Automatic Differentiation in C++

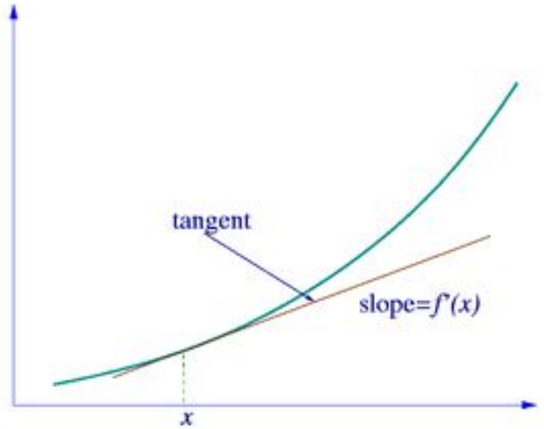
Vassil Vassilev (Princeton U)<v.g.vassilev@gmail.com>; Marco Foco (NVIDIA) <mfoco@nvidia.com>

Function Derivatives

Many nonlinear optimization techniques exploit gradient and curvature information about the target and constraint functions being calculated.

Derivatives also play a key role in sensitivity analysis (model validation), inverse problems (data assimilation) and simulation (design parameter choice).

The derivative of a function of a single variable at a chosen input value, when it exists, is the slope of the tangent line to the graph of the function at that point.



[Wikipedia, The tangent line at (x, f(x))]

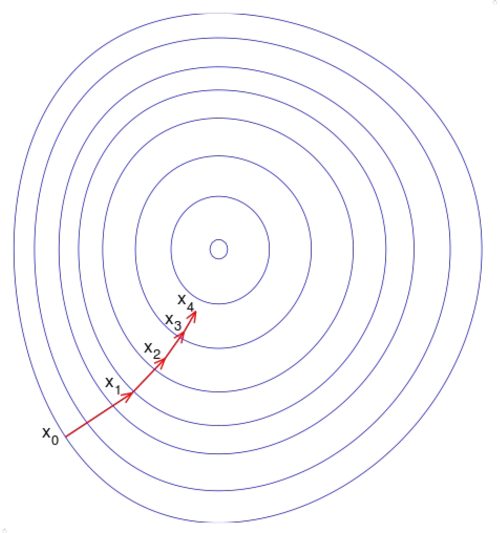
Gradient-based optimization

Gradient descent:

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$$

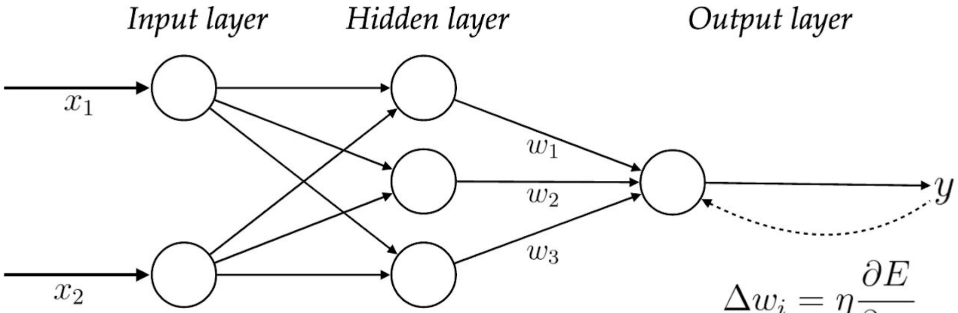
Applications:

- Function minimization
- Backpropagation for machine learning
- Fitting models to data



[Wikipedia, Gradient descent]

Backpropagation in ML



$$y = \phi\left(\sum_i w_i x_i\right)$$

$$E = \frac{1}{2}(t-y)^2$$

$$\Delta w_i = \eta \frac{\partial E}{\partial w_i}$$

Training pattern is fed, forward generating corresponding output

Error at output, the error between observed and desired state. Computed from the output *y* and seen desired output *t*.

The error propagates back, through updates of the subtracted gradient ratio from the weights.

x_i, w_i, ϕ, η *are inputs, input weights, activation function and learning rate of the neuron*

Computing Derivatives

Numerical Differentiation

- Precision loss, Rounding error problems
- Higher order and partial derivatives problems

$$f'(x) \approx \frac{f(x+h)-f(x)}{h}$$

Symbolic Differentiation

- Slow, Requires conversion of the program to a single expression, Requires closed-form expressions limiting algorithmic control flow and expressivity
- Higher order and partial derivatives problems

Algorithmic Differentiation

- Fixes all of the issues above at the cost of introducing extra software dependencies

Algorithmic/Automatic differentiation [1/2]

- Creates a function that computes the derivative(s) for you by program by replacing the domain of the variables to incorporate derivative values and redefining the semantics of the operators to propagate derivatives per the chain rule of differential calculus.
- Alternative to numerical differentiation

$$f'(x) \approx \frac{f(x+h)-f(x)}{h}$$

```
double f(double x) {
    return x * x;
}
```

```
double f_darg0(double x) {
  return 1*x + x*1;
}
```

Algorithmic/Automatic differentiation [2/2]

- *Benefits:* without additional precision loss
- *Benefits:* not limited to closed-form expressions
- *Benefits:* can take **derivatives of algorithms** (conditionals, loops, recursion)
    - Without inefficiently long expressions
- Implementations based on operator overloading/source transformation

Dual Numbers

- Forward Automatic Differentiation can be expressed in terms of Dual Numbers:
  - $a, b \in \mathcal{R}, \quad \varepsilon \notin \mathcal{R}, \ \varepsilon^2 = 0 \quad \Rightarrow \quad a + \varepsilon b$ is a dual number
- Properties ($a, b, c, d \in \mathcal{R}$:)

Interactions with $\mathcal{R}$	**Interactions between dual numbers**
$(a+\varepsilon b) + c = (a+c) + \varepsilon b$	$(a+\varepsilon b) + (c+\varepsilon d) = (a+c) + \varepsilon(b+d)$
$(a+\varepsilon b) * c = (ac) + \varepsilon(bc)$	$(a+\varepsilon b) * (c+\varepsilon d) = (ac) + \varepsilon(ad+bc) \cancel{+ \varepsilon^2 bd}$
	$(a+\varepsilon b)^2 = a^2 + \varepsilon(ab + ba) \cancel{+ \varepsilon^2 b^2} = a + 2\varepsilon(ab)$
	$(a+\varepsilon b)^n = a^n + \varepsilon(a\ldots ab + aba\ldots a + a\ldots ab) + \ldots = a^n + \varepsilon(na^{n-1}b)$

AD with Dual Numbers 1/2

f(x)	**f(z) = f(x+ε)**
a	a
x	$x + \varepsilon$
$x+a$	$(x + a) + \varepsilon$
ax	$ax + \varepsilon a$
x^n	$x^n + \varepsilon(nx^{n-1})$

AD with Dual Numbers 2/2

And finally...

$$
\begin{aligned}
f(z) &= \sum_{k=0}^{n} a_k z^k = a_0 + \sum_{k=1}^{n} a_k z^k \\
&= a_0 + \sum_{k=1}^{n} a_k (x+\varepsilon)^k \\
&= \left(a_0 + \sum_{k=1}^{n} a_k x^k\right) + \ \varepsilon \sum_{k=1}^{n} a_k k z^{k-1} \\
&= \sum_{k=0}^{n} a_k z^k + \ \varepsilon \sum_{k=0}^{n} a_{k+1}(k+1) z^k \\
&= f(x) + \ \varepsilon f'(x)
\end{aligned}
$$

AD with Dual Numbers - Code

```
auto f = [](auto x, auto y) { return x*x+y*x+y*y; };

auto dfdx = [&f](double x, double y) {
                return f(dual{x, 1.0}, y).eps();
};

auto dfdy = [&f](double x, double y) {
                return f(x, dual{y, 1.0}).eps();
};
```

Clad: Clang C/C++ AD plugin

Clad enables* ***automatic differentiation (AD) for C/C++****. It is based on the LLVM compiler infrastructure and is a plugin for Clang compiler.*

- Improve numerical stability and correctness
- Replace iterative algorithms computing gradients with a single function call (of a compiler-generated routine)
- Provide an alternative way of gradient computations

* https://github.com/vgvassilev/clad

Clad: Source Transformation

- Clad performs **automatic differentiation** on C++ functions
- For a C++ function, creates another C++ function that computes its derivative(s)

```
double f(double x) {
    return x * x * x;
}
```

Clad

```
double f_darg0(double x) {
  return 1 * x * x + x * 1 * x +
x * x * 1;
}
```

Clad: Implementation

```
double f(double x) {
    return x * x;
}
```

```
FunctionDecl f 'double (double)'
|-ParmVarDecl x 'double'
`-CompoundStmt
  `-ReturnStmt
    `-BinaryOperator 'double' '*'
      |-ImplicitCastExpr 'double' <LValueToRValue>
      | `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
      `-ImplicitCastExpr 'double' <LValueToRValue>
        `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
```

Clad

derivative AST

codegen

```
double f_darg0(double x) {
  return 1*x + x*1;
}
```

- Clad is a **Clang compiler plugin**
- Performs C++ **source code transformation**
- Operates on Clang AST (*Clang Abstract Syntax Tree*)
- AST transformation with `clang::StmtVisitor`

AD Transformation. Chain Rule

$$y = f(g(h(x))) = f(g(h(w_0))) = f(g(w_1)) = f(w_2) = w_3$$

$$\begin{aligned}
w_0 &= x \\
w_1 &= h(w_0) \\
w_2 &= g(w_1) \\
w_3 &= f(w_2) = y
\end{aligned}$$

$$\frac{dy}{dx} = \frac{dy}{dw_2}\frac{dw_2}{dw_1}\frac{dw_1}{dx}$$

The chain rule for differential calculus gives us nice visitation properties.

Forward mode `clad::differentiate`

- **Consider:** $f(x_1, x_2) = \sin(x_1) + x_1 x_2$

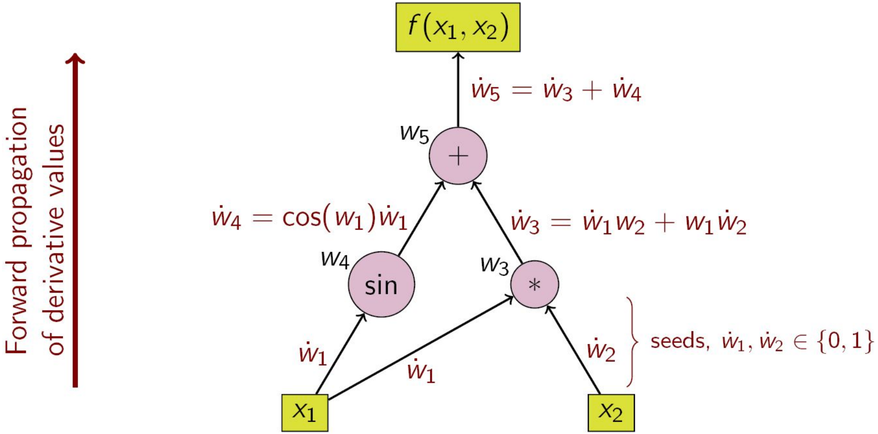
```
f(x1, x2) {
  x1 = x1
  x2 = x2
  a = x1 * x2
  b = sin(x1)
  return a + b;
}
```

```
f_dx1(x1, x2) {
  dx1 = 1
  dx2 = 0
  da = dx1*x2 + x1*dx2
  db = cos(x1) * dx1
  return da + db
}
```

```
f_dx2(x1, x2) {
  dx1 = 0
  dx2 = 1
  da = dx1*x2 + x1*dx2
  db = cos(x1) * dx1
  return da + db
}
```

Forward mode `clad::differentiate`

- **Forward mode AD** algorithm computes derivatives w.r.t. any **(single)** variable



$$f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

[Wikipedia, Automatic differentiation]

clad::differentiate

```
double f_cubed_add1(double a, double b) {
 return a * a * a + b * b * b;
}
```

clad::differentiate

```
double f_cubed_add1_darg0(double a, double b) {
    double _d_a = 1;
    double _d_b = 0;
    double _t0 = a * a;
    double _t1 = b * b;
    return (_d_a * a + a * _d_a) * a + _t0 * _d_a + (_d_b *
b + b * _d_b) * b + _t1 * _d_b;
}
```

Reverse mode

`clad::gradient`

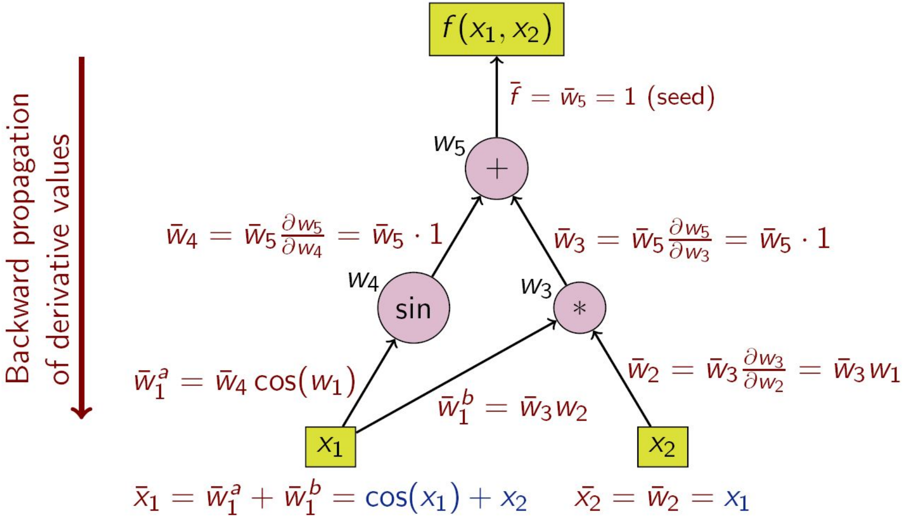
- **Consider:** $f(x_1, x_2) = \sin(x_1) + x_1 x_2$

```
f(x1, x2) {
  x1 = x1
  x2 = x2
  a = x1 * x2
  b = sin(x1)
  return a + b;
}
```

```
f_dx1(x1, x2) {
  gz = 1
  gb = gz
  ga = gz
  gx2 = x1 * ga
  gx1 = x2 * ga + cos(x1) * gb
}
```

Reverse mode `clad::gradient`

- **Reverse mode AD** computes gradients (w.r.t to **all** inputs at once)



$$f(x_1, x_2) = \sin(x_1) + x_1 x_2$$

[Wikipedia, Automatic differentiation]

clad::gradient

```
double f_cubed_add1(double a,
double b) {
 return a * a * a + b * b * b;
}
```


```
void f_cubed_add1_grad (double a, double b, double *_result)
{
    double  t0;
    double  t1;
    double  t2;
    double  t3;
    double  t4;
    double  t5;
    double  t6;
    double  t7;
     t2 = a;
     t1 = a;
     t3 =  t2 * _t1;
     t0 = a;
     t6 = b;
     t5 = b;
     t7 =  t6 * _t5;
     t4 = b;
    double f cubed_add1_return = _t3 * _t0 + _t7 * _t4;
    goto  label0;
   label0:
    {
        double  r0 = 1 *  t0;
        double  r1 =  r0 *  t1;
         result[0UL] +=  r1;
        double  r2 =  t2 *  r0;
         result[0UL] +=  r2;
        double  r3 =  t3 * 1;
         result[0UL] +=  r3;
        double  r4 = 1 *  t4;
        double  r5 =  r4 *  t5;
         result[1UL] +=  r5;
        double  r6 =  t6 *  r4;
         result[1UL] +=  r6;
        double  r7 =  t7 * 1;
        _result[1UL] += _r7;
    }
}
```

What can be differentiated

- Built-in C/C++ scalar types (e.g. double, float)
- Built-in C input arrays
- Functions that have an arbitrary number of inputs
- Functions that return a single value
- Loops
- Conditionals

Benchmarks: in High-Energy Physics Uses

```
TF1* h1 = new TF1("f1", "formula");
TFormula* f1 = h1->GetFormula();
f1->GenerateGradientPar(); // clad
```

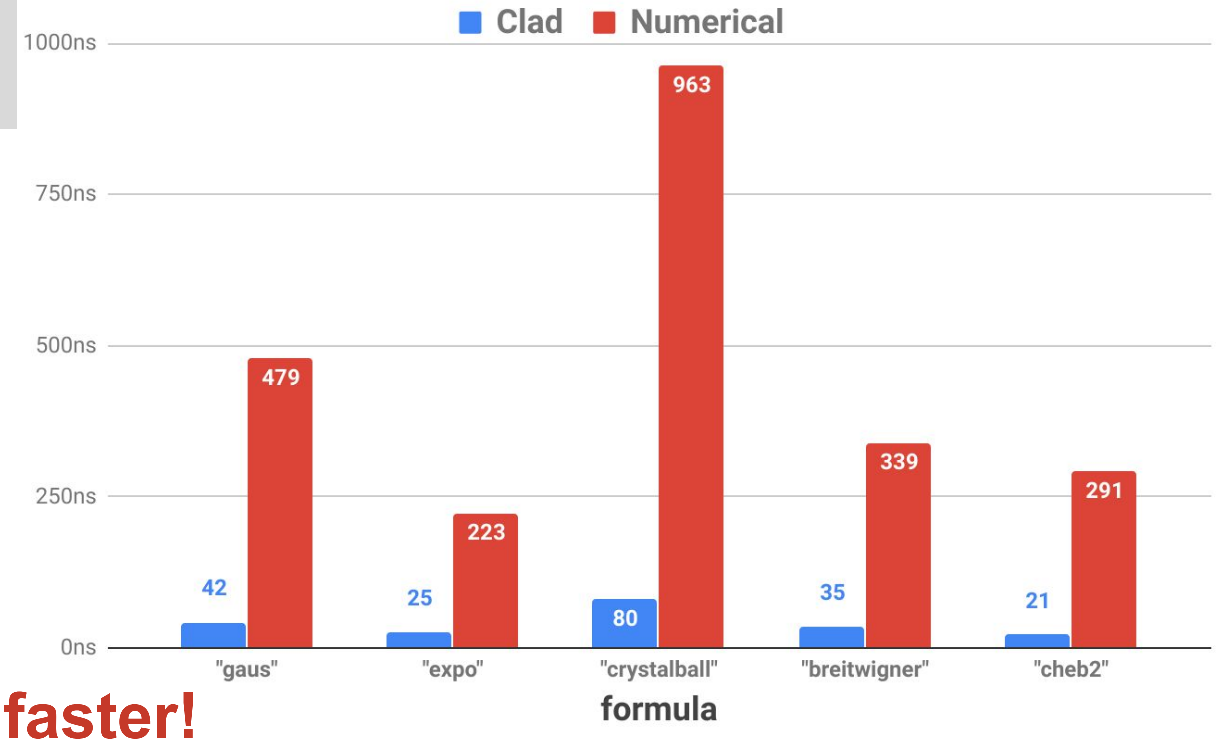
Clad:

```
f1->GradientPar(x, result);
```

Numerical:

```
h1->GradientPar(x, result);
```

- **gaus:** Npar = 3
- **expo:** Npar = 2
- **crystalball:** Npar = 5
- **breitwigner:** Npar = 5
- **cheb2:** Npar = 4



~10x faster!

Benchmarks

Tested function:

```
double sum(double* p, int dim) {
  double r = 0.0;
  for (int i = 0; i < dim; i++)
    r += p[i];
  return r;
}
```

Clad:

```
double* Clad(double* p, int dim) {
  auto result = new double[dim]{};
  auto sum_grad = clad::gradient(sum, "p");
  sum_grad.execute(p, dim, result);
  return result;
}
```

Example how to use clad

Numerical:

```
double* Numerical(double* p, int dim, double eps = 1e-8) {
  double result = new double[dim]{};
  for (int i = 0; i < dim; i++) {
    double pi = p[i];
    p[i] = pi + eps;
    double v1 = sum(p, dim);
    p[i] = pi - eps;
    double v2 = sum(p, dim);
    result[i] = (v1 - v2)/(2 * eps);
    p[i] = pi;
  }
  return result;
}
```

$$\frac{\partial f(x)}{\partial x_i} \approx \frac{f(x+h_i)-f(x-h_i)}{2h}$$

Benchmarks

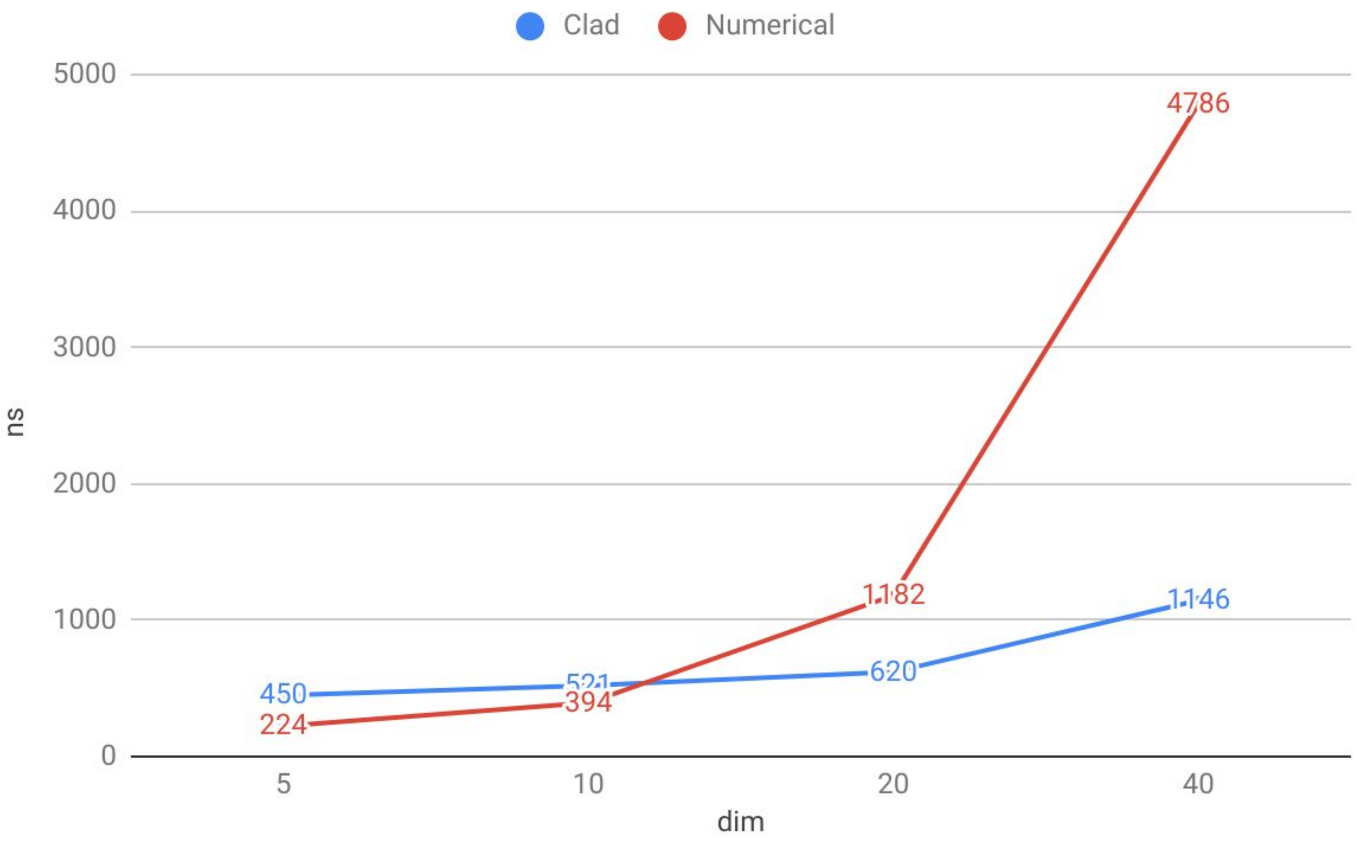
Original function:

```
double sum(double* p, int dim) {
  double r = 0.0;
  for (int i = 0; i < dim; i++)
    r += p[i];
  return r;
}
```

Clad's gradient:

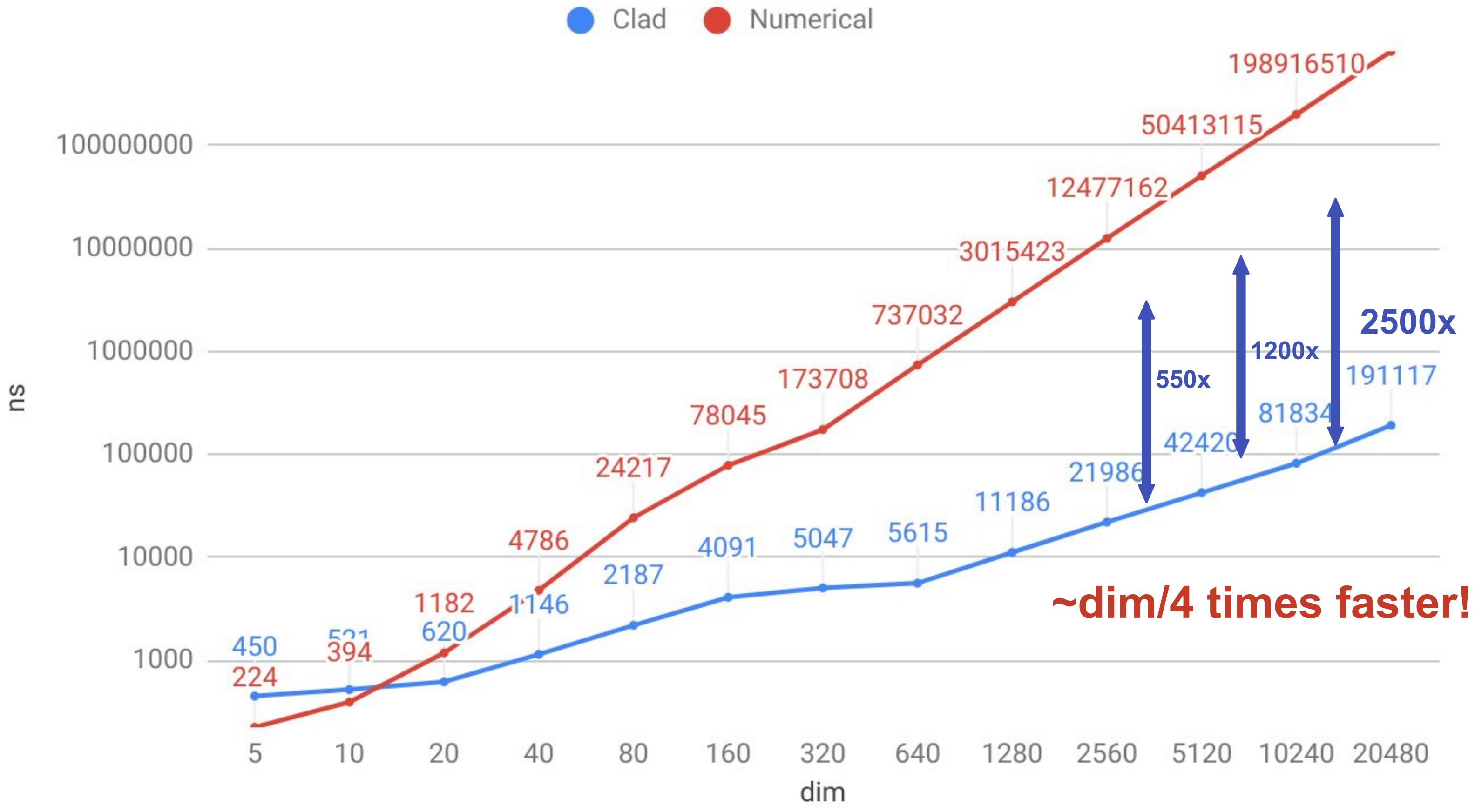
```
void sum_grad_0(double *p, int dim, double *_result) {
    double _d_r = 0;
    unsigned long _t0;
    int _d_i = 0;
    clad::tape<int> _t1 = {};
    double r = 0.;
    _t0 = 0;
    for (int i = 0; i < dim; i++) {
        _t0++;
        r += p[clad::push(_t1, i)];
    }
    double sum_return = r;
    _d_r += 1;
    for (; _t0; _t0--) {
        double _r_d0 = _d_r;
        _d_r += _r_d0;
        _result[clad::pop(_t1)] += _r_d0;
        _d_r -= _r_d0;
    }
}
```

Benchmarks



Clad
Numerical
5000
4000
3000
2000
1000
0
ns
4786
1182
1146
620
521
450
394
224
5
10
20
40
dim

Benchmarks



Clad
Numerical
198916510
50413115
12477162
3015423
737032
173708
78045
24217
4786
1182
394
224
450
521
620
1146
2187
4091
5047
5615
11186
21986
42420
81834
191117
550x
1200x
2500x
~dim/4 times faster!
100000000
10000000
1000000
100000
10000
1000
ns
5
10
20
40
80
160
320
640
1280
2560
5120
10240
20480
dim

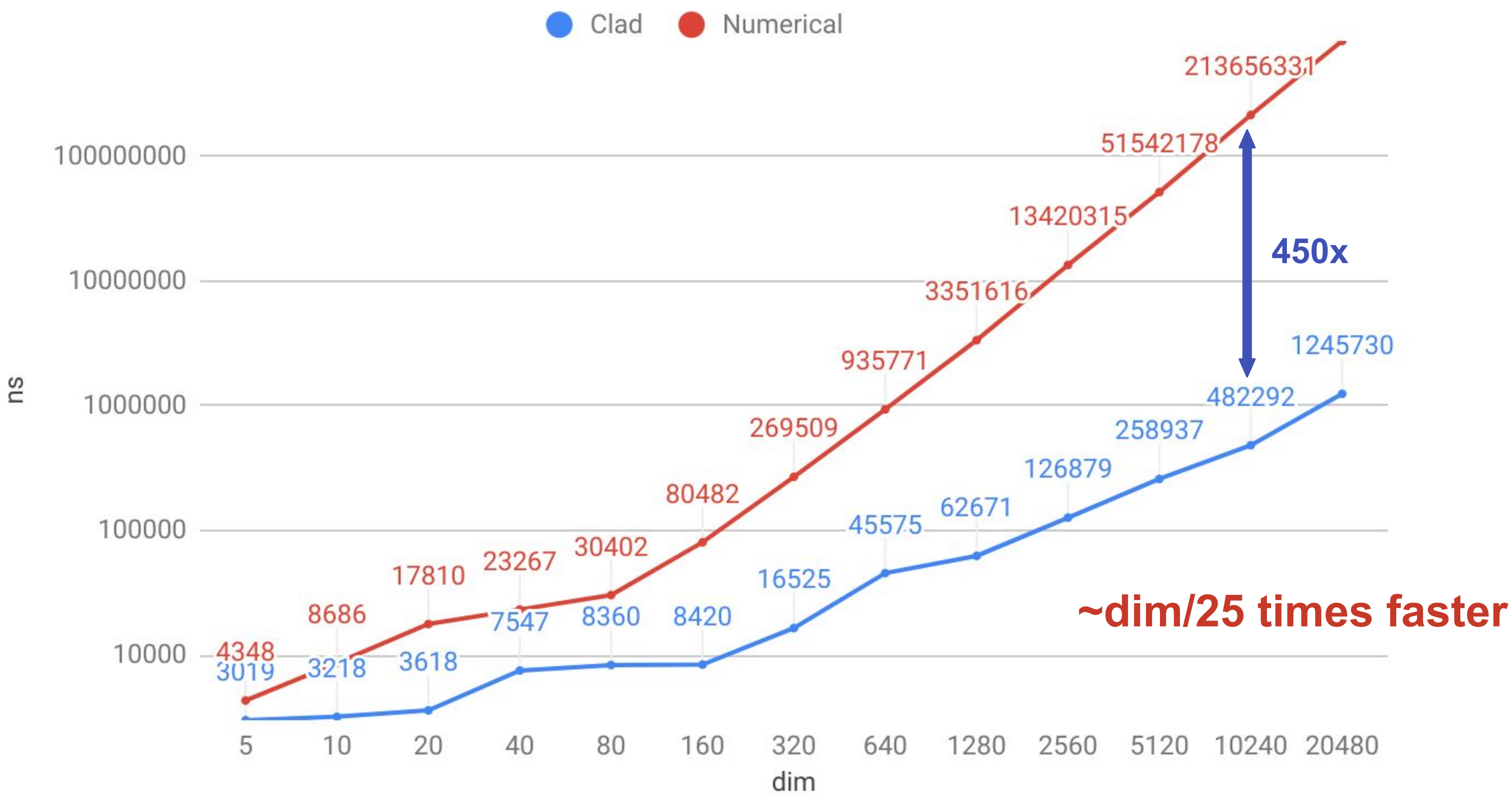
Benchmarks

Original function:

```
double gaus(double* x, double* p /*means*/, double sigma, int dim) {
  double t = 0;
  for (int i = 0; i < dim; i++)
    t += (x[i] - p[i])*(x[i] - p[i]);
  t = -t / (2*sigma*sigma);
  return std::pow(2*M_PI, -n/2.0) * std::pow(sigma, -0.5) * std::exp(t);
}
```

$$\frac{1}{\sqrt{(2\pi)^{dim}\sigma}} e^{-\frac{||x-p||_2^2}{2\sigma^2}}$$

Benchmarks



Clad
Numerical
ns
dim
100000000
10000000
1000000
100000
10000
5
10
20
40
80
160
320
640
1280
2560
5120
10240
20480
4348
8686
17810
23267
30402
80482
269509
935771
3351616
13420315
51542178
213656331
3019
3218
3618
7547
8360
8420
16525
45575
62671
126879
258937
482292
1245730
450x
~dim/25 times faster

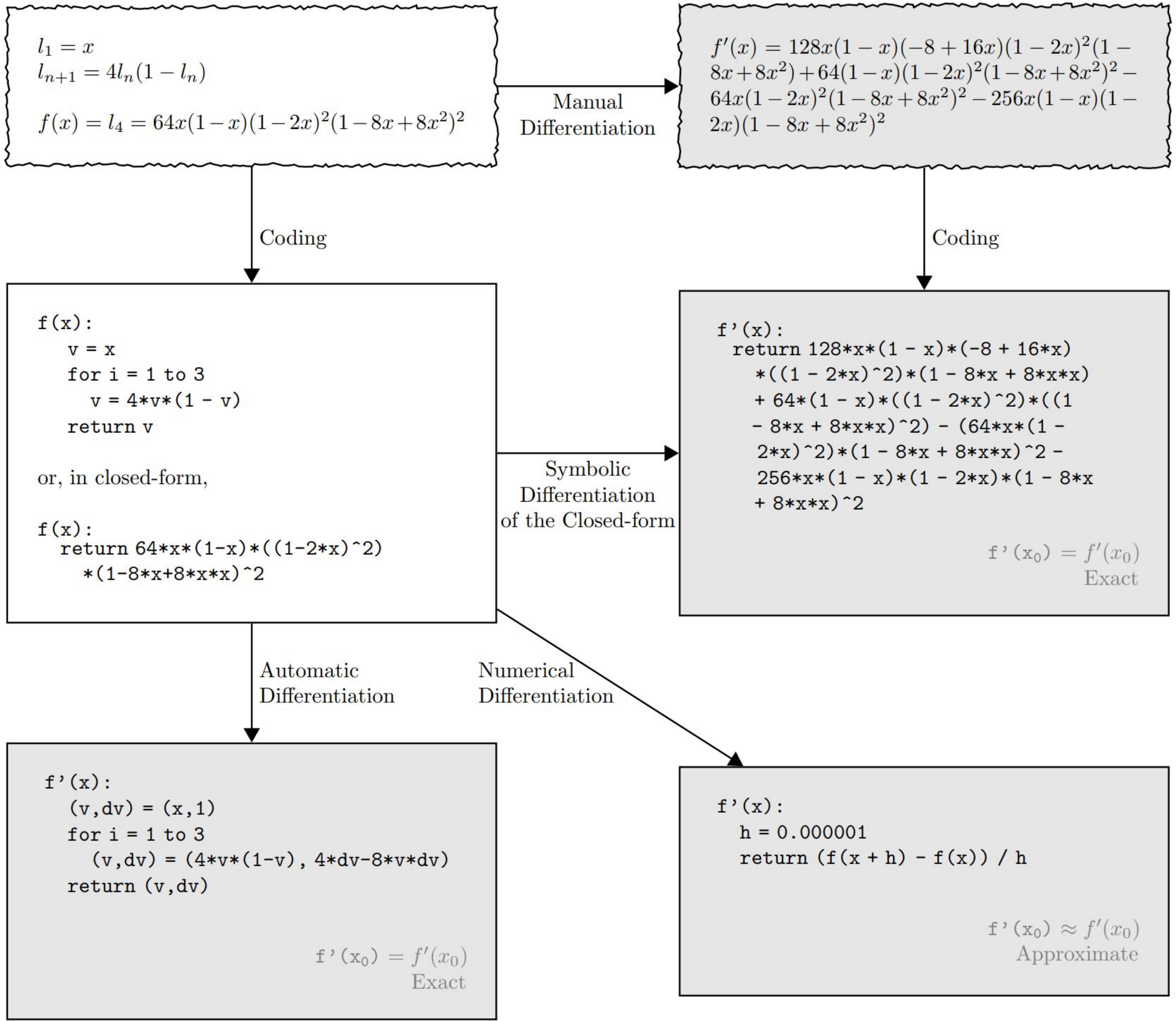
Future Work

- Hessians
    - Finding a way to calculate the determinant
    - Resolving the 1-dimension array issue to allow for 2d array input and output
    - Benchmarking row-by-row approach
- Jacobians
    - Finding a way to compose forward and reverse mode together, i.e. clad::differentiate(clad::gradient(f))
- Support OpenCL and CUDA

Thank you!

- Clad: **https://github.com/vgvassilev/clad**
- Special thanks to: A. Efremov, A. Penev, M. Vasilev, O. Shadura, V. Ilieva, J. Qui
- More about automatic differentiation: **http://www.autodiff.org**

Backup



[Baydin et al., Automatic Differentiation in Machine Learning: a Survey, 2018]

Clad functionality comparison

Feature\Tool	Swift AD	Autograd (Python)	Tangent (Python)	ADOL-C	CppAD	Clad
Basic forward and reverse-mode AD	Supported	Supported	Supported	Supported	Supported	Supported
Loops, conditionals, recursion	Supported	Supported	Supported	Supported	Supported	Supported
Works with third-party libraries, e.g. TensorFlow	TensorFlow (Supported)	Numpy (Supported)	TensorFlow (Supported)	Not Supported	Not Supported	Not Supported
User-defined numeric types/custom type inputs	Supported	Not Supported	Not Supported	Not Supported	Not Supported	Not Supported
Works with vector functions / nested containers e.g. tuple(tuple)	Supported	Supported	Supported	Supported	Supported	Not Supported
Custom-defined derivatives/gradients	Supported	Supported	Supported	Not Supported	Not Supported	Supported
Can mix and match differential operators (e.g. mix/match forward and reverse modes)	Supported	Supported	Supported	Supported	Supported	Supported
Error diagnostics that pinpoint exact location of failure / has own debugging tool	Supported	Not Supported	Supported	Not Supported	Not Supported	Not Supported
Has a marker/attribute to tell tool max amount times to differentiate	Supported	Not Supported	Not Supported	Not Supported	Not Supported	Not Supported
#differential(f): Produces a function that takes the original arguments and returns the differential of f.	Supported	Not Supported	Not Supported	Supported	Supported	Not Supported
#pullback(f): Produces a function that takes the original arguments and returns the pullback of f.	Supported	Not Supported	Not Supported	Not Supported	Not Supported	Not Supported
CUDA/GPU Support/Multithreading	Not Supported	Not Supported	Not Supported	Partially Supported	Supported	Not Supported
Checkpointing	Not Supported	Supported	Not Supported	Supported	Supported	Not Supported
Traceless forward differentiation (Source code transformation forward mode)	Not Supported	Not Supported	Supported	Supported	Not Supported	Supported
Classes	Not Supported	Supported	Not Supported	Supported	Not Supported	Supported
Tensor evaluation	Not Supported	Not Supported	Not Supported	Supported	Not Supported	Not Supported
Jacobians	Supported	Supported	Supported	Supported	Supported	Not Supported
Hessians	Supported	Supported	Supported	Supported	Supported	Not Supported
Exploits sparsity of Jacobian/Hessian	Not Supported	Not Supported	Not Supported	Supported	Supported	Not Supported
Nested functions / lambdas	Not Supported	Supported	Not Supported	Not Supported	Not Supported	Not Supported
Nested calls to functions	Supported	Supported	Supported	Supported	Supported	Supported
Closures	Supported	Supported	Not Supported	Unfair Comparison	Unfair Comparison	Unfair Comparison
Complex Numbers	Not Supported	Supported	Supported	Supported	Supported	Not Supported
Static optimisation/dead code eliminiation	Not Supported	Not Supported	Supported	Not Supported	Supported	Not Supported
Templates	Unfair Comparison	Unfair Comparison	Unfair Comparison	Supported	Supported	Supported
Works with atomic functions	Unfair Comparison	Unfair Comparison	Unfair Comparison	Not Supported	Supported	Not Supported

Work is done by GSOC student Jack Qui

Key	Supported	Not Supported	Partially Supported	Unfair Comparison

What automatic differentiation is

- Technique for evaluating the derivatives of mathematical functions
- Applies differentiation rules to each arithmetical operation in the code

```
double c = a + b;
```

→

```
double d_c = d_a + d_b;
```

```
double c = a * b;
```

→

```
double d_c = a * d_b + d_a * b;
```

...

What automatic differentiation is

- Not limited to closed-form expressions
- Can take **derivatives of algorithms** (conditionals, loops, recursion)

Example: loops

```
double pow(double x, int n) {
    double r = 1;
    for (int i = 0; i < n; i++)
        r = r * x;
    return r;
}
```

```
double pow_darg0(double x, int n) {
    double d_r = 0;
    double r = 1;
    for (int i = 0; i < n; i++) {
        d_r = d_r*x + r*1;
         r = r*x;
    }
    return dr;
}
```

Automatic differentiation in Clad

- At the moment supports functions with:
  - **multiple** (*scalar*) inputs
  - **single scalar** output value

$$f : \mathbb{R}^n \to \mathbb{R}$$

```
double f(double x0, double x1, ..., double xn);
```

- Will be extended soon with:
  - **vector** inputs

```
double f(vector<double> x);
```

```
double f(double* x);
```

- Can be extended with:
  - multiple outputs

$$f : \mathbb{R}^n \to \mathbb{R}^{m}$$

```
vector<double> f(vector<double> x);
```

Automatic differentiation in Clad

- For $f : \mathbb{R}^n \to \mathbb{R}$ can generate:
  - single derivative $\frac{\partial f}{\partial x_i}$ `clad::differentiate(f, i);`
  - gradient $\nabla f = \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_n}\right)$ `clad::gradient(f);`
- Supports both ***forward*** and ***reverse*** mode AD:
  - `clad::differentiate` uses forward mode
  - `clad::gradient` uses reverse mode

Current state

Support of C++ constructs:

- Tested with built-in floating point types: **float**, **double**
- In principle, should work with user-defined scalar types, needs testing
- Arithmetic operators, function calls, variable declarations, if statements …
- In **forward** mode:
  - variable mutation (reassignments), for loops

TODO:

- Arrays/vectors, struct/class methods, custom data structures…
- Occasional missing C++ constructs
- Rigorous documentation, error/warning handling

Why is the speedup factor higher than theoretical limit of ~Npar?

From TF1::GradientPar():

...

```
// save original parameters
Double_t par0 = parameters[ipar];

parameters[ipar] = par0 + h;
f1 = func->EvalPar(x, parameters);
parameters[ipar] = par0 - h;
f2 = func->EvalPar(x, parameters);
parameters[ipar] = par0 + h / 2;
g1 = func->EvalPar(x, parameters);
parameters[ipar] = par0 - h / 2;
g2 = func->EvalPar(x, parameters);

// compute the central differences
h2 = 1 / (2. * h);
d0 = f1 - f2;
d2 = 2 * (g1 - g2);

T grad = h2 * (4 * d2 - d0) / 3.;

// restore original value
parameters[ipar] = par0;

return grad;
```

- some initial bookkeeping
- 4 calls to **f**
- additional ops to improve accuracy

Hessians - How it is implemented

- Generated through using forward mode AD, then reverse mode AD
- Iteratively calculates each column of the Hessian at a time, which is encapsulated within a second-order partial derivative function
- Combines all of these helper functions that correspond to columns of a Hessian into a single Hessian function
- Encapsulated in Clad API through clad::hessian

$$\mathbf{H} = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

Work is done by GSOC student Jack Qui

Hessians

- Square n x n matrix containing all second order partial derivatives w.r.t to all inputs
- Useful for optimisation problems and as a second derivative test

$$\mathbf{H} = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\[2.2ex] \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\[2.2ex] \vdots & \vdots & \ddots & \vdots \\[2.2ex] \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

Work is done by GSOC student Jack Qui

Hessians - Demo

```
double f_cubed_add1(double a, double b) {
 return a * a * a + b * b * b;
}
```

```
auto func = clad::hessian(f_cubed_add_1);
func.dump();
```

```
void f_cubed_add1_hessian(double a, double b, double *hessianMatrix){
  f_cubed_add1_darg0_grad(a, b, &hessianMatrix[0UL]);
  f_cubed_add1_darg1_grad(a, b, &hessianMatrix[2UL]);
}
```