Differentiable Scripting

Uwe Naumann
Department of Computer Science, RWTH Aachen University
52056 Aachen, Germany
naumann@stce.rwth-aachen.de

Abstract

In Computational Science, Engineering and Finance (CSEF) scripts typically serve as the “glue” between potentially highly complex and computationally expensive external subprograms. Differentiability of the resulting programs turns out to be essential in the context of derivative-based methods for error analysis, uncertainty quantification, optimization or training of surrogates. We argue that it should be enforced by the scripting language itself through exclusive support of differentiable (smoothed) external subprograms and differentiable intrinsics combined with prohibition of nondifferentiable branches in the data flow. Illustration is provided by a prototype adjoint code compiler for a simple Python-like scripting language.

1 Motivation

In an ideal world, libraries for numerical simulation would provide a complete collection of the state of the art in the target domain implemented as easy-to-use, efficient, scalable and sustainable software ... and corresponding adjoints. Considerable progress in this direction has been made over the past three decades thanks to activities in Algorithmic (also: Automatic) Differentiation (AD) [9] including software tool development and applications in CSEF as well as evolution of its theoretical foundations. A good overview is provided by the proceedings of so far seven international AD conferences, e.g. [2, 4, 5]. See www.autodiff.org for links to research groups and software tools in addition to an extensive bibliography on the subject.

Numerical simulation in CSEF relies on a hierarchy of software library components implementing multivariate vector functions $F : \mathbb{R}^n \rightarrow \mathbb{R}^m : y = F(x)$ (also: primals) including subprograms for linear algebra, model calibration, Monte Carlo simulation and solvers for algebraic and differential equations. Substantial effort has been put into the implementation of adjoints $\bar{F} : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n : \bar{x} = \bar{F}(x, \bar{x}, \bar{y}) \equiv \bar{x} + F'(x)^T \cdot \bar{y}$ while ensuring or at least assuming differentiability of $F$ at all points of interest. Very large implementations in C/C++, Fortran and other general-purpose programming languages can be handled by state of the art AD software tools. Both source-to-source transformation [6] and operator/function overloading combined with template metaprogramming techniques [18] have been developed and applied successfully for several decades. Cutting-edge solutions run on large CPU, e.g. [17], or GPGPU clusters, e.g. [7].

Simulation scenarios of interest are often synthesized from a set of differentiable subprograms using both syntactically and semantically relatively simple instructions provided by domain-specific scripting languages. The latter typically do not require the same complexity exhibited by general-purpose programming languages. Their users should not be required to have the same level of software development expertise as their colleagues who implement the core numerical libraries. Simple flow of control over the basic arithmetic and relational operators in addition to a set of differentiable intrinsics / subprograms often suffices. The automatic generation of adjoint scripts becomes relatively straightforward in this case.

Conditions for differentiable scripting are formulated in the following section. Their integration into a single-pass adjoint code compiler for a simple Python-like scripting language is the subject of Section 3. A case study is presented in Section 4 followed by final remarks in Section 5.
2 Differentiable Scripting

A scripting language SL is differentiable if all arithmetic operations and intrinsic functions as well as all callable external subprograms are differentiable and if active branches in the flow of control are prohibited. For illustration we introduce a simple imperative Python-like scripting language supporting collections of (internal) subprograms

```
subprogram : DEF NAME '(' arguments ')' '{' statements RETURN argument '}'
```

over statements defined as

```
statement : assignment | if | while | for | call | ...
```

with assignments

```
assignment : variable '=' expression
```

of the results of right-hand sides of type

```
expression : expression '*' expression | EXP '(' expression ')' | ... 
```

to scalar variables. Intraprocedural flow of control includes conditional branches

```
if : IF condition '{' statements '}' ELSE '{' statements '}'
```

and two types of loops. Internal as well as external subprograms can be called as

```
call : NAME '=' NAME '(' arguments ')
```

Active in- and outputs of subprograms need to be vectors. This restriction (as well as others) is likely to be lifted in upcoming versions of SL. Its development should be considered as work in progress.

We present a single-pass compiler which translates SL into Python. It is implemented in C-style C++ using the scanner and parser generators flex and bison[15]. Grammar rules are specified in bison syntax. [Non-]Terminal symbols are written in [lower-]uppercase letters. The entire source code can be found on github.com/un110076/AD4SL including a complete specification of the SL grammar. All results in this paper can thus be reproduced.

2.1 Differentiable Intrinsics

The differentiable arithmetic operations +,−,∗,/ over scalar floating-point variables are supported as well as commonly used differentiable arithmetic functions such as the exponential function represented by the terminal symbol EXP. As an example for a smoothed not everywhere differentiable intrinsic we consider max(x,0) implemented as part of the SL runtime library in C++ as

```
float gt0(float x) { return fmax(x,0.0); }
```

Differentiability at x = 0 can be ensured, for example, by sigmoidal smoothing yielding the following implementation of the derivative of gt0 with respect to its input argument:

```
float d_gt0(float x) {
    const float h=1e-3;
    if (x<h) return 0;
    else if (x>h) return 1;
    else return 1./(1.+exp(-(x)/h));
}
```

The change in tangent slope at x = 0 is globalized in dependence of the hyperparameter h. Suitable choices for values of h depend on the simulation to be implemented. Less static ways of specifying the value of h may be required in practice. Discontinuities can be smoothed similarly. Alternatively, central finite difference approximations of the derivative can be implemented. Moreover, there is a rich body of published work to be considered, e.g. [8, 13, 14]. For the purpose of this paper, all external subprograms and intrinsics are assumed to be (made) differentiable independent of

---

1We use a tiny subset of Python and curly brackets instead of “pythonic” indentation.
2pybind11 (github.com/pybind/pybind11) is used to link the SL runtime library with the adjoint script.
the actual smoothing technique. Nondifferentiable intrinsics might still be permitted. If one is evaluated at (or within a neighborhood of) a point of nondifferentiability, then an exception should be raised and handled appropriately. At the very least, users should be informed about nondifferentiability in order to not loose sight of potentially serious numerical implications.

### 2.2 Passive Branches

To guarantee differentiability of an SL script, branch conditions must not depend on active variables. This constraint can be enforced by static activity analysis as described in [10]. The iterative nature of static data flow analysis makes it unsuitable for syntax-directed (i.e., single-pass) compilation. Instead, variables in SL are partitioned into active and passive using names starting with lowercase and uppercase letters, respectively. This conservative approach allows for propagation of the potential activity of expressions by augmenting the SL grammar with a synthesized attribute for forward activity, referred to as *variedness* in [10]. Attributes of terminal symbols (leafs of the parse tree) are initialized according to the case of their respective first letters followed by conjunctive bottom-up propagation, for example,

```plaintext
eexpression : expression 'astar' expression {
  $$ . v = \$1 . v || $$ . v;
}
```

where nonterminal symbols are referenced by their position within the right-hand side of the production rule ($1$ and $3$) and the left-hand side is accessed by $$ . For example, variedness of the first term is indicated by $1 . v = \text{true}$.

The actual treatment of active branches as errors or mere warnings is up to the language designers. In our prototype we use assertions (from `<cassert>`), for example,

```plaintext
if : IF condition ' { ' statements ' } ' {
  assert (!$$ . v); } ELSE ...
```

### 3 Single-Pass Adjoints

Adjoint SL code generated by our single-pass compiler follows the state of the art in adjoint code generation according to the well-known AD principles implemented, for example, by Tapenade [11]. To implement the fundamental requirement of data flow reversal, adjoint SL subprograms consist of forward (synthesized in the string attribute $$ . f$) and reverse (in $$ . s$ and $$ . a$) sections. The forward section corresponds to the primal code (in $$ . p$) including storage of required values that are overwritten. Some primal statements may not be required for the evaluation of the adjoint. Their generation as part of the forward section can be suppressed explicitly by using `#pragma noprimal`. Similarly, storage as well as subsequent recovery of overwritten values which are not required by the adjoint can be avoided by using `#pragma notbr`. The adjoint code remains correct if pragmas are not used. Memory requirement and runtime efficiency may suffer though. Incorrect placement of pragmas results in erroneous adjoint code.

In the reverse section all assignments are decomposed into single-assignment code (sac; in $$ . s$) through storage of the results of all operations in locally unique program variables. Corresponding adjoint statements are synthesized in $$ . a$. See Section 4 for an example.

Syntax-directed translation [11] is a conceptually elegant and light-weight approach to source-to-source transformation for typically relatively simple scripting languages. Their grammar can be augmented with attributes for synthesis of adjoint code during a single pass of a shift-reduce parser. Explicit construction of an intermediate representation of the primal program is not required. A compact, easily maintainable source-to-source transformation engine can be built with low effort at the expense of not being able to perform iterative static program analysis. This compromise turns out to be reasonable under the assumption that the potential for code optimization at the scripting level is low.

Adopting the approach proposed in [16] we use `flex/bison` to generate a generalized operator-precedence LR(1) parser for a (not quite; see below) S-attributed grammar for SL. Production rules are augmented with semantic actions over those attributes, for example
An inherited attribute \((s4.j)\) is used to enumerate the sac variables in the right-hand sides of assignments. It is implemented as a global counter \(j\) which is reset to zero prior to parsing a new right-hand side (see line 1). Assignment of active values to passive variables is not permitted (line 2). The primal code is unparsed as is (line 3). It is also used in the forward section of the adjoint code preceded by storage of the value of the left-hand side (lines 5 and 8). Optionally, both the primal assignment and/or storage and recovery of its left-hand side can be omitted through use of the previously introduced pragmas. Again, the corresponding static dead code \([1]\) and to-be-recorded \([10]\) analyses do not comply with the single-pass compilation paradigm. Adjoint code is generated for active assignments exclusively (lines 9 and 10). The stack handlers \(\text{push}_s, \text{pop}_s\) in addition to vector versions and stack access for reversal of flow of control) are part of the SL runtime library.

Right-hand sides of assignments are defined recursively as expressions resulting from arithmetic operations or intrinsic functions applied to (sub-)expressions. Their sac is synthesized in \$$s\$$.

Each reduction of a handle (right-hand side of a production rule) triggers the evaluation of the three synthesized string attributes \$$p, \$$s and \$$a\$. Enumeration of sac variables requires the inherited attribute \$$j\$$(line 2). Two auxiliary functions generate sac variables \((V)\) and their adjoints \((A)\). Adjoints of active sac variables are incremented (lines 6 and 7). Hence, they must be reset to zero after use as a left-hand side of an assignment (line 8). Refer to lines 6–10 of the adjoint code in Section 4 for an example.

The flow of control is reversed by flagging branches and by counting loop iterations as suggested in \([16]\). Within an if statement, execution of the if branch yields storage of 1 (true). The else branch is marked by 0 (false). Loop iterations are counted by incrementing counter. The adjoint loop body is executed as often as the primal loop body. Simple for loops can be reversed explicitly; see Section 4. Nesting is supported. Subprogram calls may require storage \(\text{push}_v\) and recovery \(\text{pop}_v\) of values overwritten by their results.
Active arguments are augmented with corresponding adjoint arguments. The effect of using the aforementioned pragmas is similar to the assignment case. Indentation (corresponding code omitted from listings) is handled correctly by the compiler.

4 Case Study

As a case study we consider a Monte Carlo pricer for a European call option [12] implemented in SL as follows:

```python
from numpy import *
from intrinsic import *
from external import *

def payoff (d,p) {
    #pragma noprimal
    p[0]=gt0 (d[1]-d[0])
    return p
}

def black_scholes_call (x,y,M) {
    s=[0.0]*M
    #pragma notbr
    s=mc (x,s,M)
    d=[0.0]*2
    p=[0.0]*1
    for I in range(M) {
        #pragma notbr
        d[0]=x[3]
        d[1]=s[1]
        #pragma notbr
        p=payoff (d,p)
        #pragma notbr
        y[0]=y[0]+exp(-x[1])*p[0]
    }
    #pragma noprimal
    y[0]=y[0]/M
    return y
}
```

The function `black_scholes_call` takes four active inputs collected in the array `x` consisting of asset price, interest rate, volatility and strike. `M` sample paths are allocated in line 12 and simulated by calling the function `mc` in line 14. The Monte Carlo simulation of the Black-Scholes stochastic differential equation [3] is implemented in C++. The corresponding adjoint Monte Carlo simulation can be generated by your favorite AD tool. We provided a handwritten adjoint. Both are part of `external` (line 3). Vectors `d` and `p` need to be allocated (lines 15 and 16) prior to calling `payoff` (line 22). Discounted local payoffs are added up for all paths in line 24 and averaged to get an estimate for the overall payoff `y[0]` in line 27. The function `payoff` reduces to calling the previously discussed intrinsic `gt0` in line 7 with smoothed derivative provided by `intrinsic` (line 2). The primal code does not contain any active branches.

The `noprimal` pragma is applied to the last assignments in each subprogram, respectively (lines 6 and 26). Overwrites of `s` (line 14), `d[0]` (line 19), `p` (line 22), and `y[0]` (in lines 24 and 27) do not result in loss of required values making `#pragma notbr` applicable.

The compiler transforms the primal code into the following adjoint:

```python
def a_payoff (d,a_d,p,a_p) :
    v=[0.0]*4; a_v=[0.0]*4
    # forward section
    # p[0]=gt0 (d[1]-d[0]) omitted due to #pragma noprimal
    # reverse section
    # sac
    v[0]=d[1]; v[1]=d[0]; v[2]=v[0]-v[1]; v[3]=gt0 (v[2])
    # adjoint sac
    a_v[3]=a_v[3]+a_p[0]; a_p[0]=0.0
```
a_v[2] = a_v[2] + d_gt0(v[2]) * a_v[3]; a_v[3] = 0.0

return a_d

def a_black_scholes_call(x, a_x, y, a_y, M):

# forward section
s = [0.0] * M; a_s = [0.0] * M
# push_v(s) omitted due to #pragma notbr
s = mc(x, s, M)

for i in range(M):
    push_s(d[1])
    d[1] = s[1]
    # push_v(p) omitted due to #pragma notbr
    p = payoff(d, p)
    # push_v(y) omitted due to #pragma notbr
    y[0] = y[0] + exp(-x[1]) * p[0]
    # y[0] = y[0] / M omitted due to #pragma no primal

# reverse section
v[0] = y[0]

a_y[0] = a_y[0] + a_v[0]
a_v[0] = 0.0

for i in reversed(range(M)):
    d[1] = pop_s()
    # p = pop_v() omitted due to #pragma notbr
    a_d = a_payoff(d, a_d, p, a_p)
    # s = pop_v() omitted due to #pragma notbr
    a_x = a_mc(x, a_x, s, a_s, M)
return a_x

Adjoint versions of both subprograms are generated. The listing was edited to comply with the overall space restrictions and to add crucial comments. In a_payoff the primal intrinsic gt0 is omitted in the forward section (line 4). Its smoothed adjoint is called in the reverse section (line 10). Four sac variables and their adjoints are required (line 2).

The results of the M primal Monte Carlo path simulations are augmented with storage for the corresponding adjoints in line 17. Reversal of the simple for loop in line 21 does not require additional information to be stored in the forward section.

The reverse section starts in line 30 with the adjoint of line 27 of the primal code. The adjoint simple for loop in line 35 iterates backwards over the Monte Carlo paths thus ensuring correct recovery of all required values (of d[1] stored in line 23). Finally, the adjoint Monte Carlo simulation is called in line 42 yielding the four adjoints of interest in a_x. Several intermediate statements are omitted due to space restriction.

5 Final Remarks

Differentiability of scripts for CSEF can and should be enforced by the scripting language to prevent non-expert users from unintentional implementation of nondifferentiable programs. The problem is shifted to a large extent to the design of a library of differentiable intrinsics and differentiable callable external subprograms. At the very least, “differentiation-aware programming” should be facilitated.

References

[1] A. Aho, M. Lam, R Sethi, and J. Ullman. *Compilers: Principles, Techniques, and Tools*. Addison Wesley, 2nd edition, August 2006.
[2] C. Bischof, M. Bucker, P. Hovland, U. Naumann, and J. Utke, editors. *Advances in Automatic Differentiation*, volume 64 of *Lecture Notes in Computational Science and Engineering*. Springer, Berlin, 2008.

[3] F. Black and M. Scholes. The pricing of options and corporate liabilities. *Journal of political economy*, 81(3):637, 1973.

[4] B. Christianson, S. Forth, and A. Griewank, editors. *Special issue of Optimization Methods & Software: Advances in Algorithmic Differentiation*. Taylor & Francis, 2018.

[5] S. Forth, P. Hovland, E. Phipps, J. Utke, and A. Walther, editors. *Recent Advances in Algorithmic Differentiation*, volume 87 of *Lecture Notes in Computational Science and Engineering*. Springer, Berlin, 2012.

[6] R. Giering and T. Kaminski. Recipes for adjoint code construction. *ACM Transactions on Mathematical Software*, 24(4):437–474, 1998.

[7] F. Gremse, A. Hoefter, L. Razik, F. Kiessling, and U. Naumann. GPU-accelerated adjoint algorithmic differentiation. *Computer Physics Communications*, 200:300–311, 2016.

[8] A. Griewank. On stable piecewise linearization and generalized algorithmic differentiation. *Optimization Methods and Software*, 28(6):1139–1178, 2013.

[9] A. Griewank and A. Walther. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Number 105 in Other Titles in Applied Mathematics. SIAM, Philadelphia, PA, 2nd edition, 2008.

[10] L. Hascoët, U. Naumann, and V. Pascual. To-Be-Recorded analysis in reverse mode automatic differentiation. *Future Generation Computer Systems*, 21:1401–1417, 2005.

[11] L. Hascoët and V. Pascual. The Tapenade automatic differentiation tool: Principles, model, and specification. *ACM Transactions on Mathematical Software*, 39(3):20:1–20:43, 2013.

[12] J. Hull. *Options, Futures, and Other Derivatives*. Pearson, 10th edition, 2018.

[13] B. Kearfott. Interval extensions of non-smooth functions for global optimization and nonlinear systems solvers. *Computing*, 57(2):149–162, September 1996.

[14] K. Khan and P. Barton. Evaluating an element of the Clarke generalized Jacobian of a composite piecewise differentiable function. *ACM Trans. Math. Softw.*, 39(4):23:1–23:28, jul 2013.

[15] J. Levine. *Flex & Bison*. O’Reilly Media, Inc., 1st edition, 2009.

[16] U. Naumann. *The Art of Differentiating Computer Programs: An Introduction to Algorithmic Differentiation*. Number 24 in Software, Environments, and Tools. SIAM, Philadelphia, PA, 2012.

[17] P. Heimbach and C. Hill and R. Giering. An efficient exact adjoint of the parallel MIT general circulation model, generated via automatic differentiation. *Future Generation Computer Systems*, 21(8):1356–1371, 2005.

[18] E. Phipps and R. Pawlowski. Efficient expression templates for operator overloading-based automatic differentiation. In *[20]*, pages 309–319. 2012.