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 [uyx, uyy, uyz] = derivativesx(uy, wrt(x, y, z));
auto [uzx, uzy, uzz] = derivativesx(uz, wrt(x, y, z));
```


Overview

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.

We welcome you to use **autodiff** and recommend us any improvements you think it is necessary. You may want to do so by chatting with us on our Gitter Community Channel and/or by making proposals by creating a GitHub issue.

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:

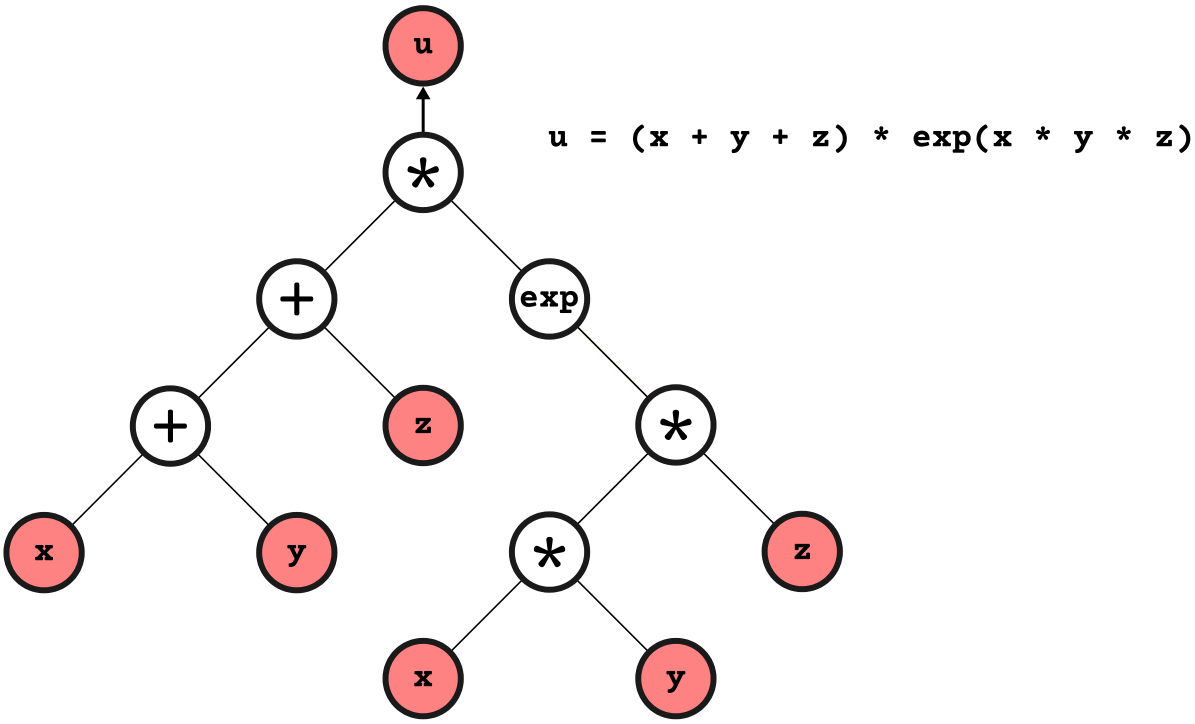
```
dual x = 1.0;
dual y = 2.0;
dual z = 3.0;
dual u = f(x, y, z);

double dudx = derivative(f, wrt(x), at(x, y, z));
double dudy = derivative(f, wrt(y), at(x, y, z));
double dudz = 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, $\partial u/\partial x$, $\partial u/\partial y$, and $\partial u/\partial z$ 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);

Derivatives dud = derivatives(u);

double dudx = dud(x);
double dudy = dud(y);
double dudz = dud(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)*, which are then stored in the object `dud`. The derivative of `u` with respect to input variable `x` (i.e., *∂u/∂x*) can then be extracted from `dud` using `dud(x)`. The operations `dud(x)`, `dud(y)`, `dud(z)` involve no computations! Just extraction of derivatives previously computed with a call to function `autodiff::derivatives`.

Development status

autodiff is planned to be a long-term maintained automatic differentiation C++ project. This means that more algorithms and number types will still be implemented and that the currently existing ones will be further enhanced. Please have in mind, however, that **autodiff** is still in a relatively early stage of development, which implies that minor breaking changes in API may be introduced to simplify its use and make it more intuitive and consistent with new library additions.

Documentation

Check the documentation website for more details:

autodiff.github.io

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