autodiff

automatic differentiation in C++ couldn't be simpler

Forward Mode (using dual)

First-Order Derivatives

```
dual x, y, z;
dual u = f(x, y, z);
```

```
double ux = derivative(f, wrt(x), at(x, y, z));
double uy = derivative(f, wrt(y), at(x, y, z));
double uz = derivative(f, wrt(z), at(x, y, z));
```

Higher-Order Cross Derivatives

```
dual3rd x, y;
dual3rd u = f(x, y);
auto [u0, ux, uxy, uxyx] =
    derivatives(f, wrt(x, y, x), at(x, y));
```

Forward Mode (using real)

First-Order Derivatives

```
real x, y, z;
real u = f(x, y, z);
double ux = derivative(f, wrt(x), at(x, y, z));
double uy = derivative(f, wrt(y), at(x, y, z));
double uz = derivative(f, wrt(z), at(x, y, z));
```

Higher-Order Directional Derivatives

```
real4th x, y, z;
real4th u = f(x, y, z);
double nx, ny, nz;      // direction n = (nx, ny, nz)
auto [un0, un1, un2, un3, un4] =
    derivatives(f, along(nx, ny, nz), at(x, y, z));
```

Reverse Mode (using var)

First-Order Derivatives

```
var x, y, z;
var u = f(x, y, z);
auto [ux, uy, uz] = derivatives(u, wrt(x, y, z));
```

Higher-Order Cross Derivatives

```
var x, y, z;
var u = f(x, y, z);
auto [ux, uy, uz] = derivativesx(u, wrt(x, y, z));
auto [uxx, uxy, uxz] = derivativesx(ux, wrt(x, y, z));
auto [uxx, uxy, uxz] = derivativesx(ux, wrt(x, y, z));
auto [uyx, uyy, uyz] = derivativesx(uy, wrt(x, y, z));
auto [uzx, uzy, uzz] = derivativesx(uz, wrt(x, y, z));
```

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autodiff

autodiff is a C++17 library that uses modern and advanced programming techniques to enable automatic computation of derivatives in an efficient, easy, and intuitive way.

Demonstration

Consider the following function *f(x, y, z)*:

```
double f(double x, double y, double z)
{
    return (x + y + z) * exp(x * y * z);
}
```

which we use use to evaluate the variable *u = f(x, y, z)*:

```
double x = 1.0;
double y = 2.0;
double z = 3.0;
double u = f(x, y, z);
```

How can we minimally transform this code so that not only *u*, but also its derivatives *∂u/∂x*, *∂u/∂y*, and *∂u/∂z*, can be computed?

The next two sections present how this can be achieved using two automatic differentiation algorithms implemented in autodiff: **forward mode** and **reverse mode**.

Forward mode

In a *forward mode automatic differentiation* algorithm, both output variables and one or more of their derivatives are computed together. For example, the function evaluation *f(x, y, z)* can be transformed in a way that it will not only produce the value of *u*, *the output variable*, but also one or more of its derivatives *(∂u/∂x, ∂u/∂y, ∂u/∂z)* with respect to the *input variables (x, y, z)*.

Enabling forward automatic differentiation for the calculation of derivatives using autodiff is relatively simple. For our previous function *f*, we only need to replace the floating-point type `double` with `autodiff::dual` for both input and output variables:

```
dual f(const dual& x, const dual& y, const dual& z)
{
    return (x + y + z) * exp(x * y * z);
}
```

We can now compute the derivatives *∂u/∂x*, *∂u/∂y*, and *∂u/∂z* as follows:

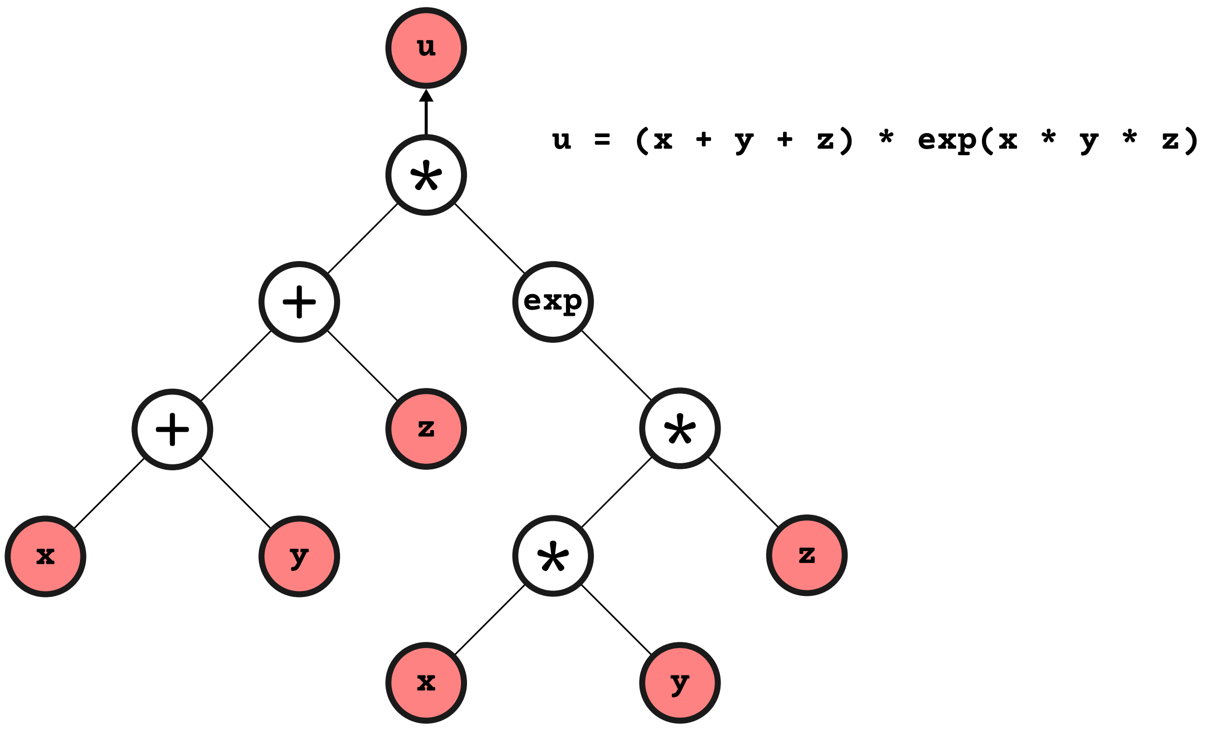
```
dual x = 1.0;
dual y = 2.0;
dual z = 3.0;
dual u = f(x, y, z);

double ux = derivative(f, wrt(x), at(x, y, z));
double uy = derivative(f, wrt(y), at(x, y, z));
double uz = derivative(f, wrt(z), at(x, y, z));
```

The auxiliary function `autodiff::wrt`, an acronym for **with respect to**, is used to indicate which input variable *(x, y, z)* is the selected one to compute the partial derivative of *f*. The auxiliary function `autodiff::at` is used to indicate where (at which values of its parameters) the derivative of *f* is evaluated.

Reverse mode

In a *reverse mode automatic differentiation* algorithm, the output variable of a function is evaluated first. During this function evaluation, all mathematical operations between the input variables are *"recorded"* in an *expression tree*. By traversing this tree from top-level (output variable as the root node) to bottom-level (input variables as the leaf nodes), it is possible to compute the contribution of each branch on the derivatives of the output variable with respect to input variables.



Thus, a single pass in a reverse mode calculation **computes all derivatives**, in contrast with forward mode, which requires one pass for each input variable. Note, however, that it is possible to change the behavior of a forward pass so that many (perhaps even all) derivatives of an output variable are computed simultaneously (e.g., in a single forward pass, *∂u/∂x*, *∂u/∂y*, and *∂u/∂z* are evaluated together with *u*, in contrast with three forward passes, each one computing the individual derivatives).

Similar as before, we can use autodiff to enable reverse automatic differentiation for our function *f* by simply replacing type `double` with `autodiff::var` as follows:

```
var f(var x, var y, var z)
{
    return (x + y + z) * exp(x * y * z);
}
```

The code below demonstrates how the derivatives *∂u/∂x*, *∂u/∂y*, and *∂u/∂z* can be calculated:

```
var x = 1.0;
var y = 2.0;
var z = 3.0;
var u = f(x, y, z);

auto [ux, uy, uz] = derivatives(u, wrt(x, y, z));
```

The function `autodiff::derivatives` will traverse the expression tree stored in variable `u` and compute all its derivatives with respect to the input variables *(x, y, z)*.

Questions?

Contact us on our GitHub Discussion Channel if you need support and assistance when using autodiff. If you would like to report a bug, then please create a new GitHub Issue.