Use of automatic differentiation (AD) in OPM

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Overview of talk

Why automatic differentiation?

Forward Mode AD

Reverse Mode AD

OPM implementation

What next?

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OPM implementation

What next?

What does AD provide

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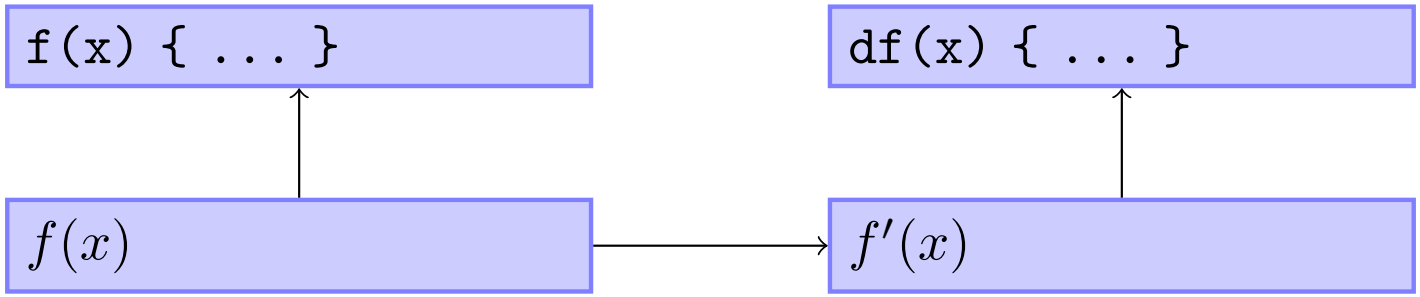
f(x) { ... }
```

```
df(x) { ... }
```

$f(x)$

$f'(x)$

What does AD provide



Traditional Process

- Human implements code to evaluate $f(x)$
- Manual or symbolic calculation to derive $f'(x)$
- Human implements code to evaluate $f'(x)$

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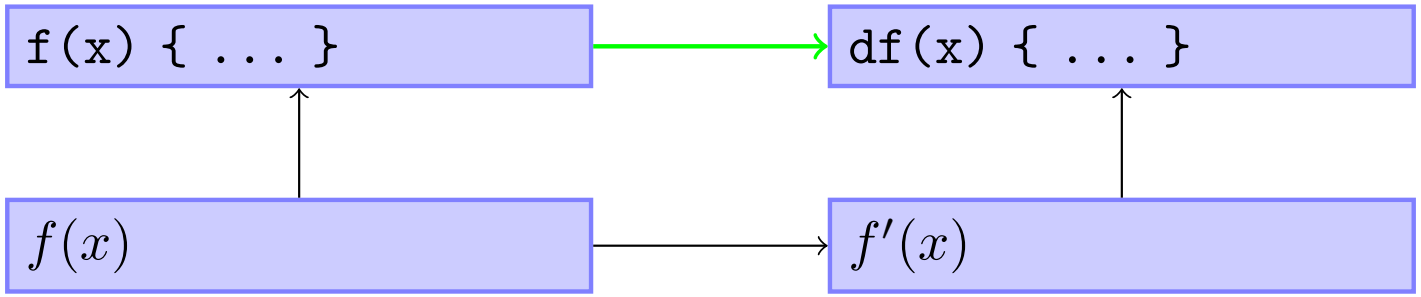

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- Human implements code to evaluate $f(x)$
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Automatic Differentiation (AD)

- Human implements code to evaluate $f(x)$
- Computer code to evaluate $f'(x)$ is automatically generated

Benefits of using AD

AD makes it easier to create simulators:

- only specify nonlinear residual equation
- automatically evaluates Jacobian
- sparsity structure of Jacobian automatically generated

Note that AD is *not* the same as finite differencing!

- no need to define a 'small' epsilon
- as precise as hand-made Jacobian
- ... but much less work!

Performance (of equation assembly) will usually be somewhat slower than a *good* hand-made Jacobian implementation.

Basic idea

A numeric computation $y = f(x)$ can be written (D = derivative)

$$
\begin{aligned}
y_1 &= f_1(x) & \frac{dy_1}{dx}(x) &= Df_1(x) \\
y_2 &= f_2(y_1) & \frac{dy_2}{dx}(x) &= Df_2(y_1) \cdot Df_1(x) \\
&\vdots \\
y &= f_n(y_{n-1}) & \frac{dy}{dx}(x) &= Df_n(y_{n-1}) \cdot Df_{n-1}(y_{n-2}) \cdots Df_1(x)
\end{aligned}
$$

Automatic Differentiation:

- make each line an elementary operation
- compute right derivative values as we go using chain rule

Implementation approaches

Two main methods:

Operator overloading

- requires operator overloading in programming language
- syntax (more or less) like before (non-AD)
- efficiency can vary a lot, depends on usage scenario
- easy to implement and experiment with
- Examples: opm-autodiff, Sacado (Trilinos), ADOL-C

Source transformation with AD tool

- can be implemented for almost any language
- may restrict language syntax or features used
- efficiency can be high (depends on AD tool)
- Examples: TAPENADE, OpenAD

Types of AD

Two different approaches.
(We compute $f(x)$, u is some intermediate variable.)

Forward Mode

Carry derivatives with respect to independent variables:

$$(u, \frac{du}{dx})$$

Reverse Mode

Carry derivatives with respect to dependent variables (adjoints):

$$(u, \frac{df}{du})$$

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Forward AD example (1)

Example function: $f(x) = x(sin(x^2) + 3x)$.
Sequence of elementary functions:

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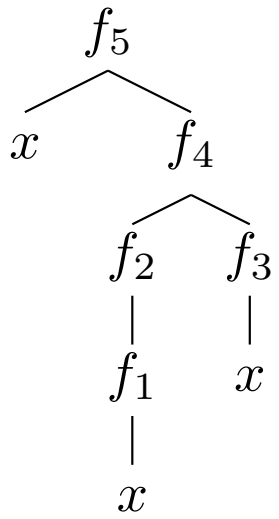
Rewritten:
$f(x) = f_5(x, f_4(f_2(f_1(x)), f_3(x)))$



Forward AD example (2)

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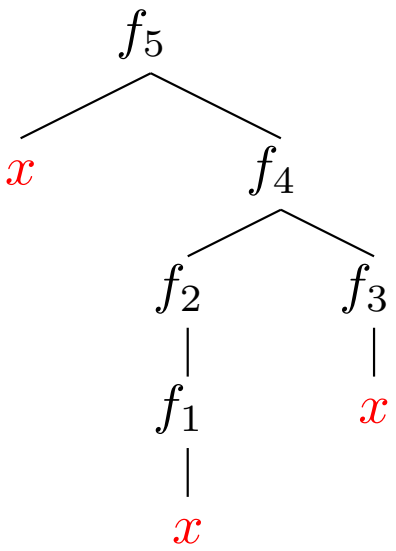

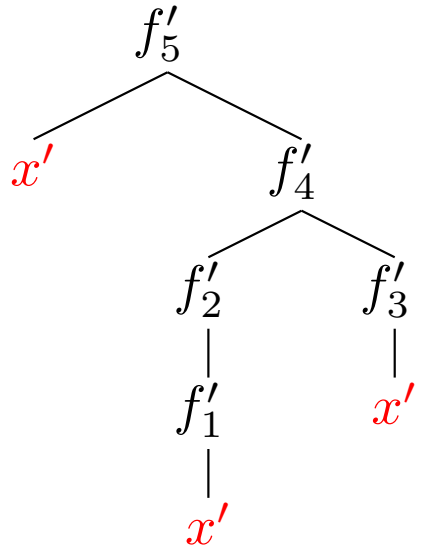

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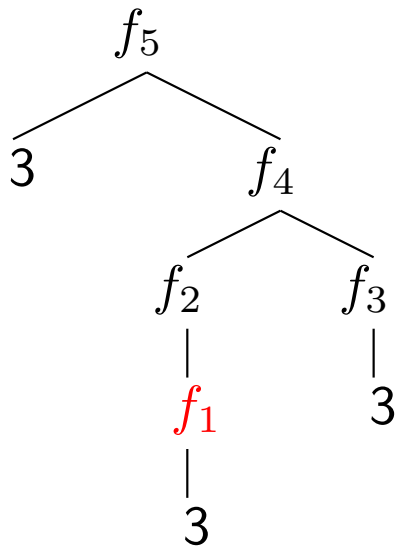

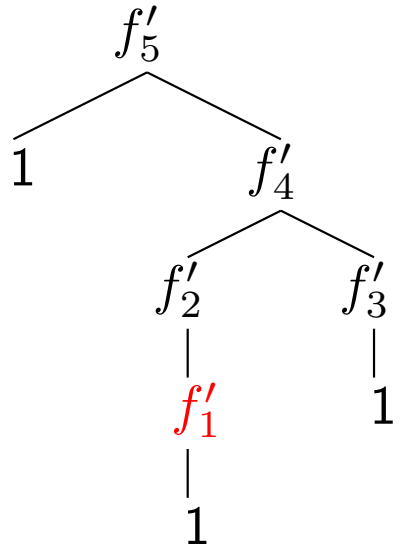

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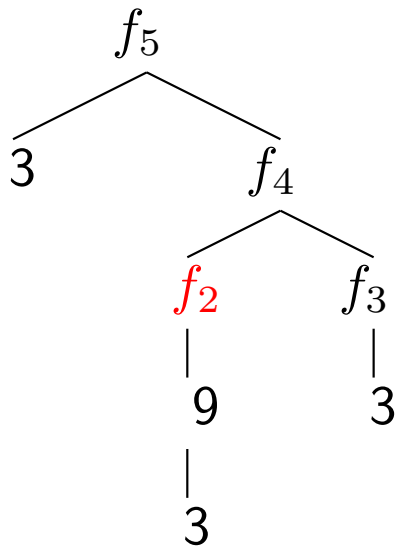

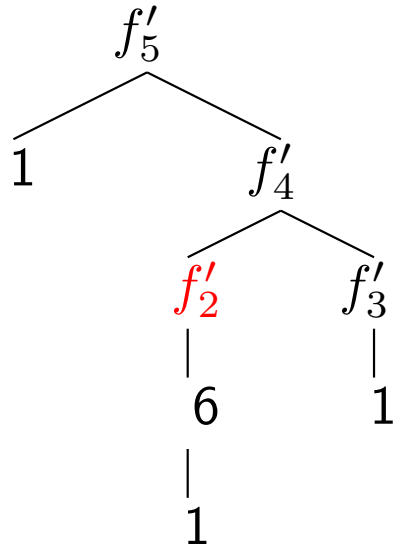

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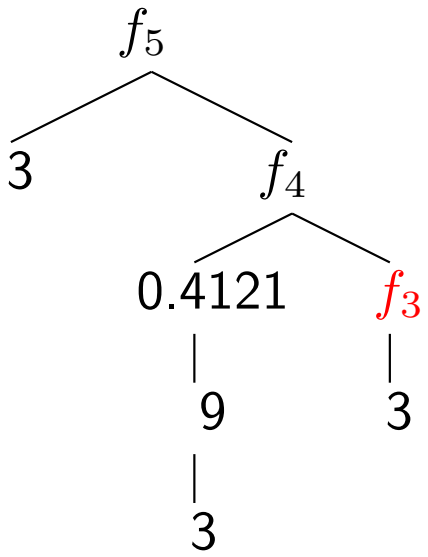

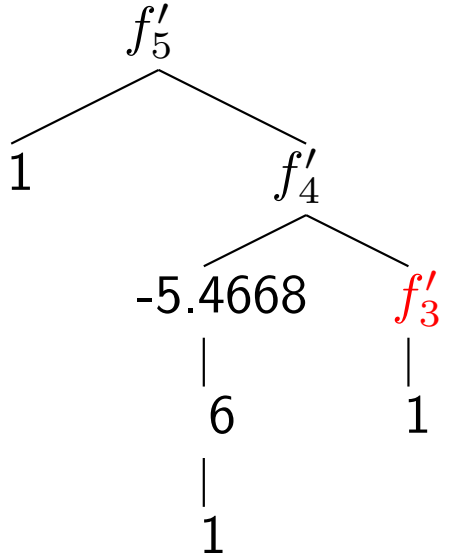

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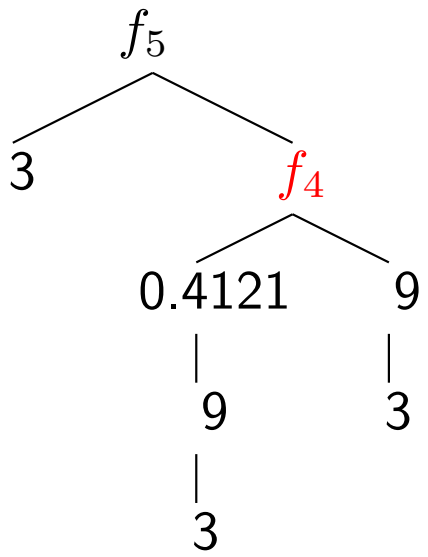

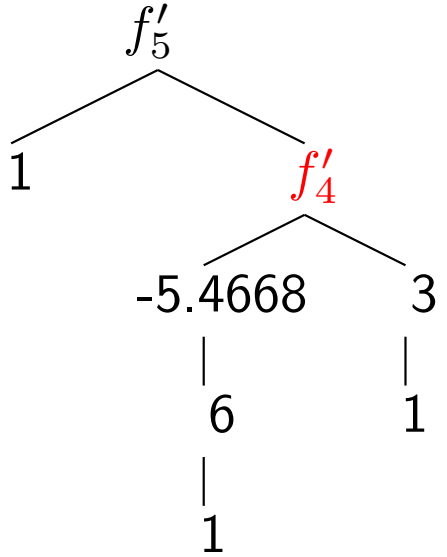

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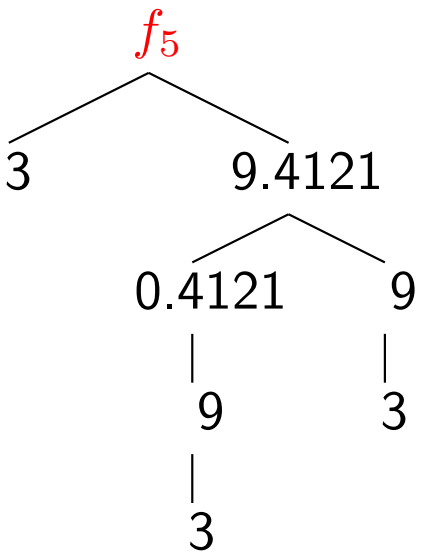

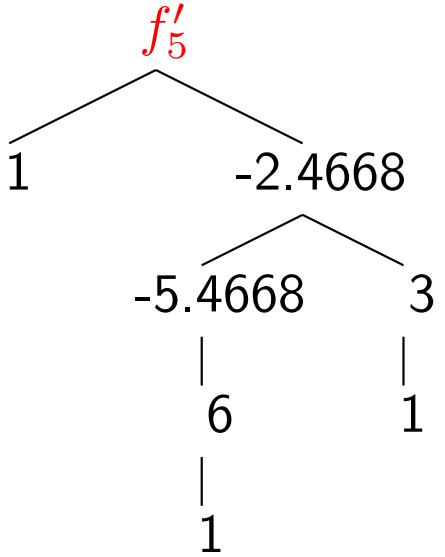

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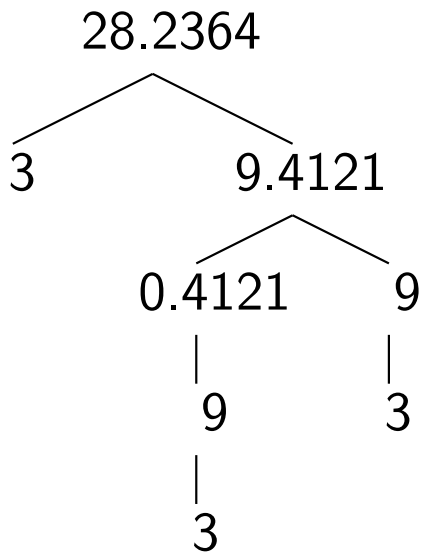

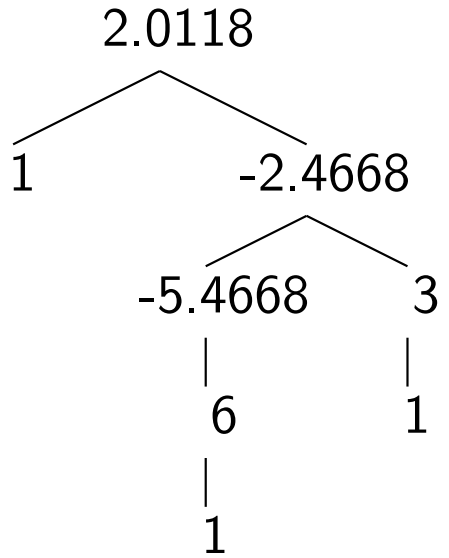

Properties of forward AD

- Easy to implement with operator overloading
- Storage required (scalar): $2\times$ normal (value, derivative).
- Storage required ($f : R^m \to R^n$): $(n+1)\times$ normal (value, derivative vector), unless sparse.

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OPM implementation

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Recall: Reverse Mode

Carry derivatives with respect to dependent variables (adjoints):

$$(u, \frac{df}{du})$$

We will use the chain rule again, but in the opposite direction:

$$\mathrm{adj}(u) = \mathrm{adj}(f_i)\frac{\partial f_i}{\partial u}.$$

Using $\mathrm{adj}(u)$ to mean the adjoint $\frac{df}{du}$.
(So $\mathrm{adj}(x)$ is our goal.)

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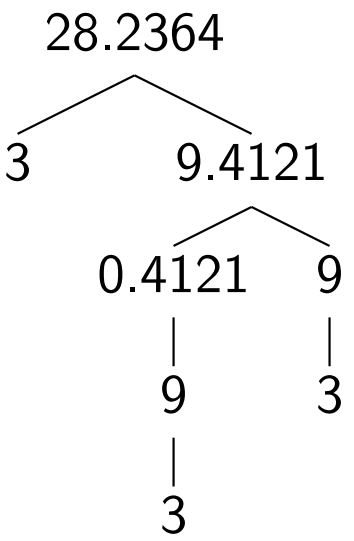

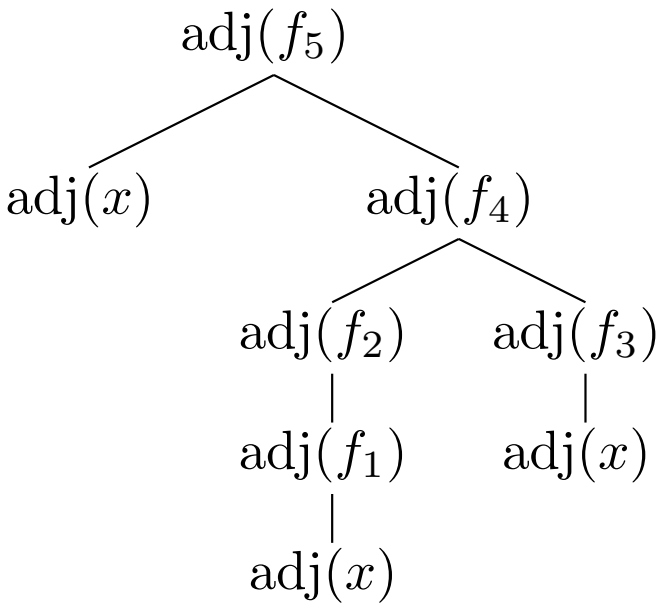

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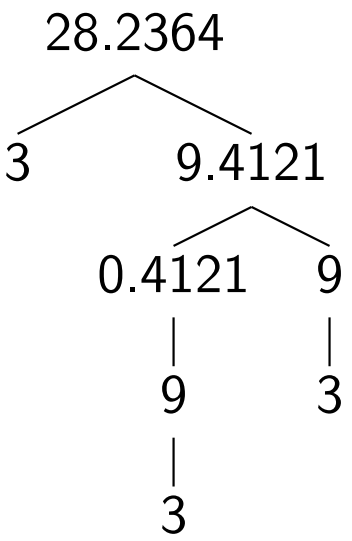

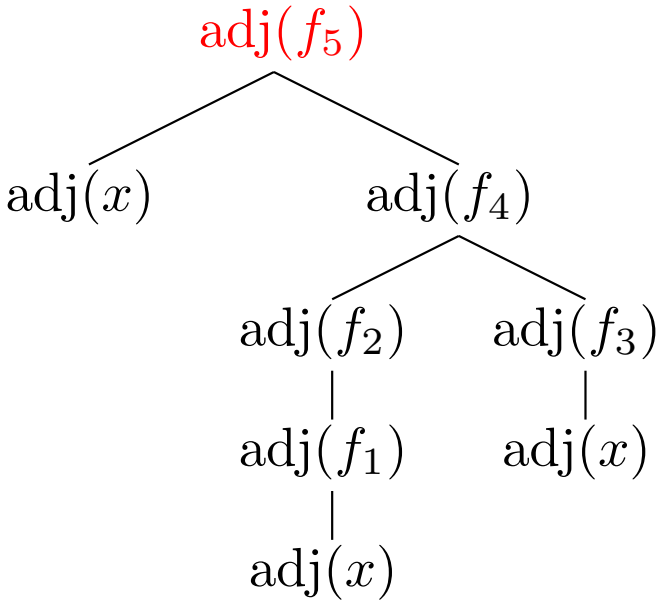

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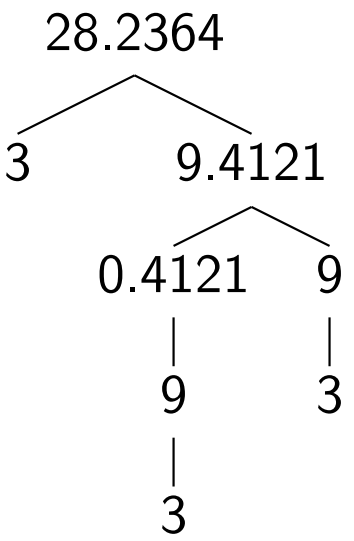

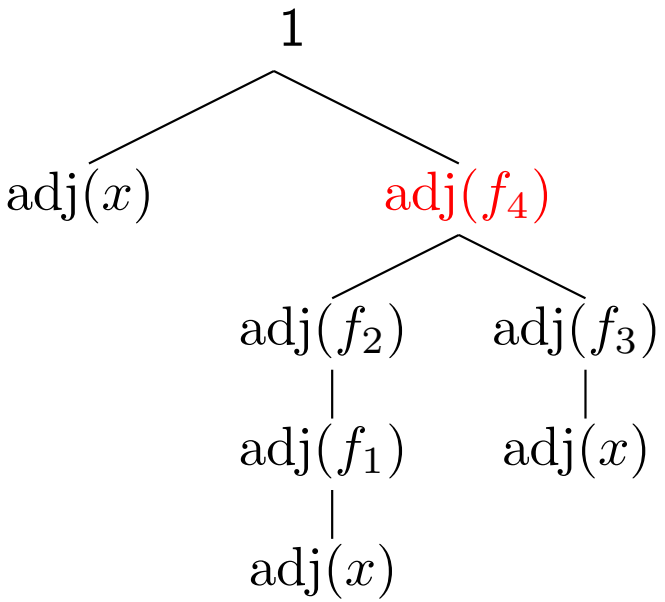

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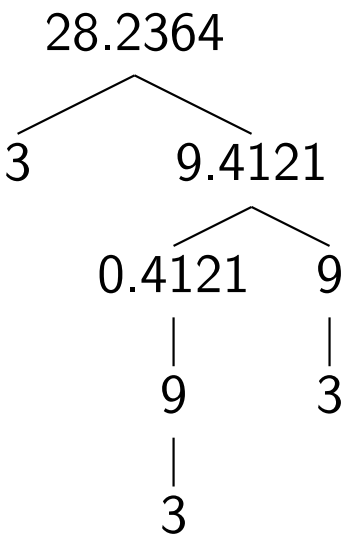

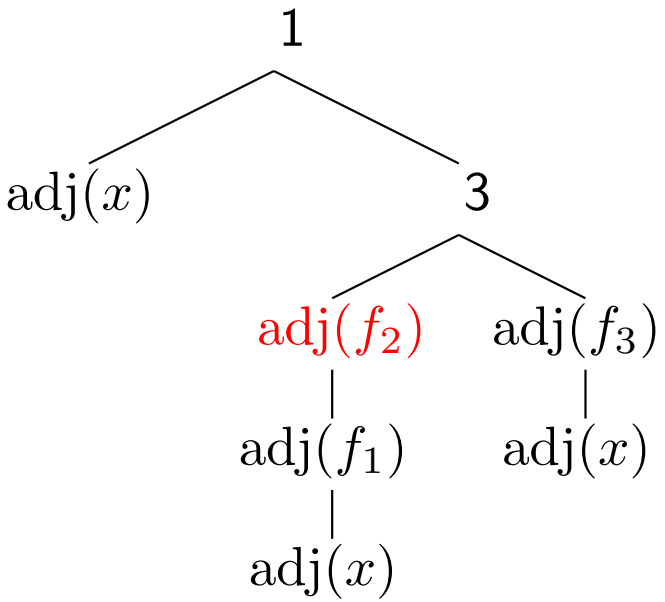

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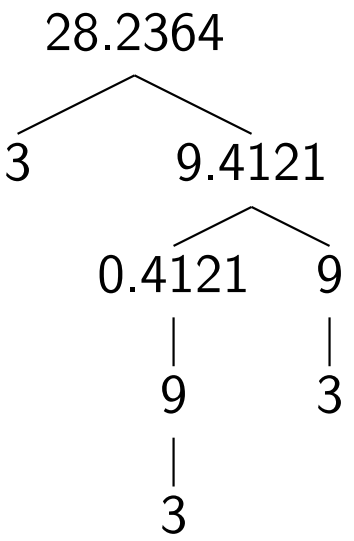

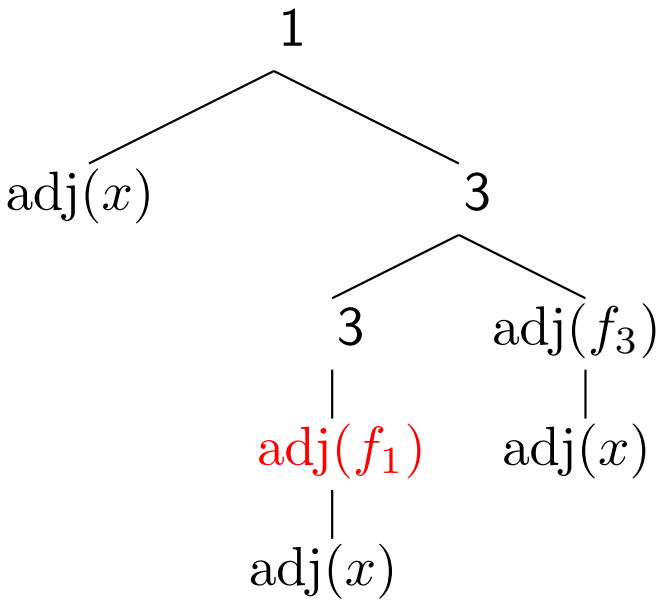

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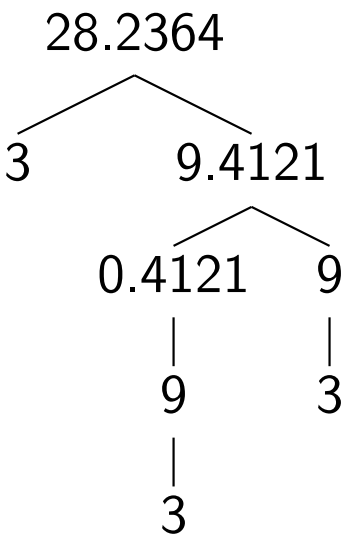

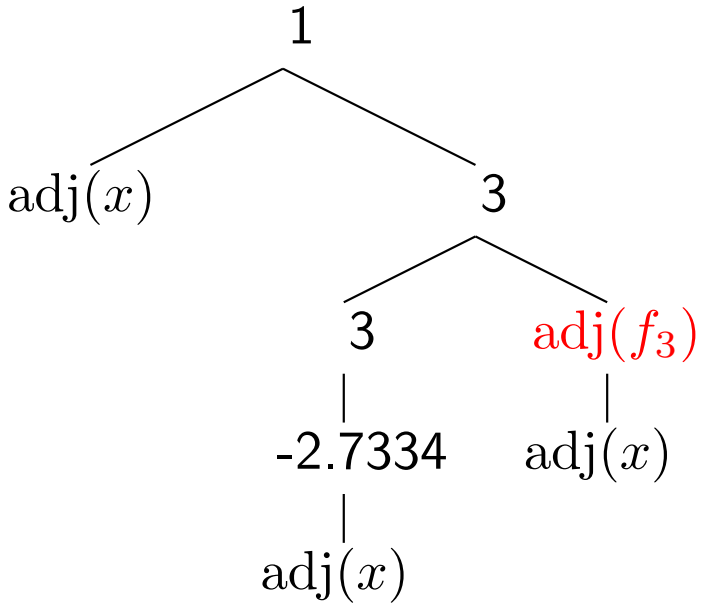

Reverse AD example

Example function: $f(x) = x(sin(x^2) + 3x)$. Computing $f(3), f'(3)$.
Sequence of elementary functions:

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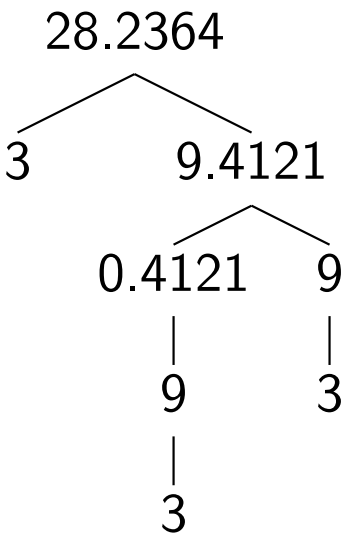
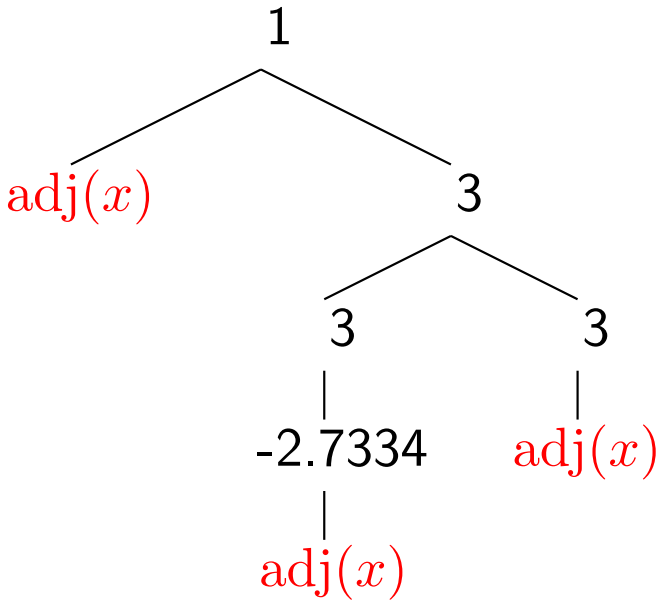
\begin{aligned}
f_1(u) &= u^2 & \mathrm{adj}(u) &= \mathrm{adj}(f_1) \cdot 2u \\
f_2(u) &= \sin(u) & \mathrm{adj}(u) &= \mathrm{adj}(f_2) \cdot \cos(u) \\
f_3(u) &= 3u & \mathrm{adj}(u) &= \mathrm{adj}(f_3) \cdot 3 \\
f_4(u,v) &= u + v & \mathrm{adj}(u) &= \mathrm{adj}(f_4), & \mathrm{adj}(v) &= \mathrm{adj}(f_4) \\
f_5(u,v) &= u \cdot v & \mathrm{adj}(u) &= \mathrm{adj}(f_5) \cdot v, & \mathrm{adj}(v) &= \mathrm{adj}(f_5) \cdot u
\end{aligned}
$$





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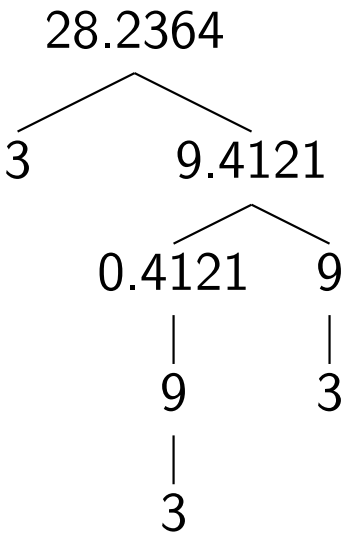

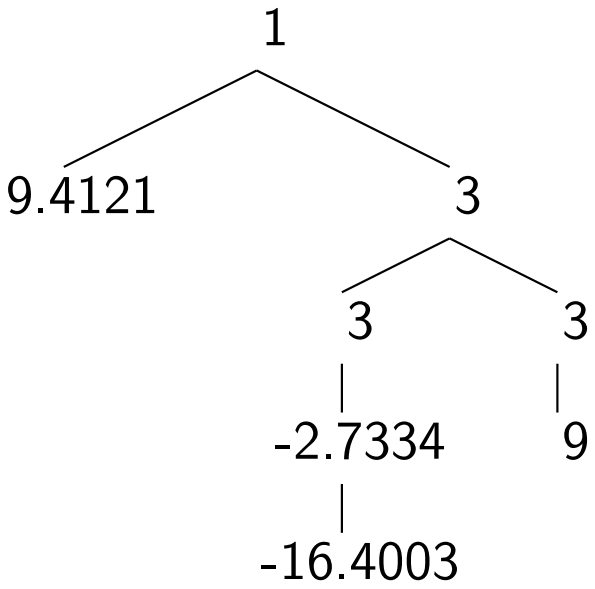

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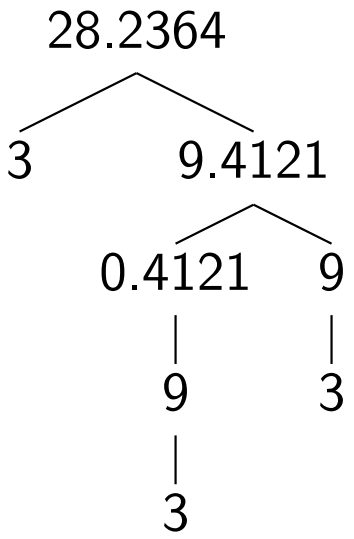

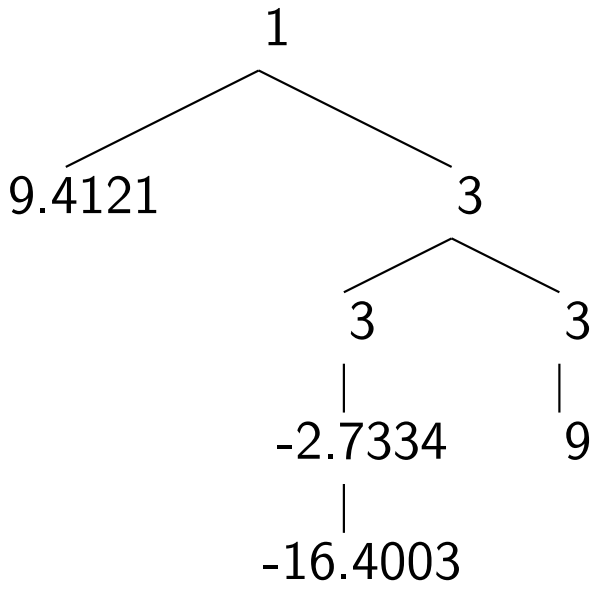

Must sum contributions:
$f'(3) = 9.4121 - 16.4003 + 9 = 2.0118.$

Overview of talk

Why automatic differentiation?

Forward Mode AD

Reverse Mode AD

OPM implementation

What next?

Automatic Differentiation: OPM implementation

AutoDiffBlock

- class implementing *forward AD* in OPM
- deals with *vectors of data* at a time
- derivatives are *sparse matrices*
- implemented with operator overloading
- based on Eigen library for basic types and operands
- helper library provides discrete operators

Automatic Differentiation: library example

```
/// Elementwise operator *
AutoDiffBlock operator*(const AutoDiffBlock& rhs) const
{
    ... // Omitted some code dealing with constants
    int num_blocks = numBlocks();
    std::vector<M> jac(num_blocks);
    assert(numBlocks() == rhs.numBlocks());
    typedef Eigen::DiagonalMatrix<Scalar, Eigen::Dynamic> D;
    D D1 = val_.matrix().asDiagonal();
    D D2 = rhs.val_.matrix().asDiagonal();
    for (int block = 0; block < num_blocks; ++block) {
        assert(jac_[block].rows() == rhs.jac_[block].rows());
        assert(jac_[block].cols() == rhs.jac_[block].cols());
        if( jac_[block].nonZeros() == 0 && rhs.jac_[block].nonZeros() == 0 ) {
            jac[block] = M( D2.rows(), jac_[block].cols() );
        }
        else if( jac_[block].nonZeros() == 0 )
            jac[block] = D1*rhs.jac_[block];
        else if ( rhs.jac_[block].nonZeros() == 0 ) {
            jac[block] = D2*jac_[block];
        }
        else {
            jac[block] = D2*jac_[block] + D1*rhs.jac_[block];
        }
    }
    return function(val_ * rhs.val_, std::move(jac));
}
```

Automatic Differentiation: usage example

Black-oil Mass Balance Equations (w/dissolved gas)

$$\begin{cases} \partial_t(\phi b_w s_w) + \operatorname{div}(b_w v_w) = q_w \\ \partial_t(\phi b_o s_o) + \operatorname{div}(b_o v_o) = q_o \\ \partial_t(\phi(b_g s_g + R_s b_o s_o)) + \operatorname{div}(b_g v_g + R_s b_o v_o) = q_g \end{cases}$$

Automatic Differentiation: usage example

Black-oil Mass Balance Equations (w/dissolved gas)

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OPM Implementation (almost: omit dissolved gas for space)

p_o, s_w, s_g, R_s and R_v can be primary variables (depending on state in each cell)

```
...
accum[phase] =   pv_mult * b[phase] * sat[phase]
               - pv_mult0 * b0[phase] * sat0[phase];
...
dp = ops_.ngrad * pressure[phase]
tdp = transmissibilities * dp;
UpwindSelector<double> upwind(grid_, ops_, tdp.value());
mflux[phase] = upwind.select(b[phase] * mob[phase]) * tdp;
...
material_balance[phase] =
    (pv/dt) * accum[phase] + ops_.div * mflux[phase];
```

Residuals in `material_balance.value()` and the associate Jacobians in `material_balance.derivative()`.

Overview of talk

Why automatic differentiation?

Forward Mode AD

Reverse Mode AD

OPM implementation

What next?

Current issues

- Assembly performance (setting up linear systems) is worse than competition.
- Vectorized notation is great for some, perhaps not for all?

Outlook and questions

- Investigate using backward mode (some or all parts).
- Is it possible to avoid vectorization penalty (few math ops per memory access)?
- Can we gain by using expression templates?
- Look at using other implementations? ADETL?
- Alternative techniques?

Thank you for listening!