Optimizing reverse-mode automatic differentiation with advanced activity analysis

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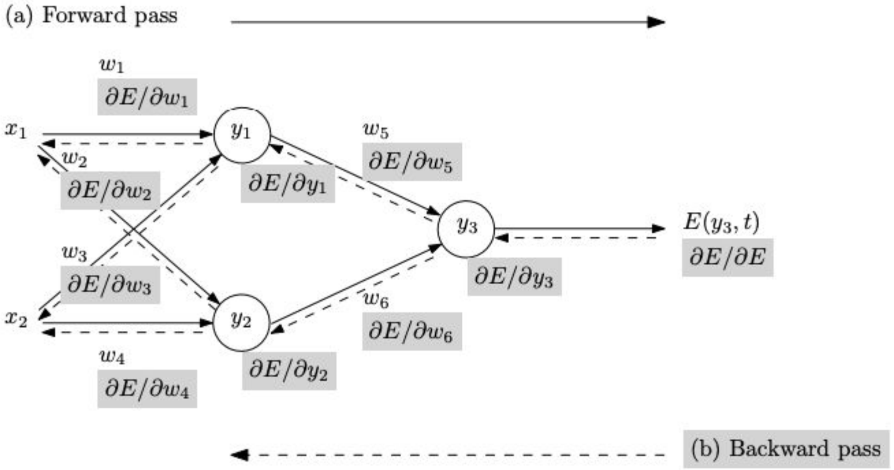
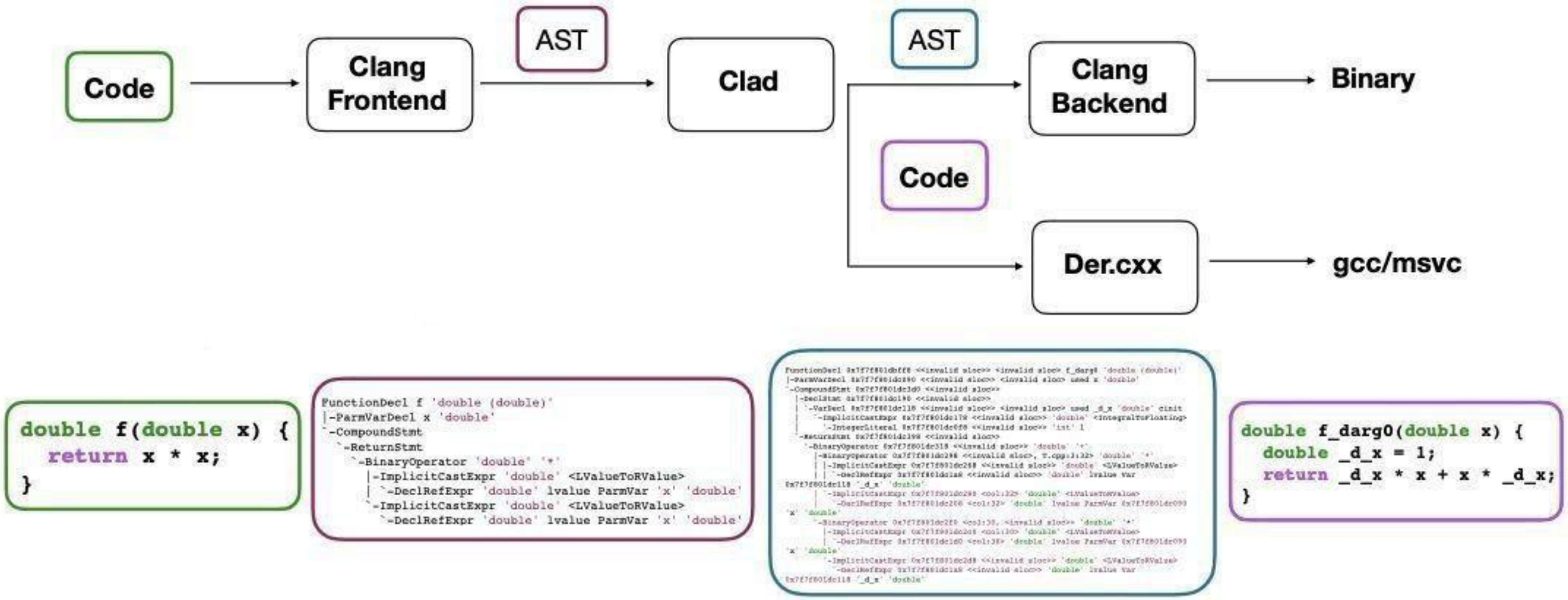
Introduction: Automatic Differentiation

Automatic differentiation is a method of differentiation of functions expressed as procedures. It involves breaking up the function into simple operations and applying chain rule to each one of them. This can be done both ways: from the input to the output (forward mode) and vice versa (reverse mode). This project focuses on the second approach which is more efficient for computing gradients. In reverse mode, we need two passes: a forward pass to store the intermediate values of all the variables and a backward pass to compute derivatives.



Introduction: Clad

Clad is an automatic differentiation Clang plugin for C++. It automatically generates code that computes derivatives of functions given by the user.



Activity Analysis

This includes removing:

- The derivatives of variables that don’t depend on the input values in a differentiable way
- The derivatives of variables that don’t influence the output values in a differentiable way
- Variables that are not used to compute the derivatives of the output values

As well as possibly:

- Removing computations that are not needed to evaluate the final derivatives
- Simplifying operations with implicit zeros

TBR (To-Be-Recorded) Analysis

Reverse-mode automatic differentiation requires storing intermediate values of variables that have impact on derivatives to restore those in the backward pass. However, we don't actually have to store all of them.

History of usage of a variable x

DECLARED → CHANGED → USED → CHANGED → USED → USED → CHANGED

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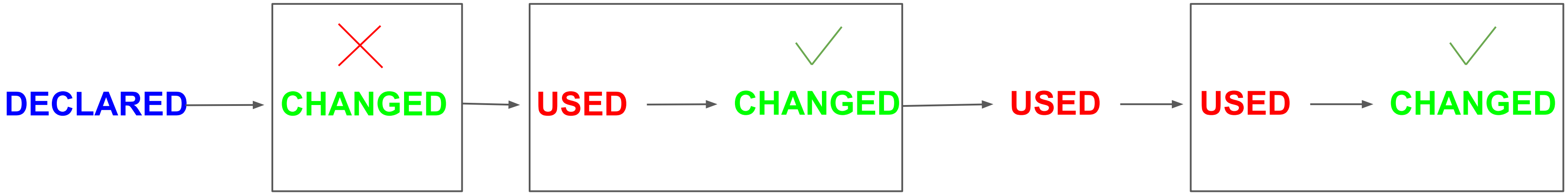
History of usage of a variable x



Examples

Original code

```
double f(double x, double y) {
  double k = 2.5;
  x += k;
  return x;
}
```

k doesn’t depend on x and y in a differentiable way!

Code differentiated by Clad

```
double _d_k = 0;
double k = 2.5;
x += k;
double f_return = x;
goto _label0;
_label0:
* _d_x += 1;
{
    double _r_d0 = * _d_x;
    * _d_x += _r_d0;
    _d_k += _r_d0;
    * _d_x -= _r_d0;
    * _d_x;
}
```

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Examples

Original code

```
double f(double x, double y) {
  double k = 2.5;
  x += k;
  return x;
}
```

k doesn’t depend on x and y in a differentiable way!

Code differentiated by Clad

Dead code

```
double _d_k = 0;
double k = 2.5;
x += k;
double f_return = x;
goto _label0;
_label0:
* _d_x += 1;
{
    double _r_d0 = * _d_x;
    * _d_x += _r_d0;
    _d_k += _r_d0;
    * _d_x -= _r_d0;
    * _d_x;
}
```

Examples

Original code

```
double f(double x, double y) {
  double k = 2 * x;
  if (k > 2)
    x *= 2;
  return x;
}
```

k doesn’t influence the return value in a differentiable way!

Code differentiated by Clad

```
  double _t0;
  double _d_k = 0;
  bool _cond0;
  _t0 = x;
  double k = 2 * _t0;
  _cond0 = k > 2;
  if (_cond0)
      x *= 2;
  double f_return = x;
  goto _label0;
_label0:
  * _d_x += 1;
  if (_cond0) {
      double _r_d0 = * _d_x;
      * _d_x += _r_d0 * 2;
      * _d_x -= _r_d0;
      * _d_x;
  }
  {
      double _r0 = _d_k * _t0;
      double _r1 = 2 * _d_k;
      * _d_x += _r1;
  }
```

Examples

Original code

```
double f(double x, double y) {
  double k = 2 * x;
  if (k > 2)
    x *= 2;
  return x;
}
```

k doesn't influence the return value in a differentiable way!

Code differentiated by Clad

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  double _t0;
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  _t0 = x;
  double k = 2 * _t0;
  _cond0 = k > 2;
  if (_cond0)
      x *= 2;
  double f_return = x;
  goto _label0;
_label0:
  * _d_x += 1;
  if (_cond0) {
      double _r_d0 = * _d_x;
      * _d_x += _r_d0 * 2;
      * _d_x -= _r_d0;
      * _d_x;
  }
  {
      double _r0 = _d_k * _t0;
      double _r1 = 2 * _d_k;
      * _d_x += _r1;
  }
```

Dead code

Goals

- Find the best optimizing strategy for Clad and implementing it
- Investigate the potential of the Clang static analysis and data-flow analysis infrastructure to capture advanced optimization opportunities
- Investigate the possibility of enabling Clad in ADBench infrastructure
- Test in major workflows such as ROOT’s RooFit package
- Writing new tests / documentation
- Create benchmarks to compare the efficiency with activity analysis on and off