

The background of the slide features a complex, abstract pattern of thin, black, overlapping lines that form various geometric shapes and polygons, creating a sense of depth and movement. The lines are scattered across the entire page, with a higher density in the upper-left quadrant.

IMPROVING AUTOMATIC DIFFERENTIATION OF OBJECT-ORIENTED PARADIGMS USING CLAD

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WHAT WE ACHIEVED

- Enhanced the clad object-oriented differentiable model by incorporating non-differentiable attributes.
- Introduced support for reference return types in clad's reverse mode.
- Upon facilitating the reference return type, we also activated operator overloading in both forward and reverse modes.
- Enabled user-defined derivative functions for operator overloads.

WHAT WE ACHIEVED

- <https://github.com/vgvassilev/clad/pull/568>
- <https://github.com/vgvassilev/clad/pull/605>
- <https://github.com/vgvassilev/clad/pull/601>(complete, waiting to be merged)
- <https://github.com/vgvassilev/clad/pull/619>(complete, will be rebased on PR601)

- NON-DIFFERENTIABLE ATTRIBUTES.

```
non_differentiable double product(double value) {  
    return x * y * value;  
}  
double mem_fn(double value) {  
    return product(value) * value;  
}
```

- `non_differentiable` is an attribute that marks specific fields or methods in a class, indicating they should not be differentiated.
- Here, the `product` method in the `SimpleFunctions` class has been tagged with this attribute, signifying that any differentiation tools or routines should bypass or ignore this method.

- NON-DIFFERENTIABLE ATTRIBUTES.

```
non_differentiable double product(double value) {  
    return x * y * value;  
}  
double mem_fn(double value) {  
    return product(value) * value;  
}
```

```
clad::ValueAndPushforward<double, double> mem_fn_pushforward(double value,  
    SimpleFunctions *_d_this, double _d_value) {  
    double _t0 = this->product(value);  
    return {_t0 * value, 0 * value + _t0 * _d_value};  
}
```

- NON-DIFFERENTIABLE ATTRIBUTES.

```
class non_differentiable SimpleFunctions2 {  
public:  
    SimpleFunctions2() noexcept : x(0), y(0) {}  
    SimpleFunctions2(double p_x, double p_y) noexcept : x(p_x), y(p_y) {}  
    double x;  
    double y;  
    double mem_fn(double i, double j) { return (x + y) * i + i * j * j; }  
    SimpleFunctions2 operator+(const SimpleFunctions2& other) const {  
        return SimpleFunctions2(x + other.x, y + other.y);  
    }  
};
```

- When applied to a class, it suggests that differentiation tools should bypass or ignore all of its fields and member functions.

- OPERATOR OVERLOADS

```
SimpleFunctions& operator+=(double value) {  
    x += value;  
    return *this;  
}
```

```
double fn2(SimpleFunctions& v, double value) {  
    v += value;  
    return v.x;  
}
```

```
auto fn2_grad = clad::gradient(fn2);
```

- The above example demonstrates the differentiation of operator overloads using clad.
- A crucial enhancement added is the support for operators with reference return types, such as the operator+= in the SimpleFunctions class.

- REFERENCE RETURN TYPE

```
SimpleFunctions& operator+=(double value) {  
    x += value;  
    return *this;  
}
```

```
clad::ValueAndAdjoint<SimpleFunctions &, SimpleFunctions &> operator_plus_equal_forw(double value,  
    clad::array_ref<SimpleFunctions> _d_this, clad::array_ref<SimpleFunctions> _d_value) {  
    this->x += value;  
    return {*this, (* _d_this)};  
}
```

- A crucial enhancement added is the support for operators with reference return types, such as the operator+= in the SimpleFunctions class.
- We introduce a “_forw” function for reference return type.

- REFERENCE RETURN TYPE

```
// derivative declarations
double _d_a = 0;
double& _d_a_ref = _d_a;

// forward pass
double& a_ref = a;
```

- In the above example, we can easily point `_d_a_ref` to `_d_a` because the derivative of `a` is known at compile time. This is not always the case, for example, consider the following code.

```
double& someFn(double& i, double& j, double& k) { ... }

double fn(double i, double j, double k) {
| double& ref = someFn(i, j, k);
}
}
```

- REFERENCE RETURN TYPE

```
double& someFn(double& i, double&j, double& k) { ... }  
  
double fn(double i, double j, double k) {  
    double& ref = someFn(i, j, k);  
}
```

- We cannot determine which variable `ref` is referencing at compile time. Thus, we also cannot determine which derivative should `_d_ref` refer to.
- That's why we need “`_forw`” function.

- REFERENCE RETURN TYPE

```
double& someFn(double& i, double& j) {  
    double& k = i;  
    double& l = j;  
    if (...)  
        return k;  
    else  
        return l;  
}
```

```
// derivative declarations  
double* _d_ref = nullptr;  
  
// forward pass  
double t0 = i;  
double t1 = j;  
clad::ValueAndAdjoint<double&, double&> t = someFn_forw(i, j, &_d_i, &_d_j);  
_d_ref = &t.adjoint;  
double& ref = t.value;  
  
// reverse pass  
someFn_pullback(t0, t1, /*pullback=*/double(), &_d_i, &_d_j);  
...
```

- REFERENCE RETURN TYPE

```
double& someFn(double& i, double& j) {  
    double& k = i;  
    double& l = j;  
    if (...)  
        return k;  
    else  
        return l;  
}
```

- The corresponding someFn_forw will be:

```
clad::ValueAndAdjoint<double&, double&  
someFn_forw(double& i, double& j, clad::array_ref<double> _d_i,  
            clad::array_ref<double> _d_j) {  
    double* _d_k = nullptr;  
    double* _d_l = nullptr;  
  
    // forward pass  
    _d_k = &* _d_i;  
    double& k = i;  
  
    _d_l = &* _d_j;  
    double& l = j;  
  
    if (...)  
        return {k, *_d_k};  
    else  
        return {l, *_d_l};  
}
```

- CUSTOM DERIVATIVES FOR SPECIAL MEMBER FUNCTIONS

```
namespace clad {  
  namespace custom_derivatives {  
    namespace class_functions {
```

```
void operator_plus_equal_pullback(SimpleFunctions* v, double value,  
  SimpleFunctions _d_y, SimpleFunctions* _d_v, double* _d_value) {  
  v->x += value;  
  goto _label0;  
_label0:  
  ;  
  {  
    double _r_d0 = (* _d_v).x;  
    (* _d_v).x += _r_d0;  
    * _d_v += _r_d0;  
    (* _d_v).x -= _r_d0;  
  }  
}
```

- The code showcases user-defined derivatives for operator overloads, allowing for custom differentiation behavior.
- By employing the `clad::custom_derivatives` namespace, users can specify custom derivatives for operators like `operator+=`, tailoring differentiation to specific class implementations.

MISSING SUPPORT FOR CPP FEATURE

- Support try-catch blocks to enable some std namespace functions differentiation.
- Support switch statements in the reverse mode.
- Support special member functions like constructors in both the forward and the reverse mode.
- Support custom derivatives for special member functions.



THANK YOU!