Clad - Clang plugin for Automatic Differentiation

Aleksandr Efremov

Mentors: Vassil Vassilev, Oksana Shadura

What automatic differentiation is

- Technique for evaluating the derivatives of mathematical functions
- Applicable to computer programs (e.g. C++ code)
- Alternative to numerical differentiation

Numerical differentiation

$$f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

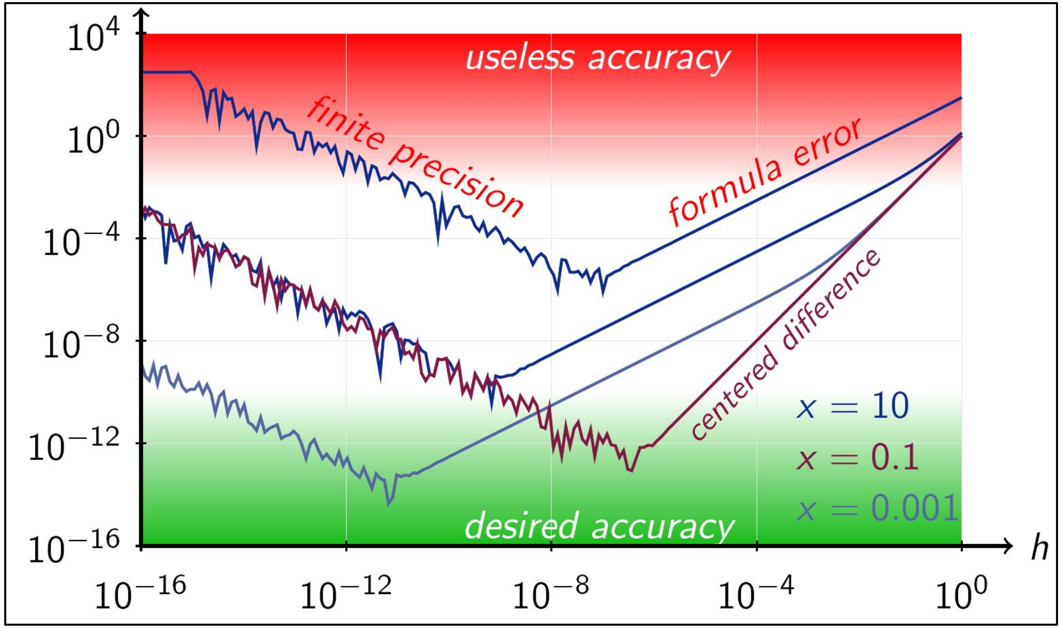
Finite difference method:

$$f'(x) \approx \frac{f(x+h)-f(x)}{h}$$

(for small value of h)

Numerical differentiation

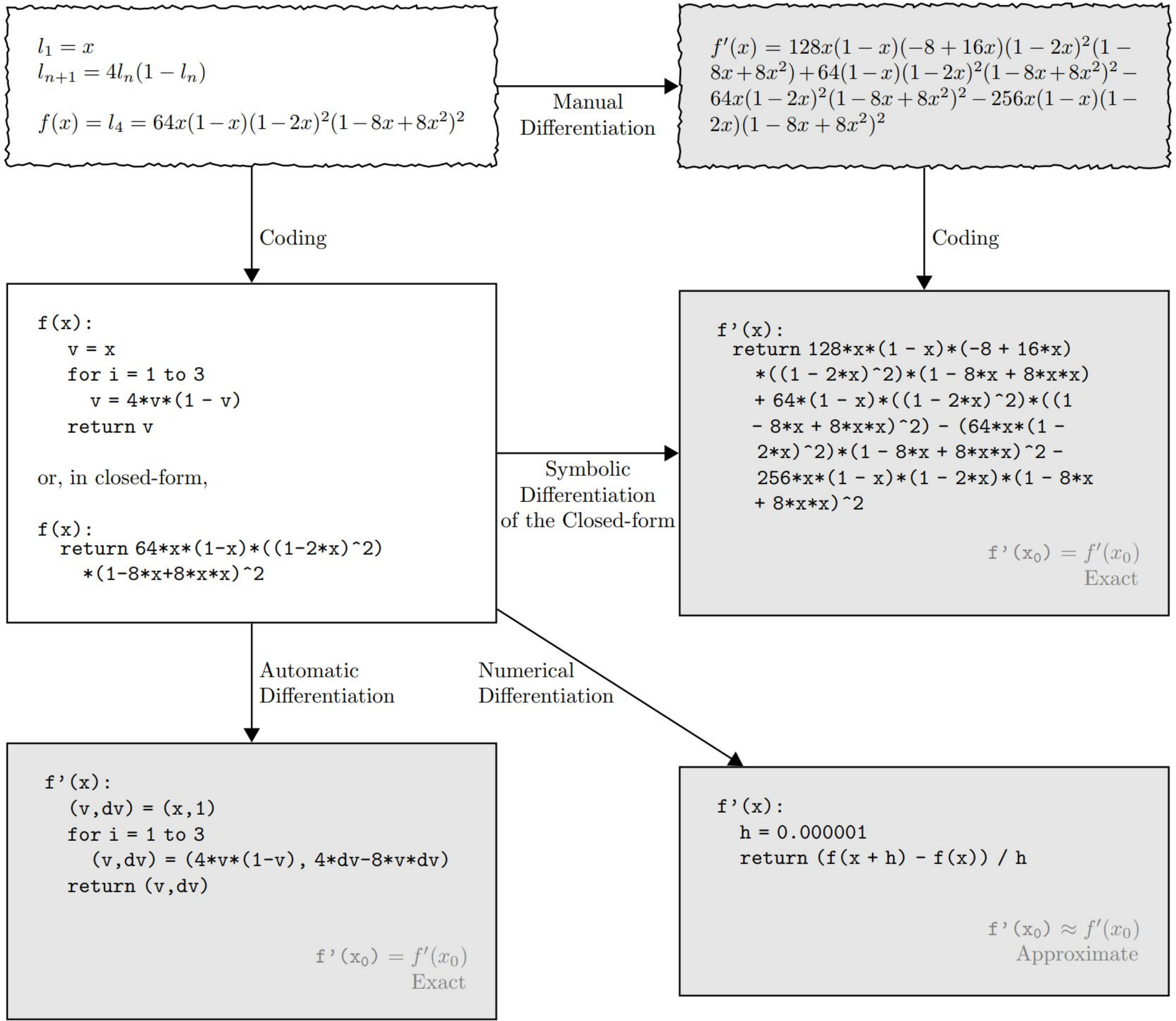
$$f'(x) \approx \frac{f(x+h)-f(x)}{h}$$



[Wikipedia, Numerical differentiation]

Disadvantages:

- Need to evaluate f twice
- Slow gradient computation
- Prone to numerical errors
- How to select h?



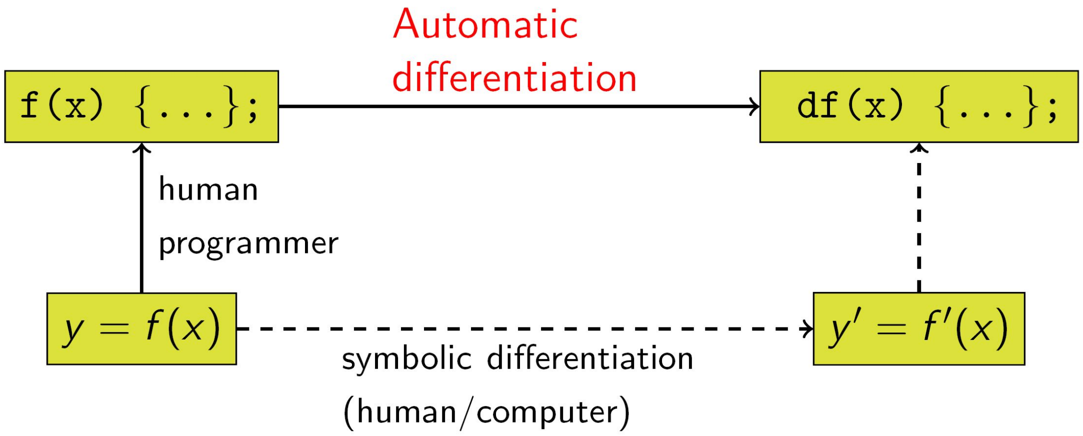
What automatic differentiation is

- Applies basic rules of symbolic differentiation
- To the source code of the original function
- The result is the code of the function that computes value of the derivative
- Without additional precision loss
- Without inefficiently long expressions

[Baydin et al., Automatic Differentiation in Machine Learning: a Survey, 2018]

Alternative to symbolic differentiation

- Not limited to closed-form expressions
- Can take derivatives of algorithms (conditionals, loops, recursion)



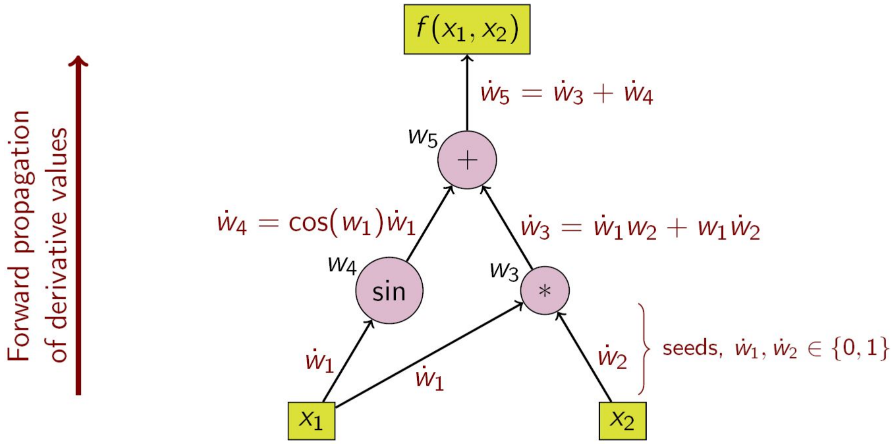
[Wikipedia, Automatic differentiation]

Automatic differentiation

- **Forward mode AD** algorithm allows to compute derivatives w.r.t. any (single) variable
- Theoretical result guarantees that the derivative can be computed in **at most 2.5 times** more arithmetic operations than the original function
- Propagates derivatives from the dependent towards the independent variables

$$f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

[Wikipedia, Automatic differentiation]



Computing gradients

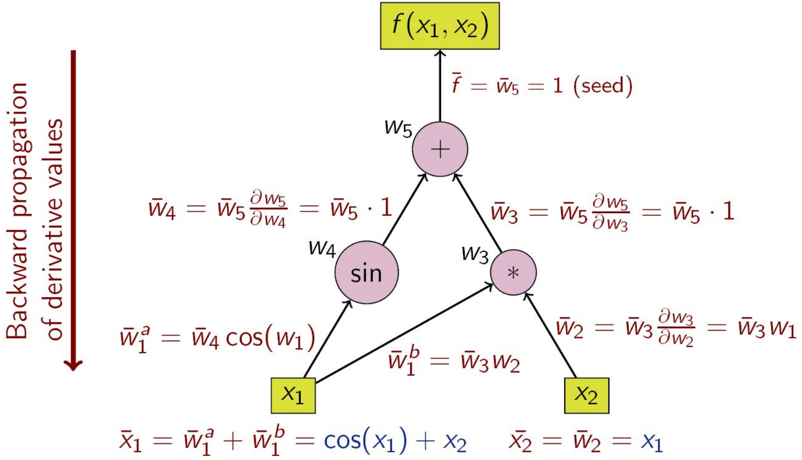
- What if we want to compute a gradient (vector of derivatives w.r.t. every variable)?
- For a function of N inputs, we have to call N functions produced by the forward mode
- Total complexity is O(2.5*N*M), where M is the complexity of the original function
- **Reverse mode** allows to compute gradients with complexity of O(4*M), independently of N, which is much more efficient for functions with many parameters

Automatic differentiation

- **Reverse mode AD** allows to compute gradients
- Gradients can be computed in **at most 4 times** more arithmetic operations than the original function **(independently of the number of input variables)**
- Propagates derivatives from the independent variables towards the result of the function

$$f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

[Wikipedia, Automatic differentiation]



AD implementations

- Source transformation
- Operator overloading
- Several implementations exist, see: http://www.autodiff.org/?module=Tools

Automatic differentiation in Clad

- Clad is a **Clang compiler plugin**
- Performs C++ **source code transformation**, based on Clang AST

```
double f(double x) {
    return x * x;
}
```

AST

```
FunctionDecl f 'double (double)'
|-ParmVarDecl x 'double'
`-CompoundStmt
  `-ReturnStmt
    `-BinaryOperator 'double' '*'
      |-ImplicitCastExpr 'double' <LValueToRValue>
      | `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
      `-ImplicitCastExpr 'double' <LValueToRValue>
        `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
```

Automatic differentiation in Clad

- Given some C++ function **f**
- **(no source modification needed, but must be visible for the compiler)**
- User specifies the function, independent variables, differentiation mode
- Clad performs the transformation **(in compile time)**
- Another C++ function for **f’** is produced

Automatic differentiation in Clad

```
double f(double x) { return x*x; }
```

User marks f for differentiation

```
...
clad::differentiate(f, 0);
...
```

Clad generates a new function

```
double f_darg0(double x) { return 1*x + x*1; }
```

Derivative is ready to be used in the same program as a ‘normal’ function

```
std::cout << f_darg0(1) << ‘\n’;
// Prints 2
```

Clad capabilities

- Most C++ construct are (will be) supported
- As long as the function is differentiable

Example: temporary variable declarations

```
double f(double x, double y) {
    double t = x*x;
    return t + y;
}
```

```
double f_darg0(double x, double y) {
    double dt = 1*x + x*1;
    return dt + 0;
}
```

Clad capabilities

Example: loops

```
double pow(double x, int n) {
    double r = 1;
    for (int i = 0; i < n; i++)
        r = r*x;
    return r;
}
```

```
double pow_darg0(double x, int n) {
    double dr = 0;
    double r = 1;
    for (int i = 0; i < n; i++) {
        dr = dr*x + r*1;
        r = r*x;
    }
    return dr;
}
```

Contributions

- Implemented **Reverse mode AD** for efficient gradients computation
- Extended the functionality to support control flow and variable reassignments
- Integrated Clad into **ROOT** (CERN’s framework for data analysis), available through **TFormula**, to be used in minimization and fitting

Potential applications

Any gradient-based optimization methods, for example:

- Function minimization
- Backpropagation for machine learning
- Fitting models to data

In **ROOT**:

- Minuit
- TMVA
- RooFit

Future work

- Support more C++ constructs, enable differentiation of any C++ code in general
- Improve user interface to allow more expressiveness for independent variables, differentiation mode specification
- Support OpenCL/CUDA code differentiation
- Implement advanced features of forward/reverse mode AD to produce optimal code
- Efficient differentiation of functions with multiple outputs (Jacobians), Hessians

Thank you!