push(v5); v5=sin(v4);
12 push(v6); v6=v1*v5;
13 push(x); x=v6;
14 push(v1); v1=x;
15 push(v2); v2=y;
16 push(v3); v3=v1*v2;
17 push(y); y=v3;
18 push(v1); v1=x;
19 push(v2); v2=sin(v1);
20 push(x); x=v2;
21 pop(x); v2_=x_; x_=0;
22 pop(v2); v1_=cos(v1)*v2_;
23 pop(v1); x_+=v1_;
24 pop(y); v3_=y_; y_=0;
25 pop(v3); v1_=v3_*v2; v2_=v3_*v1;
26 pop(v2); y_+=v2_;
27 pop(v1); x_+=v1_;
28 pop(x); v6_=x_; x_=0;
29 pop(v6); v1_=v6_*v5; v5_=v6_*v1;
30 pop(v5); v4_=cos(v4)*v5_;
31 pop(v4); v2_=v4_*v3; v3_=v4_*v2;
32 pop(v3); y_+=v3_;
33 pop(v2); x_+=v2_;
34 pop(v1); x_+=v1_;
```

3 Adjoint Straight-Line Programs

As in [Nau05] we consider straight-line programs according to the following definition

Definition 1. *A* straight-line program (SLP) *is a sequence of scalar assignments described by the context-free grammar $G = (N, T, P, s)$ with nonterminal symbols*

$$N = \left\{ s \text{ (straight-line program)} \quad a \text{ (assignment)} \quad e \text{ (expression)} \right\}$$

terminal symbols

$$T = \left\{ \begin{array}{ll} V & (\textit{program variables; see line 14 in Appendix A.1, Listing 1.6}) \\ C & (\textit{constants; line 20}) \\ F & (\textit{unary intrinsic; line 13}) \\ O & (\textit{binary operator; line 26}) \\ \;,\;;\;)\;(& (\textit{remaining single character tokens; line 26}) \end{array} \right\}$$

start symbol s, and production rules

$$P = \left\{ \begin{array}{lll} (P1) & s :: a & (\textit{see line 28 in Appendix A.1, Listing 1.7}) \\ (P2) & s :: as & (\textit{line 29}) \\ (P3) & a :: V = e; & (\textit{line 40}) \\ (P4) & e :: V & (\textit{line 84}) \\ (P5) & e :: C & (\textit{line 95}) \\ (P6) & e :: F(e) & (\textit{line 73}) \\ (P7) & e :: eOe & (\textit{line 50 and line 62}) \end{array} \right\}$$

Any comments made in [Nau05] on the structure of this grammar, its use in the context of lexical and syntax analysis using `flex` and `bison`, and its sufficiency as a proof-of-concept implementation of the theoretical ideas presented in this paper apply in the current context as well. Again, we use an LALR(1)-parsing algorithm based on a push-down automaton with a characteristic finite automaton as in [Nau05, Equations (7) and (8)].

```
s (6)  →  a (5)
               |→  V("y")
               |→  =
               |→  e (4)
                        |→  F(" sin ")
                        |→  (
                        |→  e (3)
                                 |→  e (1)  →  V("x")
                                 |→  O(" * ")
                                 |→  e (2)  →  C("2")
                        |→  )
```

Fig. 3. Abstract Syntax tree of "$y = \sin(x * 2);$".

The production rules for syntax-directed compilation of adjoint SLPs are derived below. Both counters ν and c are initialized with one. Examples are provided based on the bottom-up derivation of the assignment "$y = \sin(x * 2);$" by performing the reductions **(P4)**, **(P5)**, **(P7)**, **(P6)**, **(P3)**, and **(P1)** to get the abstract syntax tree shown in Figure 3. The augmented forward section is synthesized in attribute $\mathbf{v}_\nu.a^f$ and the adjoint section in $\mathbf{v}_\nu.a^r$ for $\nu = 1, \ldots, 6$. Hence, the entire adjoint code consists of $\mathbf{v}_6.a^f$ followed by $\mathbf{v}_6.a^r$. Figure 4 shows the corresponding output as generated by `sdac`. Note that as a result of bottom-up parsing the examples provided with the extended reduction rules need to be read in the order of the reductions as performed by the parser, that is **(P4)**, **(P5)**, ..., **(P1)**.

We use syntax that is analogous to that used in [Nau05]. For example, $V.\bar{a}^f$ refers to the string that marks the adjoint of the variable marked by the string $V.a^f$, that is, if $V.a^f =$ "x", then $V.\bar{a}^f =$ "$\bar{x}$". In **(P6)** the symbolic transformation

$$\frac{\partial F.a}{\partial \text{ "}v_{[\mathbf{v}_{\nu-1}.j]}\text{"}}$$

is defined according to the differentiation rules of the elemental functions, for example, if $F.a =$ " cos " and "$v_{[\mathbf{v}_{\nu-1}.j]}$" $=$ "v_1", then

$$\frac{\partial F.a}{\partial \text{ "}v_{[\mathbf{v}_{\nu-1}.j]}\text{"}} = \frac{\partial \text{ " }\cos(v_1)\text{"}}{\partial \text{ "}v_1\text{"}} = \text{" } -\sin(v_1)\text{"} \quad .$$

(P1) $s :: a$

$$\begin{aligned} &\mathbf{v}_\nu.a^f = \mathbf{v}_{\nu-1}.a^f \\ &\mathbf{v}_\nu.a^r = \mathbf{v}_{\nu-1}.a^r \\ &\nu{+}{+} \end{aligned}$$

(See line 28 in Appendix A.1, Listing 1.7.)

Example: After the last reduction the entire augmented forward code has been synthesized in $\mathbf{v}_6.a^f$. The adjoint code is in $\mathbf{v}_6.a^r$.

$$\begin{aligned} \mathbf{v}_6.a^f = \text{"}&push(v_1);\ v_1 = x; \\ &push(v_2);\ v_2 = 2; \\ &push(v_3);\ v_3 = v_1 * v_2; \\ &push(v_4);\ v_4 = \sin(v_3); \\ &push(y);\ y = v_4;\text{"} \\ \mathbf{v}_6.a^r = \text{"}&pop(y);\ \bar{v}_4 = \bar{y};\ \bar{y} = 0; \\ &pop(v_4);\ \bar{v}_3 = \cos(v_3) * \bar{v}_4; \\ &pop(v_3);\ \bar{v}_1 = v_2 * \bar{v}_3;\ \bar{v}_2 = v_1 * \bar{v}_3; \\ &pop(v_2); \\ &pop(v_1);\ \bar{x}{+}{=}\bar{v}_1;\text{"} \end{aligned}$$

(P2) $s :: as$

$$\begin{aligned} &\mathbf{v}_\nu.a^f = \mathbf{v}_{\mu_1}.a^f + \mathbf{v}_{\mu_2}.a^f \\ &\mathbf{v}_\nu.a^r = \mathbf{v}_{\mu_2}.a^r + \mathbf{v}_{\mu_1}.a^r \\ &\qquad \text{where } \mathbf{v}_{\mu_1} \hat{=} a \text{ and } \mathbf{v}_{\mu_2} \hat{=} s \text{ in } as \\ &\nu{+}{+} \end{aligned}$$

(See lines 29–39.)

Example: This rule is not used as we are dealing with only one assignment. As in [Nau05] we use the notation "$\hat{=}$" in the sense of "corresponds to", that is, for example, $\mathbf{v}_{\mu_2}$ is the vertex in the abstract syntax tree that corresponds to the second non-terminal on the right-hand side of rule **(P2)**. The counter ν for the vertices in the abstract syntax tree is incremented by each reduction.

(P3) $a :: V = e;$

$$
\begin{aligned}
\mathbf{v}_\nu.a^f &= \mathbf{v}_{\nu-1}.a^f + \text{"}push\text{"} + \text{"(" } + V.a^f + \text{")"} + \text{";"} \\
&\quad + V.a^f + \text{" = "} + \text{"}v_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{";"} \\
\mathbf{v}_\nu.a^r &= \text{"}pop\text{"} + \text{"(" } + V.a^f + \text{")"} + \text{";"} \\
&\quad + \text{"}\bar{v}_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{" = "} + V.\bar{a}^f + \text{";"} \\
&\quad + V.\bar{a}^f + \text{" = 0;"} \\
&\quad + \mathbf{v}_{\nu-1}.a^r \\
c &= 1 \\
\nu&{+}{+}
\end{aligned}
$$

(See lines 40–49.)

Example: The augmented forward code is synthesized from the augmented forward code of the right-hand side ($\mathbf{v}_{\nu-1}.a^f$), the *push* statement that stores the overwritten value of the left-hand side (y), and the assignment of the value of the code list variable that holds the value of the right-hand side (v_4) to the variable on the left-hand side.

$$
\begin{aligned}
\mathbf{v}_5.a^f = \; & \text{"}push(v_1);\; v_1 = x; \\
& push(v_2);\; v_2 = 2; \\
& push(v_3);\; v_3 = v_1 * v_2; \\
& push(v_4);\; v_4 = \sin(v_3); \\
& push(y);\; y = v_4;\text{"}
\end{aligned}
$$

The adjoint code consists of a *pop* statement to restore the value of the variable on the left-hand side ($V.a^f$ = "y") followed by overwriting the adjoint of the code list variable that corresponds to the right-hand side ("$\bar{v}_{[\mathbf{v}_{\nu-1}.j]}$" = "$\bar{v}_4$") with the adjoint of the left-hand side ($V.\bar{a}^f$ = "$\bar{y}$"), the reinitialization of $V.\bar{a}^f$ with zero, and all this synthesized with the adjoint code of the right-hand side ($\mathbf{v}_{\nu-1}.a^r$). The data flow in the adjoint code is reversed with respect to that of the forward code. The code list counter c is reset to one in anticipation of the next statement-level code list to be built potentially (not in this simple example).

$$\begin{aligned}\mathbf{v}_5.a^r = \ & "pop(y);\ \bar{v}_4 = \bar{y};\ \bar{y} = 0;\\ & pop(v_4);\ \bar{v}_3 = \cos(v_3) * \bar{v}_4;\\ & pop(v_3);\ \bar{v}_1 = v_2 * \bar{v}_3;\ \bar{v}_2 = v_1 * \bar{v}_3;\\ & pop(v_2);\\ & pop(v_1);\ \bar{x}{+}{=}\bar{v}_1;"\\ \nu = 6 & \end{aligned}$$

(P4) $e :: V$

$$\begin{aligned}\mathbf{v}_\nu.j &= c{+}{+}\\ \mathbf{v}_\nu.a^f &= "push" + "(" + "v_{[\mathbf{v}_\nu.j]}" + ")" + ";"\\ &\quad + "v_{[\mathbf{v}_\nu.j]}" + " = " + V.a^f + ";"\\ \mathbf{v}_\nu.a^r &= "pop" + "(" + "v_{[\mathbf{v}_\nu.j]}" + ")" + ";"\\ &\quad + V.\bar{a}^f + "{+}{=}" + "\bar{v}_{[\mathbf{v}_\nu.j]}" + ";"\\ \nu{+}{+} & \end{aligned}$$

(See lines 84–94.)

Example: The value of the next code list variable "$v_{[\mathbf{v}_\nu.j]}$" is stored on the stack before the variable is overwritten with the value of the program variable $V.a^f$.

$$\begin{aligned}\mathbf{v}_1.j &= 1\\ c &= 2\\ \mathbf{v}_1.a^f &= "push(v_1);\ v_1 = x;"\end{aligned}$$

The value of the code list variable "$v_{[\mathbf{v}_\nu.j]}$" is restored and the adjoint $V.\bar{a}^f$ of the program variable is incremented with the adjoint of "$v_{[\mathbf{v}_\nu.j]}$", that is "$\bar{v}_{[\mathbf{v}_\nu.j]}$".

$$\begin{aligned}\mathbf{v}_1.a^r &= "pop(v_1);\ \bar{x}{+}{=}\bar{v}_1;"\\ \nu &= 2\end{aligned}$$

The value of a^r is the empty string for all terminal symbols, Hence, it can be omitted in the synthesis of $\mathbf{v}_\nu.a^r$.

```
double v1, v1_;
double v2, v2_;
double v3, v3_;
double v4, v4_;
push(v1); v1=x;
push(v2); v2=2;
push(v3); v3=v1*v2;
push(v4); v4=sin(v3);
push(y); y=v4;
pop(y); v4_=y_; y_=0;
pop(v4); v3_=cos(v3)*v4_;
pop(v3); v1_=v3_*v2; v2_=v3_*v1;
pop(v2);
pop(v1); x_+=v1_;
```

(a)

```
#include <stack>
using namespace std;

static stack<double> stack_v;

void push(double v) {
  stack_v.push(v);
}
void pop(double& v) {
  v=stack_v.top();
  stack_v.pop();
}
```

(b)

Fig. 4. (a) `sdac` output for "`y=sin(x*2);`" The correctness has been verified with `sdtlc` [Nau05] and finite difference approximation. (b) Implementation of stack.

(P5) $e :: C$

$$
\begin{aligned}
\mathbf{v}_\nu.j &= c{+}{+} \\
\mathbf{v}_\nu.a^f &= \text{"}push\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{"};\text{"} \\
&\quad + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"} = \text{"} + C.a^f + \text{"};\text{"} \\
\mathbf{v}_\nu.a^r &= \text{"}pop\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{"};\text{"} \\
\nu&{+}{+}
\end{aligned}
$$

(See lines 95–105.)

Example: The augmented forward code is analogous to that of **(P4)**.

$$
\begin{aligned}
\mathbf{v}_2.j &= 2 \\
c &= 3 \\
\mathbf{v}_2.a^f &= \text{"}push(v_2);\ v_2 = 2;\text{"}
\end{aligned}
$$

The adjoint code simply restores the value of the code list variable that was overwritten by the augmented forward code.

$$
\begin{aligned}
\mathbf{v}_2.a^r &= \text{"}pop(v_2);\text{"} \\
\nu &= 3
\end{aligned}
$$

(P6) $e :: F(e)$

$$
\begin{aligned}
\mathbf{v}_\nu.j &= c{+}{+}\\
\mathbf{v}_\nu.a^f &= \mathbf{v}_{\nu-1}.a^f\\
&\quad + \text{"}push\text{"} + \text{"(" } + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{")"} + \text{";"}\\
&\quad + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{" = "} + F.a^f + \text{"("} + \text{"}v_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{")"} + \text{";"}\\
\mathbf{v}_\nu.a^r &= \text{"}pop\text{"} + \text{"("} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{")"} + \text{";"}\\
&\quad + \text{"}\bar{v}_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{" = "} + \frac{\partial F.a^f}{\partial\text{"}v_{[\mathbf{v}_{\nu-1}.j]}\text{"}} + \text{" * "} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{";"}\\
&\quad + \mathbf{v}_{\nu-1}.a^r\\
\nu{+}{+}
\end{aligned}
$$

(See lines 73–83.)

Example: As before and succeeding the augmented forward code generated so far, the value of the expression that corresponds to the right-hand side of the production rule is assigned to the next code list variable "$v_{[\mathbf{v}_\nu.j]}$" whose old value needs to be stored before that.

$$
\begin{aligned}
\mathbf{v}_4.j &= 4\\
\mathbf{v}_4.a^f &= \text{"}push(v_1);\ v_1 = x;\\
&\qquad push(v_2);\ v_2 = 2;\\
&\qquad push(v_3);\ v_3 = v_1 * v_2;\\
&\qquad push(v_4);\ v_4 = \sin(v_3);\text{"}
\end{aligned}
$$

The adjoint code restores this value and it increments the adjoint of the code list variable that holds the value of the expression forming the argument of the unary intrinsic $F.a^f$ with the product of the corresponding local partial derivative and the adjoint of "$v_{[\mathbf{v}_\nu.j]}$".

$$
\begin{aligned}
\mathbf{v}_4.a^r &= \text{"}pop(v_4);\ \bar{v}_3 = \cos(v_3) * \bar{v}_4;\\
&\qquad pop(v_3);\ \bar{v}_1 = v_2 * \bar{v}_3;\ \bar{v}_2 = v_1 * \bar{v}_3;\\
&\qquad pop(v_2);\\
&\qquad pop(v_1);\ \bar{x} {+}{=} \bar{v}_1;\text{"}\\
\nu &= 5
\end{aligned}
$$

(P7) $e :: eOe$

$$
\begin{aligned}
\mathbf{v}_\nu.j &= c{+}{+}\\
\mathbf{v}_\nu.a^f &= \mathbf{v}_{\mu_1}.a^f + \mathbf{v}_{\mu_2}.a^f\\
&\quad + \text{"}push\text{"} + \text{"("} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{")"} + \text{";"}\\
&\quad + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{" = "} + \text{"}v_{[\mathbf{v}_{\mu_1}.j]}\text{"} + O.a^f + \text{"}v_{[\mathbf{v}_{\mu_2}.j]}\text{"} + \text{";"}
\end{aligned}
$$

$$
\begin{aligned}
&\mathbf{v}_\nu.a^r = \text{"}pop\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{";"} \\
&\quad + \text{"}\bar{v}_{[\mathbf{v}_{\mu_1}.j]}\text{"} + \text{"} = \text{"} + \frac{\partial O.a^f}{\partial \text{"}v_{[\mathbf{v}_{\mu_1}.j]}\text{"}} + \text{"} * \text{"} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{";"} \\
&\quad + \text{"}\bar{v}_{[\mathbf{v}_{\mu_2}.j]}\text{"} + \text{"} = \text{"} + \frac{\partial O.a^f}{\partial \text{"}v_{[\mathbf{v}_{\mu_2}.j]}\text{"}} + \text{"} * \text{"} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{";"} \\
&\quad + \mathbf{v}_{\mu_1}.a^r + \mathbf{v}_{\mu_2}.a^r \\
&\qquad\qquad \text{where } \mathbf{v}_{\mu_1} \hat{=} e^1 \text{ and } \mathbf{v}_{\mu_2} \hat{=} e^2 \text{ in } e^1 O e^2 \\
&\nu{+}{+}
\end{aligned}
$$

(See lines 50–72.)

Example: The augmented forward code is analogous to that of **(P6)**.

$$
\begin{aligned}
\mathbf{v}_3.j &= 3 \\
\mathbf{v}_3.a^f &= \text{"}push(v_1);\ v_1 = x; \\
&\quad\ push(v_2);\ v_2 = 2; \\
&\quad\ push(v_3);\ v_3 = v_1 * v_2;\text{"}
\end{aligned}
$$

In the adjoint code the adjoints of both code list variables that store the values of the two arguments of the binary operator $O.a^f$ need to be incremented with the product of the corresponding local partial derivative and the adjoint of the code list variable that holds the value of the expression that is reduced according to the right-hand side of the production rule.

$$
\begin{aligned}
\mathbf{v}_3.a^r &= \text{"}pop(v_3);\ \bar{v}_1 = v_2 * \bar{v}_3;\ \bar{v}_2 = v_1 * \bar{v}_3; \\
&\quad\ pop(v_2); \\
&\quad\ pop(v_1);\ \bar{x} {+}{=} \bar{v}_1;\text{"} \\
\nu &= 4
\end{aligned}
$$

4 Adjoint Subroutines

As in [Nau05] we consider subroutines defined syntactically as follows.

Definition 2. *A* subroutine *is described by the following context-free grammar* $G = (N, T, P, r)$.

$$
N = \left\{ \begin{array}{ll} r \text{ (sequence of statements)} & s \text{ (statement)} \\ e \text{ (expression)} & c \text{ (condition)} \end{array} \right\}
$$

$$
T = \left\{ \begin{array}{rl} \vdots & \textbf{\textit{(see Definition 1)}} \\ IF & (\textit{unary intrinsic; see line 14 in Appendix A.2, Listing 1.9}) \\ WHILE & (\textit{binary operator; line 15}) \end{array} \right\}
$$

start symbol r*, and production rules*

$$P = \left\{ \begin{array}{lll} (P1) & r :: s & (\textit{see line 45 in Appendix A.2, Listing 1.10}) \\ (P2) & r :: sr & (\textit{line 46}) \\ (P3) & s :: V = e; & (\textit{line 122}) \\ & \vdots \ \textbf{\textit{(see Definition 1)}} & \\ (P8) & s :: IF(c)\{s\} & (\textit{see line 76 in Appendix A.2, Listing 1.10}) \\ (P9) & s :: WHILE(c)\{s\} & (\textit{line 96}) \\ (P10) & c :: V < V & (\textit{line 116}) \end{array} \right\}.$$

The presence of control-flow structures in a subroutine has a significant impact on the way the adjoint code is generated. In Section (3) we saw that the data-flow in the adjoint section of the code is reversed compared with that of the forward code (or, equivalently, the augmented forward section of the adjoint code). Hence, the flow of control needs to be reversed too as it defines the data flow between the basic blocks. Informally, loops need to be executed in reverse order and the same branches need to be executed both by the augmented forward and the adjoint section of the adjoint code. The obvious solution is to enumerate the basic blocks and to push their indexes onto a *control stack* during the evaluation of the augmented forward code. The adjoint code then simply restores the indexes of all basic blocks followed by the execution of the corresponding adjoint basic blocks. From Section (3) we know how to generate the latter. The stack that enables the reversal of the data flow by storing the values of overwritten variables is referred to as the *data stack*.

As for SLP's the first attribute a^f that is associated with all vertices in the AST is used to synthesize the augmented forward code. Due to the selected approach to the reversal of the flow of control the adjoint basic blocks need to be synthesized individually making the second attribute a^r a vector of length equal to the number of basic blocks in the subroutine.

In the following we present a set of extended shift and reduce actions that make the syntax-directed generation of adjoint code for entire subroutines as defined in Definition 2 work. We focus on the differences from the set of rules given in Section (3) by using " $\vdots$ " to avoid obvious duplication. We comment on the single rules without presenting examples as we did in Section (3). Instead an adjoint code generated automatically by `sdac` is discussed in Section (5).

(P1) $r :: s$

$$\begin{aligned} &\mathbf{v}_\nu.a^f = \mathbf{v}_{\nu-1}.a^f \\ &\mathbf{v}_\nu.a^r_i = \mathbf{v}_{\nu-1}.a^r_i \quad i = 0, \ldots, idxBB \\ &\nu{+}{+} \end{aligned}$$

The adjoints of all basic blocks that have been parsed so far need to be copied. Note that the requirement to synthesize all entries in a^r is restricted to vertices that may occur above assignments (see **(P3)**) in the AST, that is, AST vertices that are generated as the result of the reductions **(P1)**, **(P2)**, **(P8)**, and **(P9)**. The remaining reductions lead to AST vertices for which $\mathbf{v}_\nu.a^r_i$ is equal to the empty string for $i \neq idxBB$.

(P2) $r :: sr$

$$\begin{aligned}
\mathbf{v}_\nu.a^f &= \mathbf{v}_{\mu_1}.a^f + \mathbf{v}_{\mu_2}.a^f \\
\mathbf{v}_\nu.a_i^r &= \mathbf{v}_{\mu_2}.a_i^r + \mathbf{v}_{\mu_1}.a_i^r \quad i = 0, \ldots, idxBB \\
&\quad \text{where } \mathbf{v}_{\mu_1} \hat{=} s \text{ and } \mathbf{v}_{\mu_2} \hat{=} r \text{ in } sr \\
\nu&{++}
\end{aligned}$$

The adjoint basic blocks are synthesized by concatenating the values of the corresponding attributes of both successors of the AST vertex $\mathbf{v}_\nu$.

(P3) $s :: V = e;$

$$\begin{aligned}
\mathbf{v}_\nu.a^f &= \begin{cases} \text{"}push_c\text{"} + \text{"("} + idxBB + \text{")"} + \text{";"} & \text{if } newBB \vee \neg idxBB \\ \text{""} & \text{otherwise} \end{cases} \\
\mathbf{v}_\nu.a^f &= \mathbf{v}_{\nu-1}.a^f + \text{"}push\text{"} + \text{"("} + V.a^f + \text{")"} + \text{";"} \\
&\quad + V.a^f + \text{" = "} + \text{"}v_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{";"} \\
\mathbf{v}_\nu.a^r_{idxBB} &= \text{"}pop\text{"} + \text{"("} + V.a^f + \text{")"} + \text{";"} \\
&\quad + \text{"}\bar{v}_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{" = "} + V.\bar{a}^f + \text{";"} \\
&\quad + V.\bar{a}^f + \text{" = 0;"} \\
&\quad + \mathbf{v}_{\nu-1}.a^r_{idxBB} \\
c &= 1 \\
\nu&{++}
\end{aligned}$$

If the assignment is the first in the current basic block, that is, if $(newBB \vee \neg idxBB)$ returns TRUE, then the index of this basic block needs to be pushed onto the control stack. The value of the variable on the left-hand side ($V.a^f$) is stored on the data stack prior to getting overwritten with the value of the code list variable, that is the value of the expression on the right-hand side.

The adjoint of the assignment that is currently parsed is preceded by restoring the value of $V.a^f$, and it is followed by resetting the adjoint of $V.a^f$ to zero. The adjoint of the section of the current basic block ($idxBB$) that has been parsed so far is appended. As before, the code list variable counter c is reset to 1 to set the ground for correctly building the code list of the next assignment. All reduce actions end with the incrementation of the AST vertex counter ν.

(P4) $e :: V$

$$\begin{aligned}
&\vdots \\
\mathbf{v}_\nu.a^r_{idxBB} &= \text{"}pop\text{"} + \text{"("} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{")"} + \text{";"} \\
&\quad + V.\bar{a}^f + \text{"+="} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{";"} \\
\nu&{++}
\end{aligned}$$

The synthesis of the adjoint code is restricted to the current basic block as pointed out in the discussion of **(P1)**.

(P5) $e :: C$

$$\begin{aligned}
&\vdots \\
\mathbf{v}_\nu.a^r_{idxBB} &= \text{"}pop\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{"};\text{"} \\
\nu{+}{+}&
\end{aligned}$$

We simply restore the value of the code list variable that was overwritten with the constant $C.a^f$.

(P6) $e :: F(e)$

$$\begin{aligned}
&\vdots \\
\mathbf{v}_\nu.a^r_{idxBB} &= \text{"}pop\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{"};\text{"} \\
&+ \text{"}\bar{v}_{[\mathbf{v}_{\nu-1}.j]}\text{"} + \text{"} = \text{"} + \frac{\partial F.a^f}{\partial\text{"}v_{[\mathbf{v}_{\nu-1}.j]}\text{"}} + \text{"} * \text{"} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{"};\text{"} \\
&+ \mathbf{v}_{\nu-1}.a^r_{idxBB} \\
\nu{+}{+}&
\end{aligned}$$

The only difference from Section (3) is the restriction to the current basic block.

(P7) $e :: eOe$

$$\begin{aligned}
&\vdots \\
\mathbf{v}_\nu.a^r_{idxBB} &= \text{"}pop\text{"} + \text{"}(\text{"} + \text{"}v_{[\mathbf{v}_\nu.j]}\text{"} + \text{"})\text{"} + \text{"};\text{"} \\
&+ \text{"}\bar{v}_{[\mathbf{v}_{\mu_1}.j]}\text{"} + \text{"} = \text{"} + \frac{\partial O.a^f}{\partial\text{"}v_{[\mathbf{v}_{\mu_1}.j]}\text{"}} + \text{"} * \text{"} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{"};\text{"} \\
&+ \text{"}\bar{v}_{[\mathbf{v}_{\mu_2}.j]}\text{"} + \text{"} = \text{"} + \frac{\partial O.a^f}{\partial\text{"}v_{[\mathbf{v}_{\mu_2}.j]}\text{"}} + \text{"} * \text{"} + \text{"}\bar{v}_{[\mathbf{v}_\nu.j]}\text{"} + \text{"};\text{"} \\
&+ \mathbf{v}_{\mu_1}.a^r_{idxBB} + \mathbf{v}_{\mu_2}.a^r_{idxBB} \\
&\qquad \text{where } \mathbf{v}_{\mu_1} \hat{=} e^1 \text{ and } \mathbf{v}_{\mu_2} \hat{=} e^2 \text{ in } e^1 O e^2 \\
\nu{+}{+}&
\end{aligned}$$

The treatment is analogous to **(P6)**.

(P8) $s :: IF(c)\{r\}$

Shift Action:

$$newBB = 1$$

Reduce Action:

$$\mathbf{v}_\nu.a^f = "if" + "(" + \mathbf{v}_{\mu_1}.a^f + ")" + "\{" \mathbf{v}_{\mu_2}.a^f + "\}"$$
$$\text{where } \mathbf{v}_{\mu_1} \hat{=} c \text{ and } \mathbf{v}_{\mu_2} \hat{=} r \text{ in } IF(c)\{r\}$$
$$\mathbf{v}_\nu.a_i^r = \mathbf{v}_{\mu_2}.a_i^r \quad i = 0, \ldots, idxBB$$
$$newBB = 1$$
$$\nu{+}{+}$$

Prior to parsing the branch body r, that is, while shifting through the right-hand side of the production rule, we need to ensure that the next assignment is correctly recognized as the first entry of the next basic block. For the same reason, we need to set $newBB = 1$ after parsing the IF-statement.

(P9) $s :: WHILE(c)\{r\}$
The treatment is analogous to **(P8)**.

(P10) $c :: V < V$

$$\mathbf{v}_\nu.a^f = V^{(1)}.a^f + " < " + V^{(2)}.a^f$$
where $V^{(1)}$ and $V^{(2)}$ correspond to the tokens preceding and succeeding the $<$ token, respectively.
$$\nu{+}{+}$$

Conditions get simply unparsed.

5 Implementation

Our simple proof-of-concept implementation (called `sdac` for syntax-directed adjoint code compiler) uses the compiler tools `flex`[3] and `bison`[4] The source code is shown in Appendix A.2. Furthermore, we present a simplified version that generates adjoint SLP's in Appendix A.1. `sdac` is meant to serve as a starting point for further development of more complete syntax-directed adjoint code compilers that provide better coverage for the commonly used programming languages. The source code can be downloaded from the project website.

In the following we present a small case study that is supposed to illustrate the current functionality of `sdac`.

Listing 1.2 shows a small input file that needs to be transformed into adjoint code. The same example has been used in [Nau05], thus providing a point for comparison of the numerical results.

Listing 1.2. test.in

```
t=0;
while (x<t) {
  if (x<y) {
```

[3] `http://www.gnu.org/software/flex/`
[4] `http://www.gnu.org/software/bison/`

```
    x=y+1;
  }
  x=sin(x*y);
}
```

We call `sdac test.in > test.out` to obtain the output in Listing 1.3.

Listing 1.3. test.out

```
double v1, v1_;
double v2, v2_;
double v3, v3_;
double v4, v4_;
push_c(0);
push_v(v1); v1=0;
push_v(t); t=v1;
while (x<t) {
if (x<y) {
push_c(1);
push_v(v1); v1=y;
push_v(v2); v2=1;
push_v(v3); v3=v1+v2;
push_v(x); x=v3;
}
push_c(2);
push_v(v1); v1=x;
push_v(v2); v2=y;
push_v(v3); v3=v1*v2;
push_v(v4); v4=sin(v3);
push_v(x); x=v4;
}
int i_;
while (pop_c(i_)) {
if (i_==0) {
pop_v(t); v1_=t_; t_=0;
pop_v(v1);
}
else if (i_==1) {
pop_v(x); v3_=x_; x_=0;
pop_v(v3); v1_=v3_; v2_=v3_;
pop_v(v2);
pop_v(v1); y_+=v1_;
}
else if (i_==2) {
pop_v(x); v4_=x_; x_=0;
pop_v(v4); v3_=cos(v3)*v4_;
pop_v(v3); v1_=v3_*v2; v2_=v3_*v1;
pop_v(v2); y_+=v2_;
pop_v(v1); x_+=v1_;
}
}
```

To verify the correctness of the transformation we provide a driver that compares the values of the two gradient entries as computed by the adjoint code with an approximation obtained by applying forward finite differences. The driver contains wrappers for the original code (lines 29–32) and the adjoint code (lines 34–37) in the form of the subroutines `test` and `test_`. Furthermore it implements the data and control stack together with the corresponding storage and retrieval functions (lines 3, 7–27).

Note that only one call of the adjoint routine is required in Listing 1.4, line 55 as opposed to two calls for the finite difference approximation (or, similarly, of the tangent-linear routine as discussed in [Nau05]).

Listing 1.4. test.cpp

```
1 #include <cmath>
2 #include <iostream>
3 #include <stack>
4
5 using namespace std;
6
7 static stack<double> stack_v;
8 static stack<int> stack_c;
9
10 void push_v(double v) {
11   stack_v.push(v);
12 }
13 void pop_v(double& v) {
14   v=stack_v.top();
15   stack_v.pop();
16 }
17 void push_c(int c) {
18   stack_c.push(c);
19 }
20 int pop_c(int& c) {
21   if (!stack_c.empty()) {
22     c=stack_c.top();
23     stack_c.pop();
24     return 1;
25   }
26   return 0;
27 }
28
29 void test ( double &x, double y) {
30 double t;
31 #include "test.in"
32 }
33
34 void test_ ( double &x, double& x_, double y, double& y_) {
35 double t,t_;
36 #include "test.out"
37 }
38
39 int main() {
40 {
41   cout << "finite differences:" << endl;
42   double h=1e-6, x=-.5, y=-5., x_=x+h, y_=y;
43   test(x,y);
44   test(x_,y_);
45   cout << "dx/dx=" << (x_-x)/h << endl;
46
47   x=-.5, x_=x, y_=y+h;
48   test(x,y);
49   test(x_,y_);
50   cout << "dx/dy=" << (x_-x)/h << endl;
51 }
52 {
53   cout << "adjoint code:" << endl;
54   double x=-.5, y=-5, x_=1., y_=0.;
```

```
  test_(x,x_,y,y_);
  cout << "dx/dx=" << x_ << endl;
  cout << "dx/dy=" << y_ << endl;
}
  return 0;
}
```

The numerical results are identical with those in [Nau05].

```
finite differences:
dx/dx=4.00571
dx/dy=0.400572
adjoint code:
dx/dx=4.00572
dx/dy=0.400572
```

6 Conclusions and Outlook

The syntax-directed generation of adjoint code is elegant and relatively simple to implement. No internal representation of the forward code needs to be generated. A resulting disadvantage is the lack of data flow analysis which makes a full domain-specific optimization of the generated code impossible. Standard optimizations are performed potentially by the compiler that is used to translate the adjoint into object code.

The proposed approach represents a reasonable trade-off between the effort required for the tool development and the quality of the generated code. Moreover, the question about where the limits of the syntax-directed approach in the context of adjoint code generation are is still open and the subject of ongoing research.

In part III of this series of reports on syntax-directed generation of derivative code we will focus on adjoint code for numerical programs with interprocedural flow of control induced by subroutine calls. Work is underway to increase the syntactic richness of the input accepted by `sdac` with the objective to provide a tool that covers more and more practically relevant cases.

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A A Proof-of-Concept Implementation

A.1 Adjoint SLP's

Listing 1.5. ast.h

```
typedef struct {
  int j;
  char* af;
  char* ar;
} astNodeType;

#define YYSTYPE astNodeType
```

Listing 1.6. scanner.l

```
%{
#include "ast.h"
#include "parser.tab.h"
%}

whitespace        [ \t\n]+
symbol            [a-z]
const             [0-9]

%%

{whitespace} { }
"sin" { return SIN; }
{symbol} {
  yylval.af = (char*)malloc(2*sizeof(char));
  strcpy(yylval.af,yytext);
  yylval.ar=0; yylval.j=0;
  return SYMBOL;
}
{const} {
  yylval.af = (char*)malloc((strlen(yytext)+1)*sizeof(char));
  strcpy(yylval.af,yytext);
  yylval.ar=0; yylval.j=0;
  return CONSTANT;
}
. { return yytext[0]; }

%%

void lexinit(FILE *source)
{
  yyin=source;
}
```

Listing 1.7. parser.y

```
%{

#include <stdio.h>
#include "ast.h"

extern int yylex();
extern void lexinit(FILE*);
```

```

static int c=1,cmax=1;

%}

%token SYMBOL CONSTANT SIN IF WHILE

%left '+'
%left '*'

%%

code : sequence_of_assignments
  {
    for (c=1;c<cmax;c++) printf("double v%d, v%d_;\n",c,c);
    printf("%s%s",$1.af,$1.ar);
    free($1.af); free($1.ar);
  }

  ;
sequence_of_assignments : assignment { $$=$1; }
  | assignment sequence_of_assignments
  {
    $$.af=(char*)malloc((strlen($1.af)+strlen($2.af)+1)*sizeof(char));
    sprintf($$.af,"%s%s",$1.af,$2.af);
    free($2.af); free($1.af);

    $$.ar=(char*)malloc((strlen($1.ar)+strlen($2.ar)+1)*sizeof(char));
    sprintf($$.ar,"%s%s",$2.ar,$1.ar);
    free($2.ar); free($1.ar);
  }
  ;
assignment : SYMBOL '=' expression ';'
  {
    $$.af=(char*)malloc((strlen($3.af)+2*strlen($1.af)+$3.j%10+14)*sizeof(char));
    sprintf($$.af,"%spush(%s); %s=v%d;\n",$3.af,$1.af,$1.af,$3.j);
    $$.ar=(char*)malloc((3*strlen($1.af)+$3.j%10+strlen($3.ar)+20)*sizeof(char));
    sprintf($$.ar,"pop(%s); v%d_=%s_; %s_=0;\n%s",$1.af,$3.j,$1.af,$1.af,$3.ar);
    free($3.ar); free($1.af); free($3.af);
    c=1;
  }
  ;
expression : expression '*' expression
  {
    $$.af=(char*)malloc((strlen($1.af)+strlen($3.af)+2*c%10+$1.j%10+$3.j%10+21)*sizeof(char));
    $$.j=c++; if (c>cmax) cmax=c;
    sprintf($$.af,"%s%spush(v%d); v%d=v%d*v%d;\n",$1.af,$3.af,$$.j,$$.j,$1.j,$3.j);
    free($1.af); free($3.af);

    $$.ar=(char*)malloc((2*$1.j%10+2*$3.j%10+3*$$.j%10+strlen($1.ar)+strlen($3.ar)+34)*sizeof(char));
```

```
      sprintf($$.ar,"pop(v%d); v%d_=v%d_*v%d; v%d_=v%d_*v%d;\n%s%s",$$.j,$1.j,$$.j,$3.j,$3.j,$$.j,$1.j,$3.ar,$1.ar);
      free($1.ar); free($3.ar);

    }
    | expression '+' expression
    {
      $$.af=(char*)malloc((strlen($1.af)+strlen($3.af)+2*c%10+$1.j%10+$3.j%10+21)*sizeof(char));
      $$.j=c++; if (c>cmax) cmax=c;
      sprintf($$.af,"%s%spush(v%d); v%d=v%d+v%d;\n",$1.af,$3.af,$$.j,$$.j,$1.j,$3.j);
      free($1.af); free($3.af);

        $$.ar=(char*)malloc(($1.j%10+$3.j%10+3*$$.j%10+strlen($1.ar)+strlen($3.ar)+28)*sizeof(char));
        sprintf($$.ar,"pop(v%d); v%d_=v%d_; v%d_=v%d_;\n%s%s",$$.j,$1.j,$$.j,$3.j,$$.j,$3.ar,$1.ar);
        free($1.ar); free($3.ar);
    }
    | SIN '(' expression ')'
    {
      $$.af=(char*)malloc((strlen($3.af)+2*c%10+$3.j%10+23)*sizeof(char));
      $$.j=c++; if (c>cmax) cmax=c;
      sprintf($$.af,"%spush(v%d); v%d=sin(v%d);\n",$3.af,$$.j,$$.j,$3.j);
      free($3.af);

      $$.ar=(char*)malloc((2*$3.j%10+2*$$.j%10+strlen($3.ar)+27)*sizeof(char));
      sprintf($$.ar,"pop(v%d); v%d_=cos(v%d)*v%d_;\n%s",$$.j,$3.j,$3.j,$$.j,$3.ar);
      free($3.ar);
    }
    | SYMBOL
    {
      $$.af=(char*)malloc((2*c%10+strlen($1.af)+16)*sizeof(char));
      $$.j=c++; if (c>cmax) cmax=c;
      sprintf($$.af,"push(v%d); v%d=%s;\n",$$.j,$$.j,$1.af);

      $$.ar=(char*)malloc((strlen($1.af)+2*$$.j%10+18)*sizeof(char));
      sprintf($$.ar,"pop(v%d); %s_+=v%d_;\n",$$.j,$1.af,$$.j);

      free($1.af);
    }
    | CONSTANT
    {
      $$.af=(char*)malloc((2*c%10+strlen($1.af)+16)*sizeof(char));
      $$.j=c++; if (c>cmax) cmax=c;
      sprintf($$.af,"push(v%d); v%d=%s;\n",$$.j,$$.j,$1.af);

      $$.ar=(char*)malloc((2*$$.j%10+10)*sizeof(char));
      sprintf($$.ar,"pop(v%d);\n",$$.j);
      free($1.af);
    }
    ;

%%
```

```

int yyerror(char *msg) { printf("ERROR: %s \n",msg); return -1; }

int main(int argc,char** argv)
{
  FILE *source_file=fopen(argv[1],"r");
  lexinit(source_file);
  yyparse();
  fclose(source_file);
  return 0;
}
```

A.2 Adjoint Subroutines

Listing 1.8. ast.h

```
#define maxBB 100

typedef struct {
  int j;
  char* af;
  char* ar[maxBB];
} astNodeType;

#define YYSTYPE astNodeType
```

Listing 1.9. scanner.l

```
%{
#include "ast.h"
#include "parser.tab.h"
%}

whitespace      [ \t\n]+
symbol          [a-z]
const           [0-9]

%%

{whitespace} { }
"if" { return IF; }
"while" { return WHILE; }
"sin" { return SIN; }
{symbol} {
  yylval.af = (char*)malloc(2*sizeof(char));
  strcpy(yylval.af,yytext);
  int i;
  for (i=0;i<maxBB;i++) yylval.ar[i]=0;
  yylval.j=0;
  return SYMBOL;
}
{const} {
  yylval.af = (char*)malloc((strlen(yytext)+1)*sizeof(char));
```

```
  strcpy(yylval.af,yytext);
  int i;
  for (i=0;i<maxBB;i++) yylval.ar[i]=0;
  yylval.j=0;
  return CONSTANT;
}

. { return yytext[0]; }

%%

void lexinit(FILE *source)
{
  yyin=source;
}
```

Listing 1.10. parser.y

```
%{

#include <stdio.h>
#include "ast.h"

extern int yylex();
extern void lexinit(FILE*);

static int c=1,cmax=1;
static int newBB=0;
static int idxBB=0;

%}

%token SYMBOL CONSTANT SIN IF WHILE

%left '+'
%left '*'

%%

code : sequence_of_statements
  {
    for (c=1;c<cmax;c++) printf("double v%d, v%d_;\n",c,c);
    printf("%s",$1.af);
    free($1.af);
    int i;
    printf("int i_;\n");
    printf("while (pop_c(i_)) {\n");
    for (i=0;i<=idxBB;i++) {
      if (i==0)
        printf("if");
      else
        printf("else if");
      if ($1.ar[i])
        printf(" (i_==%d) {\n%s}\n",i,$1.ar[i]);
      else
        printf(" (i_==%d) {\n}\n",i);
      free($1.ar[i]);
```

```
    }
    printf("}\n");
  }

  ;
sequence_of_statements : statement { $$=$1; }
  | statement sequence_of_statements
  {
    $$.af=(char*)malloc((strlen($1.af)+strlen($2.af)+1)*sizeof(char));
    sprintf($$.af,"%s%s",$1.af,$2.af);
    free($2.af); free($1.af);

    int i;
    for (i=0;i<=idxBB;i++) {
      if ($2.ar[i]&&$1.ar[i]) {
        $$.ar[i]=(char*)malloc((strlen($1.ar[i])+strlen($2.ar[i])+1)*sizeof(char));
        sprintf($$.ar[i],"%s%s",$2.ar[i],$1.ar[i]);
        free($2.ar[i]); free($1.ar[i]);
      }
      else if ($2.ar[i]) {
        $$.ar[i]=(char*)malloc((strlen($2.ar[i])+1)*sizeof(char));
        sprintf($$.ar[i],"%s",$2.ar[i]);
        free($2.ar[i]);
      }
      else if ($1.ar[i]) {
        $$.ar[i]=(char*)malloc((strlen($1.ar[i])+1)*sizeof(char));
        sprintf($$.ar[i],"%s",$1.ar[i]);
        free($1.ar[i]);
      }
    }
  }
  ;
statement : assignment { $$=$1; }
  | if_statement { $$=$1; }
  | while_statement { $$=$1; }
  ;
if_statement : IF '(' condition ')' '{'
  {
    newBB=1;
  }
  sequence_of_statements '}'
  {
    $$.af=(char*)malloc((strlen($3.af)+strlen($7.af)+12)*sizeof(char));
    sprintf($$.af,"if (%s) {\n%s}\n",$3.af,$7.af);
    free($3.af); free($7.af);
    int i;
    for (i=0;i<=idxBB;i++) {
      if ($7.ar[i]) {
        $$.ar[i]=(char*)malloc((strlen($7.ar[i])+1)*sizeof(char));
        sprintf($$.ar[i],"%s",$7.ar[i]);
        free($7.ar[i]);
      }
    }
    newBB=1;
  }
  ;
```

```
while_statement : WHILE '(' condition ')' '{'
  {
    newBB=1;
  }
  sequence_of_statements '}'
  {
    $$.af=(char*)malloc((strlen($3.af)+strlen($7.af)+15)*sizeof(char));
    sprintf($$.af,"while (%s) {\n%s}\n",$3.af,$7.af);
    free($3.af); free($7.af);
    int i;
    for (i=0;i<=idxBB;i++) {
      if ($7.ar[i]) {
        $$.ar[i]=(char*)malloc((strlen($7.ar[i])+1)*sizeof(char));
        sprintf($$.ar[i],"%s",$7.ar[i]);
        free($7.ar[i]);
      }
    }
    newBB=1;
  }
  ;
condition : SYMBOL '<' SYMBOL
  {
    $$.af=(char*)malloc((strlen($1.af)+strlen($3.af)+2)*sizeof(char));
    sprintf($$.af,"%s<%s",$1.af,$3.af);
    free($1.af); free($3.af);
  }
assignment : SYMBOL '='
  {
    if (newBB) idxBB++;
  }
  expression ';'
  {
    if (newBB||!idxBB) {
      $$.af=(char*)malloc((strlen($4.af)+idxBB%10+3*strlen($1.af)+2*$4.j%10+27)*sizeof(char));
      sprintf($$.af,"push_c(%d);\n%spush_v(%s); %s=v%d;\n",idxBB,$4.af,$1.af,$1.af,$4.j);
    }
    else {
      $$.af=(char*)malloc((strlen($4.af)+3*strlen($1.af)+2*$4.j%10+16)*sizeof(char));
      sprintf($$.af,"%spush_v(%s); %s=v%d;\n",$4.af,$1.af,$1.af,$4.j);
    }
    $$.ar[idxBB]=(char*)malloc((3*strlen($1.af)+$4.j%10+strlen($4.ar[idxBB])+22)*sizeof(char));
    sprintf($$.ar[idxBB],"pop_v(%s); v%d_=%s_; %s_=0;\n%s",$1.af,$4.j,$1.af,$1.af,$4.ar[idxBB]);
    free($4.ar[idxBB]);
    newBB=0;
    free($1.af); free($4.af);
    c=1;
  }
  ;
expression : expression '*' expression
  {
    $$.j=c++; if (c>cmax) cmax=c;
```

```
      $$.af=(char*)malloc((strlen($1.af)+strlen($3.af)+2*$$.j%10+$1.j%10+$3.j%10+20)*sizeof(char));
      sprintf($$.af,"%s%spush_v(v%d); v%d=v%d*v%d;\n",$1.af,$3.af,$$.j,$$.j,$1.j,$3.j);
      free($1.af); free($3.af);

      $$.ar[idxBB]=(char*)malloc((2*$1.j%10+2*$3.j%10+3*$$.j%10+strlen($1.ar[idxBB])+strlen($3.ar[idxBB])+36)*sizeof(char));
      sprintf($$.ar[idxBB],"pop_v(v%d); v%d_=v%d_*v%d; v%d_=v%d_*v%d;\n%s%s",$$.j,$1.j,$$.j,$3.j,$3.j,$$.j,$1.j,$3.ar[idxBB],$1.ar[idxBB]);
      free($1.ar[idxBB]); free($3.ar[idxBB]);

    }
    | expression '+' expression
    {
      $$.j=c++; if (c>cmax) cmax=c;
      $$.af=(char*)malloc((strlen($1.af)+strlen($3.af)+2*$$.j%10+$1.j%10+$3.j%10+23)*sizeof(char));
      sprintf($$.af,"%s%spush_v(v%d); v%d=v%d+v%d;\n",$1.af,$3.af,$$.j,$$.j,$1.j,$3.j);
      free($1.af); free($3.af);

        $$.ar[idxBB]=(char*)malloc((2*$1.j%10+2*$3.j%10+3*$$.j%10+strlen($1.ar[idxBB])+strlen($3.ar[idxBB])+30)*sizeof(char));
        sprintf($$.ar[idxBB],"pop_v(v%d); v%d_=v%d_; v%d_=v%d_;\n%s%s",$$.j,$1.j,$$.j,$3.j,$$.j,$3.ar[idxBB],$1.ar[idxBB]);
        free($1.ar[idxBB]); free($3.ar[idxBB]);
    }
    | SIN '(' expression ')'
    {
      $$.j=c++; if (c>cmax) cmax=c;
      $$.af=(char*)malloc((strlen($3.af)+2*$$.j%10+$3.j%10+25)*sizeof(char));
      sprintf($$.af,"%spush_v(v%d); v%d=sin(v%d);\n",$3.af,$$.j,$$.j,$3.j);
      free($3.af);

      $$.ar[idxBB]=(char*)malloc((2*$$.j%10+2*$3.j%10+strlen($3.ar[idxBB])+29)*sizeof(char));
      sprintf($$.ar[idxBB],"pop_v(v%d); v%d_=cos(v%d)*v%d_;\n%s",$$.j,$3.j,$3.j,$$.j,$3.ar[idxBB]);
      free($3.ar[idxBB]);
    }
    | SYMBOL
    {
      $$.j=c++; if (c>cmax) cmax=c;
      $$.af=(char*)malloc((2*$$.j%10+strlen($1.af)+18)*sizeof(char));
      sprintf($$.af,"push_v(v%d); v%d=%s;\n",$$.j,$$.j,$1.af);

      $$.ar[idxBB]=(char*)malloc((strlen($1.af)+2*$$.j%10+20)*sizeof(char));
      sprintf($$.ar[idxBB],"pop_v(v%d); %s_+=v%d_;\n",$$.j,$1.af,$$.j);
      free($1.af);
    }
    | CONSTANT
    {
```

```
      $$.j=c++; if (c>cmax) cmax=c;
      $$.af=(char*)malloc((2*$$.j%10+strlen($1.af)+18)*sizeof(char));
      sprintf($$.af,"push_v(v%d); v%d=%s;\n",$$.j,$$.j,$1.af);

      $$.ar[idxBB]=(char*)malloc(($$.j%10+12)*sizeof(char));
      sprintf($$.ar[idxBB],"pop_v(v%d);\n",$$.j);
      free($1.af);
    }
    ;

%%

int yyerror(char *msg) { printf("ERROR: %s \n",msg); return -1; }

int main(int argc,char** argv)
{
  FILE *source_file=fopen(argv[1],"r");
  lexinit(source_file);
  yyparse();
  fclose(source_file);
  return 0;
}
```

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