From Bayesian Inference to LLMs

Modern C++ Optimizations for Reverse-Mode Automatic Differentiation

STEVE BRONDER

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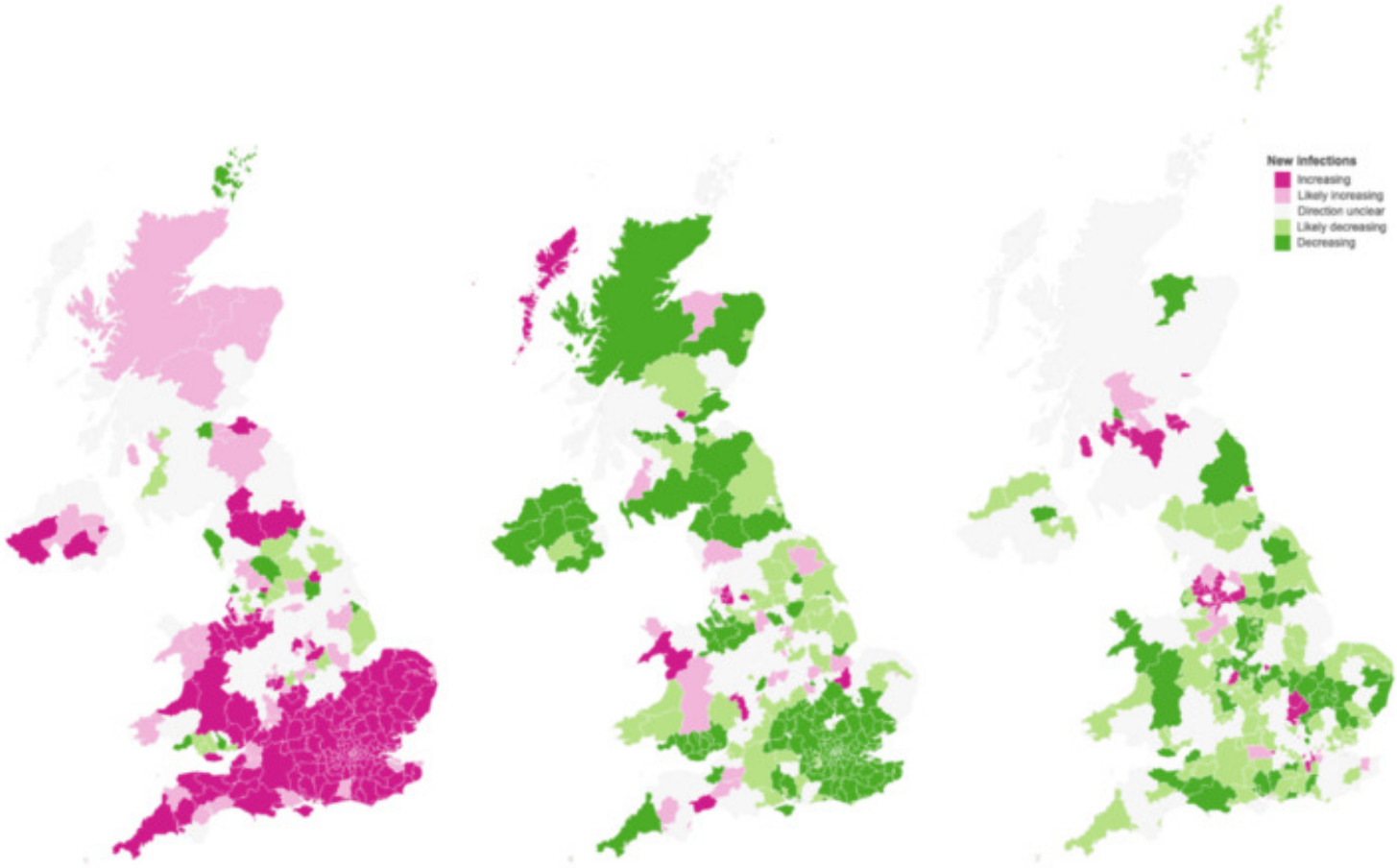
Estimating COVID Infection Rates For Policy



(a) 25 Dec 2020 (b) 21 Jan 2021 (c) 30 May 2021

Figure: Probability of epidemic growth by local area

Go to ChatGPT. Autodiff is the mitochondria of machine learning. AD allows for efficient estimation of many statistical models.

What is Automatic Differentiation?

Automatically compute exact gradients by treating a program as a graph of elementary operations and applying the chain rule on that graph

Reverse-mode automatic differentiation (AD) lets us get derivatives of a program's output with respect to its inputs without doing algebra by hand. Imagine the code as a computational graph of simple ops (add, multiply, sin, etc.). In the forward pass, we execute the code normally, get the output, and save intermediate results. Then we do a backward pass effectively running the chain rule on the graph from the output back to the inputs. This two-pass strategy is what powers deep learning frameworks (it's basically backpropagation), and it efficiently produces gradients even for complex code.

What is a gradient?

Ex: Newton's root finding method

$$x_{n+1} = x_n - \frac{f(x_n)}{f'_x(x_n)}$$

find $f(x) = y$ where $y = 0$

- Note that f'_x is the gradient of f with respect to x

  How do we estimate solutions for equations? A simple method is the newton method.

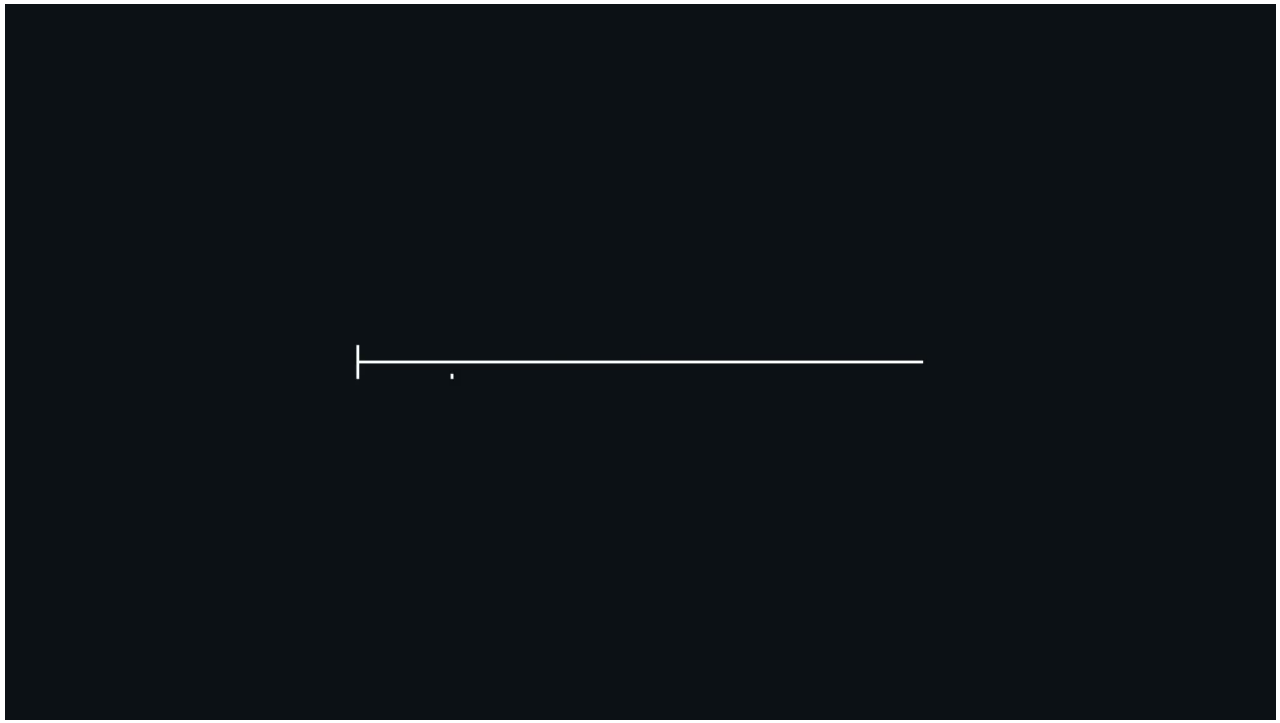
  Why are gradients useful? We use gradients to solve

  For models we want to estimate parameter values. Change the slide here so that we show how to solve for parameters using Newton's method

What is a gradient?

$$f(x) = x^3 + x^2 + x \tag{1}$$

$$f'_x(x) = 3x^2 + 2x + 1 \tag{2}$$



The gradient tells us

- The direction the function increases most quickly from x_n
- The rate of increase of the function at x_n

Why use Automatic Differentiation?

- Hamiltonian Monte Carlo:

$$\frac{dp}{dt} = \nabla_\theta \log p(\theta|y)$$

- BFGS:

$$s_k = -H_k \nabla_\theta f(\theta_k)$$

- Stochastic Gradient Descent:

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta L(\theta_t; x_t)$$

Hamiltonian Monte Carlo:

- Updates the momentum p using the (negative) gradient of the log posterior—i.e., the deterministic "force" driving the Hamiltonian dynamics.

BFGS:

- Forms the search step s_k as a quasi-Newton descent direction by preconditioning the gradient with the current inverse-Hessian estimate H_k.

Stochastic Gradient Descent:

- Updates parameters by stepping θ a learning-rate η in the direction opposite the stochastic gradient of the loss evaluated on x_t.

Why use Automatic Differentiation?

Choices:

- Write by hand
- finite difference,
- symbolic differentiation
- spectral differentiation
- automatic differentiation

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Why use Automatic Differentiation?

$$\underbrace{p(\boldsymbol{\theta} \mid \mathbf{y})}_{\textbf{posterior}} \propto \prod_{i=1}^{N} \left\{ \sum_{\mathbf{z}_i \in \{1,2,3\}^{T_i}} \left[\underbrace{\pi_{z_{i,1}} \prod_{t=2}^{T_i} \Pi_{z_{i,t-1},\, z_{i,t}}}_{\text{3-state HMM prior}} \prod_{t=1}^{T_i} \underbrace{\mathcal{N}\left(y_{i,t} \,\middle|\, \eta_{i,t},\ \sigma^2_{z_{i,t}}\right)}_{\text{state-dependent emission}} \right] \right\}$$

where $\eta_{i,t} = \underbrace{\mathbf{x}_{i,t}^\top \boldsymbol{\beta}}_{\text{fixed}} + \underbrace{\mathbf{z}_{i,t}^{(G)\top} \mathbf{b}_{g[i]} + \mathbf{z}_{i,t}^{(C)\top} \mathbf{c}_{c[i]} + u_{g[i]}}_{\text{crossed random effects}} + \underbrace{f(t_{i,t})}_{\text{GP}} + \underbrace{\mu_{z_{i,t}} + \mathbf{r}_{z_{i,t}}^\top \mathbf{w}_i}_{\text{state-specific offset + slope}}, \qquad z_{i,t} \in \{1, 2, 3\}.$

$$p(\mathbf{f} \mid \boldsymbol{\psi}) = (2\pi)^{-T/2} \, |\mathbf{K}|^{-1/2} \, \exp\Big(-\tfrac{1}{2} \mathbf{f}^\top \mathbf{K}^{-1} \mathbf{f} \Big),$$

$$\mathbf{K} = \sigma_f^2 \Big(\mathbf{K}_{\mathsf{LP}}(\ell, p, \lambda) \ + \ \rho \, \mathbf{K}_{\mathsf{SE}}(\tilde{\ell}) \Big) + \sigma_n^2 \mathbf{I}, \quad \left[\mathbf{K}_{\mathsf{LP}}\right]_{tt'} = \exp\left(-\frac{(t-t')^2}{2\ell^2} - \frac{2\sin^2\left(\pi |t-t'|/p\right)}{\lambda^2} \right),$$

$$\left[\mathbf{K}_{\mathsf{SE}}\right]_{tt'} = \exp\left(-\frac{(t-t')^2}{2\tilde{\ell}^2} \right), \qquad \mathbf{K} = \mathbf{L}_K \mathbf{L}_K^\top \ \Rightarrow \ \log|\mathbf{K}| = 2 \sum_{j=1}^{T} \log\left((\mathbf{L}_K)_{jj} \right).$$

Hierarchical mixed effects (non-centered, LKJ prior):

$$\mathbf{b}_g = \left(\mathbf{I}_{p_G} \otimes \operatorname{diag}(\boldsymbol{\tau}_b) \, \mathbf{L}_R \right) \tilde{\mathbf{b}}_g, \quad \tilde{\mathbf{b}}_g \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \mathbf{c}_c = \operatorname{diag}(\boldsymbol{\tau}_c) \, \tilde{\mathbf{c}}_c, \quad \tilde{\mathbf{c}}_c \sim \mathcal{N}(\mathbf{0}, \mathbf{I}),$$

$$\mathrm{LKJ}_{p_G}(\eta) \text{ prior on } \mathbf{R}, \quad \mathbf{L}_R \mathbf{L}_R^\top = \mathbf{R}, \quad \boldsymbol{\tau}_b \sim \prod_{j=1}^{p_G} \text{Half-}t_{\nu_b}(0, s_b), \quad \boldsymbol{\tau}_c \sim \prod_{j=1}^{p_C} \text{Half-}t_{\nu_c}(0, s_c),$$

$$u_g \sim \mathcal{N}(0, \sigma_u^2).$$

Move from this slide quickly

Why use Automatic Differentiation?

- I do not wish to write those gradients by hand

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- Allows for unknown length while and for loops

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- Allows for unknown length while and for loops
- Accurate to floating point precision

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Implementation Matters!

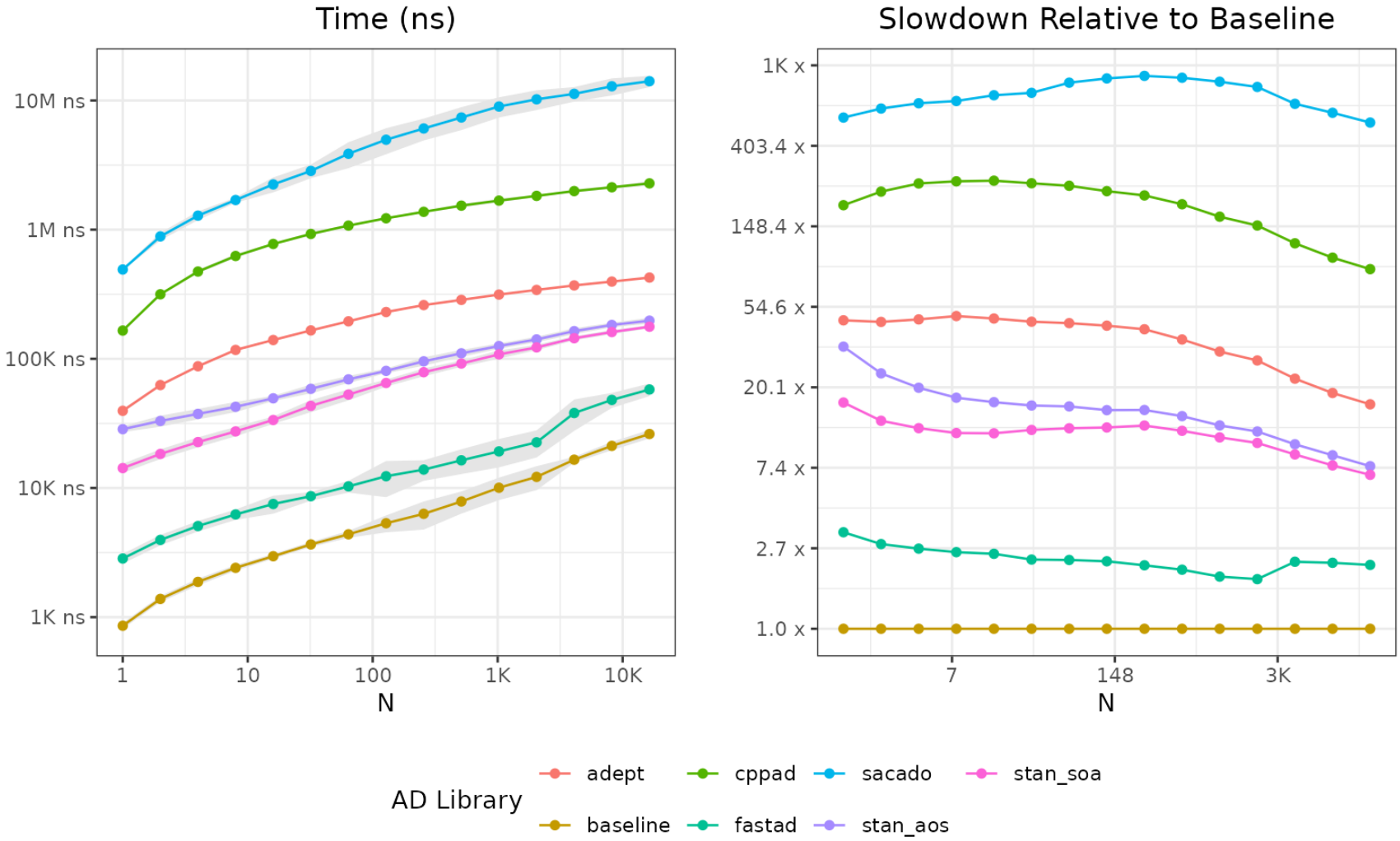

Figure: Benchmark for f and f' given $f(y) = N(y|X\theta, \sigma)$

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Goal of this talk

- How Reverse Mode Automatic Differentiation works
- Performance of high throughput memory intensive programs
- How modern C++ has led to cleaner and more efficient AD

Let v_k be the sequence of intermediate expressions for the input x and output z and let $v_K = z$ and $v_1 = x; v_0 = y$. Let $\bar{v}_k$ be the partial gradient of the kth intermediate step. Then we can apply the chain rule to each intermediate step to get the partial gradient.

What is Automatic Differentiation?

- AD computes gradients of a program by applying the chain rule to its subexpressions.

$$
\begin{aligned}
f(x, y) &= \log(x \cdot y) \\
g(x, y) &= x \cdot y \\
h(u) &= \log(u) \\
f(x, y) &= h\big(g(x, y)\big)
\end{aligned}
$$

- Emphasize: AD is mechanical chain rule over the executed program, not symbolic math or numeric differencing.
- Automatic Differentiation can do higher order partials, but here we just focus on the first order
- Now we rewrite f in terms of h and g

What is Automatic Differentiation?

- AD computes gradients of a program by applying the chain rule to its subexpressions.

$$f(x,y) = h\big(g(x,y)\big)$$
$$g(x,y) = x \cdot y \qquad g_x{}'(x,y) = y \;\; g_y{}'(x,y) = x$$
$$h(u) = \log(u) \qquad h'_u(u) = u^{-1}$$

$$\begin{aligned} f'_x(x,y) &= h'_g\big(g(x,y)\big) \cdot g'_x(x,y) \\ &= \frac{1}{g(x,y)} \cdot y = \frac{1}{x}, \end{aligned}$$

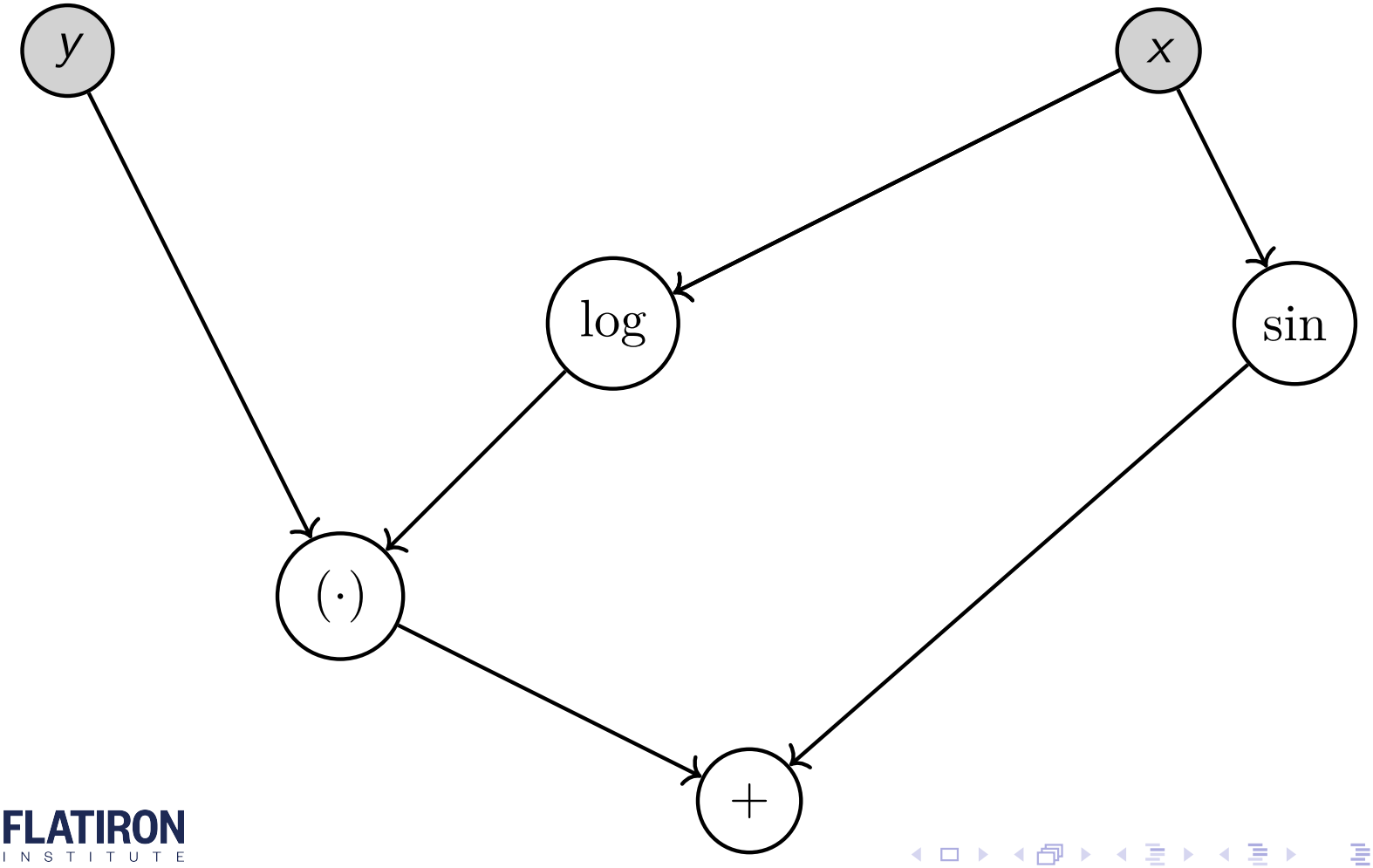
$$\begin{aligned} f'_y(x,y) &= h'_g\big(g(x,y)\big) \cdot g'_y(x,y) \\ &= \frac{1}{g(x,y)} \cdot x = \frac{1}{y}. \end{aligned}$$

Emphasize: AD is mechanical chain rule over the executed program, not symbolic math or numeric differencing.

Data Type: Expression Graph

Goal: Calculate the full gradient by accumulating partial gradients (adjoints) through the a graph of subexpressions.

$$z = \log(x) \cdot y + \sin(x)$$



- Each node of expression graph is an intermediate calculation we know the gradient of with respect to its inputs
- For each node we compute a forward pass till we get to our end node
- Once we reach our end node we can compute the reverse pass

Expression Graph: Traversal

$$f(x, y) = \log(x)y + \sin(x)$$

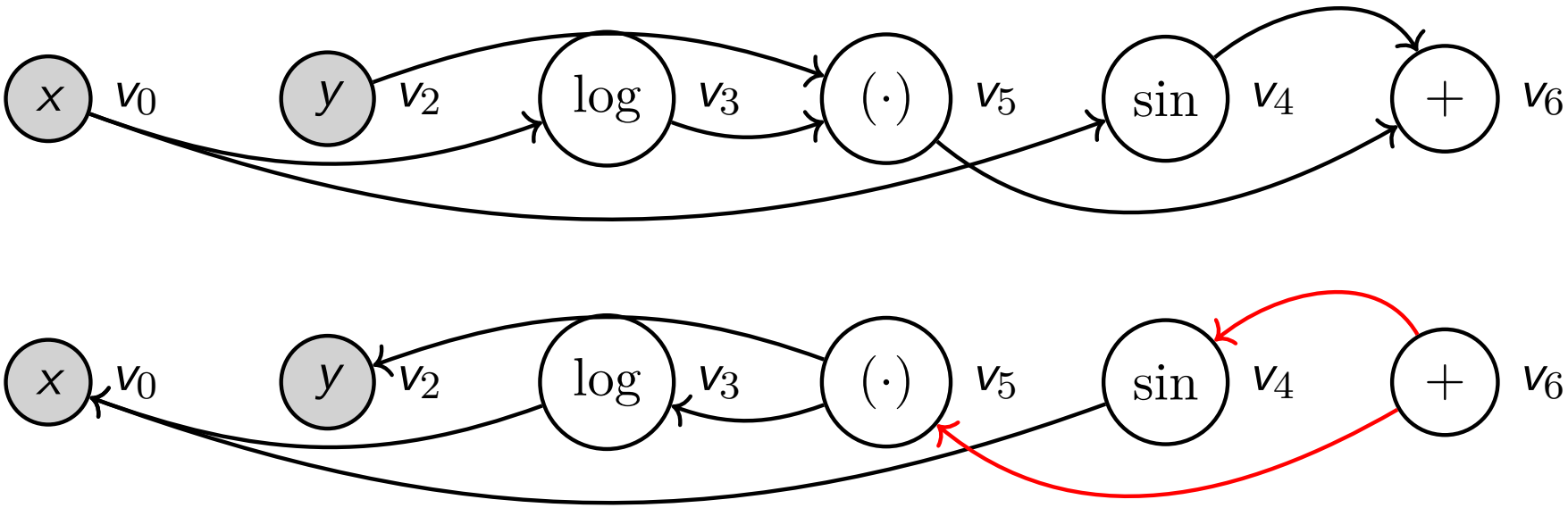


Figure: Topological sort of expression graph

- We can do a Topological sort on the graph and traverse it this way
- This is how we should execute the program linearly on a thread

Expression Graph: Node

For Reverse Mode AD, each node performs two functions.

- Forward Pass:

$$z = f(x, y)$$

- Reverse Pass: Given z's adjoint (partial gradient) $\bar{z}$
  Calculate the local adjoint-Jacobian update for x and y.

$$chain(\bar{z}, y, x) = \begin{cases} \bar{y} \mathrel{+}= \bar{z} \cdot z_y{}' \\ \bar{x} \mathrel{+}= \bar{z} \cdot z_x{}' \end{cases}$$

Adjoint = local gradient

- Each node in the graph holds an adjoint value, which is the partial derivative of the final output with respect to that node's value. It accumulates all contributions of that node to the output's gradient.

Backpropagation (chain rule):

- During the backward pass, each operation uses its adjoint and the operation's local derivative to add to its input nodes' adjoints. This is how gradients flow backward through the graph

Pseudocode for AutoDiff

```
// compute and store node.value
struct node {
  double val;
  double adj;
  virtual void chain() {}
};
node x = 2.0;
node y = 3.0;
// Forward pass calculated here
auto e_graph = log(x) * y + sin(x);
// Calculate reverse pass
e_graph.end().adj = 1.0;
for (auto& node : e_graph | std::views::reverse) {
    (*node)->chain();
}
assert(y.adj == 1.2103);
assert(x.adj == 0.2516);
```

What Do AD Libraries Care About?

- Flexibility:

  Debugging, exceptions, conditional loops, matrix subset assignment

- : Efficiency:

  Efficiently using a single CPU/GPU

- Scaling

  Efficiently using clusters with multi-gpu/cpu nodes

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How do we keep track of our reverse pass?

Source code transformation

- Unroll all forward passes and reverse passes into one function

Good: Fast

Bad: Hard to implement, very restrictive

Operator Overloading

- Nodes in the expression graph are objects which store a forward and reverse pass function

Good: Easier to implement, more flexible

Bad: Less optimization opportunities

Newer AD packages use a combination of both

flexibility, performance, and developer time

How do we keep track of our reverse pass?

Static (Fast) vs. Dynamic (Flexible) graphs

- Known expression graph size at compile time? (Static)
- Reassignment of variables (Dynamic easy, Static hard)
- How much time do I have? (Dynamic)

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Operator Overloading Approach

The operator overloading approach usually involves:

- Runtime "tape" for tracking expressions
- Arena allocator for storing AD nodes
- Pair scalar type to hold the value and adjoint

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Operator Overloading: Basic Type

```
struct var_impl {
  double val;
  double adj;
  virtual void chain() {};
}; // 24 bytes
struct var {
  var_impl* vi_;
}; // 8 bytes
```

var_impl is our base type all expression nodes inherit from

Operator Overloading: Monotonic Buffer

```
struct Tape {
std::monotonic_buffer_resource mbr{(1 << 16)};
std::polymorphic_allocator<std::byte> pa{&mbr};
std::vector<var_impl*> tape;
void clear() {
  tape.clear();
  mbr.release();
}
};
static Tape g_tape{};
template <typename T, typename Types>
auto new_node(Types&& ... args) {
  auto* ret = g_tape.pa.template
  ↪  new_object<T>(args ... );
  g_tape.tape.push_back(ret);
  return var{ret};
}
```

..

Operator Overloading: Expression Node

```
struct mul_vv : public var_impl {
  var op1_;
  var op2_;
  void chain() {
    op1_.adj() += this->adjoint_ * op2_.val();
    op2_.adj += this->adjoint_ * op1_.val();
  }
}; // 40 bytes
var operator*(var op1, var op2) {
  return new_node<mul_vv>(op1.val() * op2.val(),
    op1, op2);
}
```

..

Operator Overloading: Reverse Pass

```
void grad(var& v) {
  v.adj = 1.0;
  for (auto&& x : tape | std::views::reverse) {
    x->chain();
  }
}
```

..

Monotonic Buffer

```
void compute_grads(var x, var y) {
  var z = -10;
  while (z.val() < 20) {
    z += log(x * y);
  }
  grad(z);
}
// Later in program
for (int i = 0; i < 1e10; ++i) {
  var x = compute_x(...);
  var y = compute_y(...);
  compute_grads(x, y);
  do_something_with_grads(x.adj, y.adj);
  g_tape.clear();
}
```

..

So Many Operator Classes

```
struct mul_vv;
struct mul_vd;
struct mul_dv;
struct add_vv;
struct add_dv;
struct add_vd;
struct subtract_vv;
struct subtract_dv;
struct subtract_vd;
struct divide_vv;
struct divide_dv;
struct divide_vd;
```

..

Reduce Boilerplate

```
template <Functor F>
struct callback_var_impl : public var_impl {
  F rev_functor_;
  template <std::floating_point S>
  explicit callback_var_impl(
    S&& value, F&& rev_functor)
    : var_impl(value),
      rev_functor_(rev_functor) {}
  void chain() final { rev_functor_(*this); }
}; // 24 + 8B * N
```

..

Reduce Boilerplate

```
template <typename T1, typename T2>
requires any_var<T1, T2>
inline auto operator*(T1 op1, T2 op2) {
  return new_node<callback_var_impl>(
    value(op1) * value(op2),
    [op1, op2](auto&& ret) mutable {
      if constexpr (is_var_v<T1>) {
        adjoint(op1) += adjoint(ret) * value(op2);
      }
      if constexpr (is_var_v<T2>) {
        adjoint(op2) += adjoint(ret) * value(op1);
      }
    });
}
```

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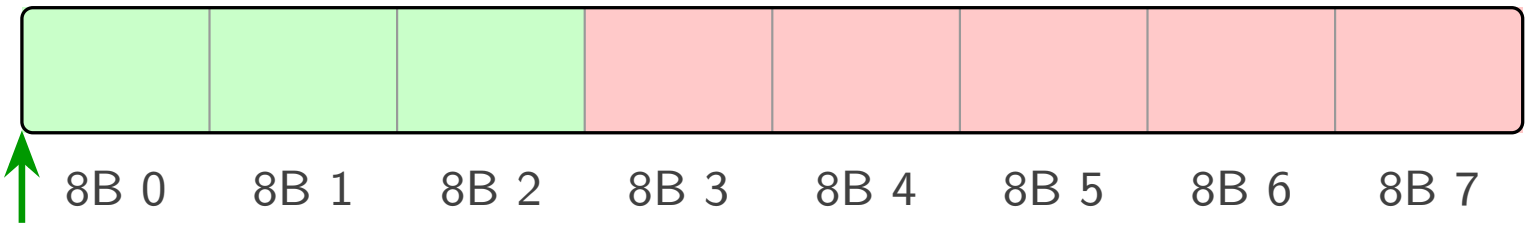
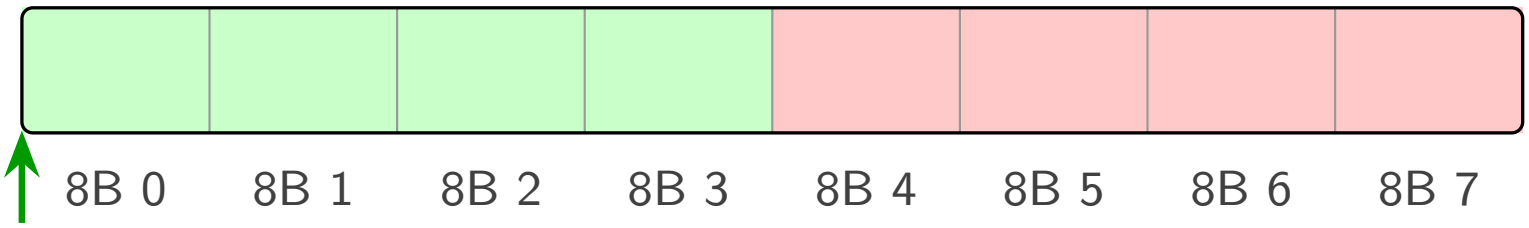
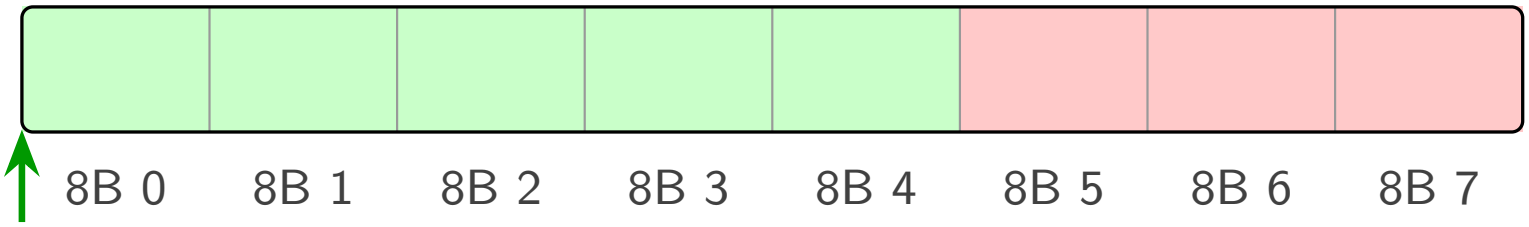
Poor Cache Use



var_impl{dbl, dbl, vptr}



unary_var{dbl, dbl, vptr, var_impl*}



binary_var{dbl, dbl, vptr, var_impl*, var_impl*}

..

Source Code Transform Ex:

```
double z = log(x * y);
```

Break it down

```
double v0 = x;
double v1 = y;
double v2 = x * y;
double v3 = log(v2)
double bar_v3 = 1;
double bar_v2 = bar_v3 * 1/v2;
double bar_v1 = bar_v2 * v0;
double bar_v0 = bar_v2 * v1;
```

..

Source Code Transform Ex:

Code like the following very hard / impossible in source code transform

```
while(error < tolerance) {
  //  ...
}
```

..

Source Code Transform Ex:

```
struct var {
    double values_;
    double adjoints_;
    var(double x) : values_(x), adjoints_(0) {}
};
```

..

Source Code Transform Ex:

```
template <typename F, typename... Exprs>
struct expr {
    var ret_;
    std::tuple<deduce_ownership_t<Exprs>...> exprs_;
    std::decay_t<F> f_;
    template <typename FF, typename... Args>
    expr(double x, FF&& f, Args&&... args) :
      ret_(x), f_(std::forward<F>(f)),
      exprs_(std::forward<Args>(args)...) {}
};
```

..

Source Code Transform Ex:

```
template <typename T1, typename T2>
requires any_var_or_expr<T1, T2>
inline auto operator*(T1&& lhs, T2&& rhs) {
  return make_expr(value(lhs) * value(rhs),
  [](auto&& ret, auto&& lhs, auto&& rhs) {
    if constexpr (!std::is_arithmetic_v<T1>) {
      adjoint(lhs) += adjoint(ret) * value(rhs);
    }
    if constexpr (!std::is_arithmetic_v<T2>) {
      adjoint(rhs) += adjoint(ret) * value(lhs);
    }
  }, std::forward<T1>(lhs), std::forward<T2>(rhs));
}
```

..

Source Code Transform Ex:

```
auto z = x * log(y) + log(x * y) * y;
expr<Lambda<Plus>,
  expr<Lambda<Mult>, var, expr<Lambda<Log>, var>>,
  expr<Lambda<Mult>,
   expr<Lambda<Log>, expr<Lambda<Mult>, var, var>>,
   var>>
```

..

Source Code Transform Ex:

```
template <typename Expr>
inline void grad(Expr&& z) {
  adjoint(z) = 1.0;
  auto nodes = collect_bfs(z);
  eval_breadthwise(nodes);
}
```

Example Godbolt

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Comparison

Table: $f(x, y) = x\log(y) + \log(xy)y$;

Method	CPU Time	% Improvement
Shared Ptr	508ns	1.0
MonoBuff	121ns	3.9x
Lambda	112ns	4.2x
Source Code Transform	26.5ns	19x
Baseline	2.82ns	180x

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Operator Overloading Approach: Matrices

```
Matrix<var> B(M, M);
Matrix<var> X(M, M);
Matrix<var> Z = X * B.transpose();
```

..

Operator Overloading Approach: Matrices

```
template <typename MatrixType>
struct arena_matrix :
  public Eigen::Map<MatrixType> {
  using Base = Eigen::Map<MatrixType>
  template <typename T>
  arena_matrix(T&& mat) :
   Base(copy_to_arena(mat.data(), mat.size()),
     mat.rows(), mat.cols()) {}
};
```

..

Operator Overloading Approach: Matrices

```
// Array of Structs
struct Matrix<var> {
  var* data_;
};
// Struct of Arrays
struct var_impl<Matrix<double>> {
  arena_matrix<double> value_;
  arena_matrix<double> adjoint_;
  virtual void chain() {}
};
```

..

Operator Overloading Approach: Matrices

```
// Array of Structs
struct Matrix<var> {
  var* data_;
};
```

- Array of Structs:
  - Simple, most algorithms Just Work™
  - Adds a lot to expression graph
  - turns off SIMD

..

Operator Overloading Approach: Matrices

```
// Struct of Arrays
struct var_impl<Matrix<double>> {
  arena_matrix<double> value_;
  arena_matrix<double> adjoint_;
  virtual void chain() {}
};
```

- Struct of Arrays:
  - Hard, everything written out manually
  - Collapses matrix expressions in tree
  - SIMD can be used on values and adjoints

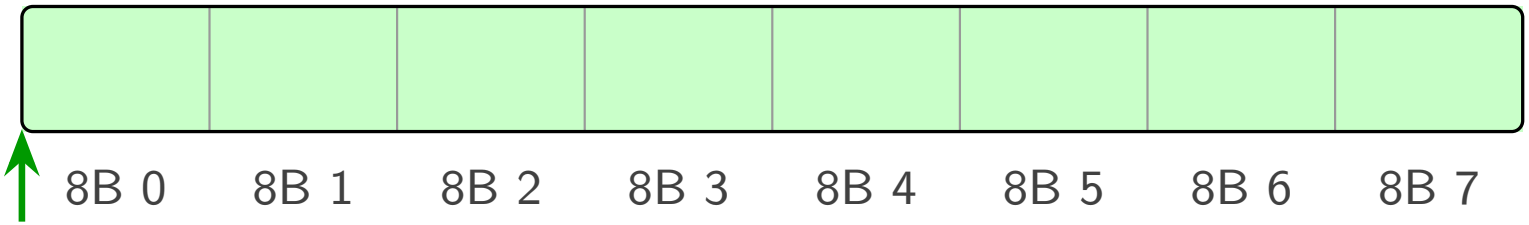
..

Matrix Multiplication Example

```
template <typename T1, typename T2>
requires any_var_matrix<T1, T2>
inline auto operator*(T1&& op1, T2&& op2) {
  return lambda_var(value(op1) * value(op2),
    [op1, op2](auto&& ret) mutable {
      if constexpr (is_var_matrix_v<T1>) {
        adjoint(op1) += adjoint(ret) *
          ↪  value(op2).transpose();
      }
      if constexpr (is_var_matrix_v<T2>) {
        adjoint(op2) += value(op1) * adjoint(ret);
      }
    });
}
```

..

Operator Overloading Approach: Matrices



mat_mul_vv{dbl*, dbl*, long int, long int, vptr, lambda[var<Mat>, var<Mat>]}

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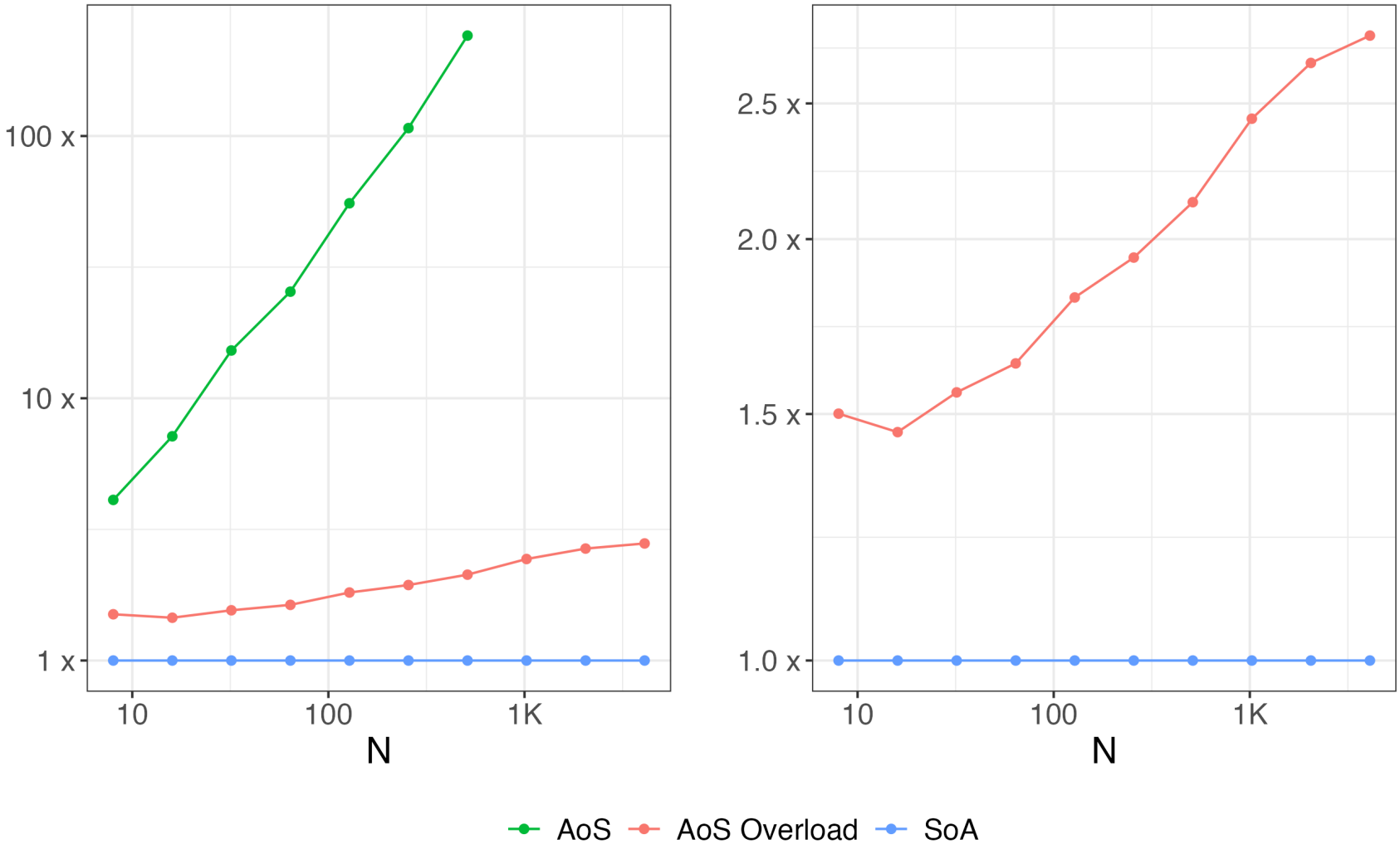
Matrix Multiplication Benchmark



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Subset Assignment

```
var<Vector<double>> y{{0, 1, 2, 3}};
var<Vector<double>> x{{0, 1, 2, 3}};
var prod = y.dot(x);
x.slice(1, 3) = x.head(3);
auto z = prod + sum(x);
```

Subset Assignment

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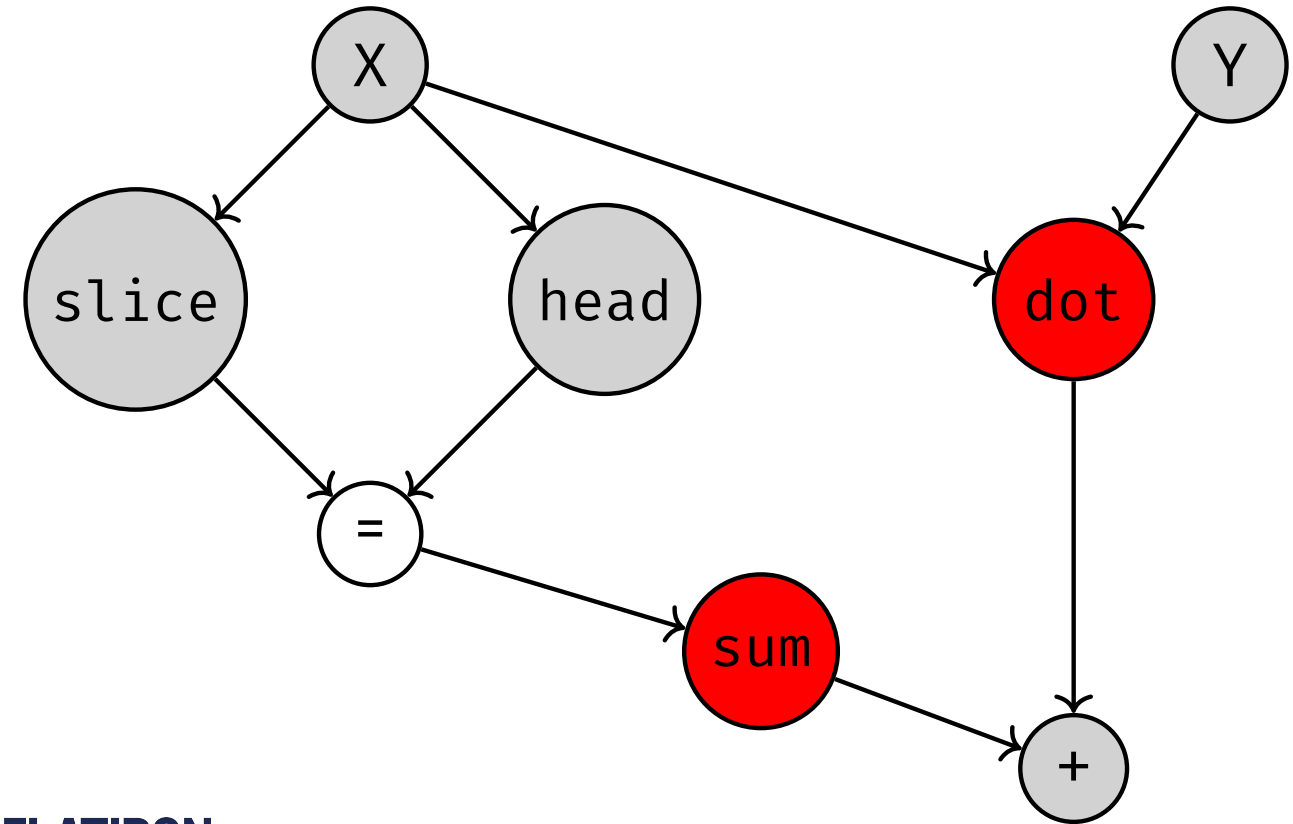

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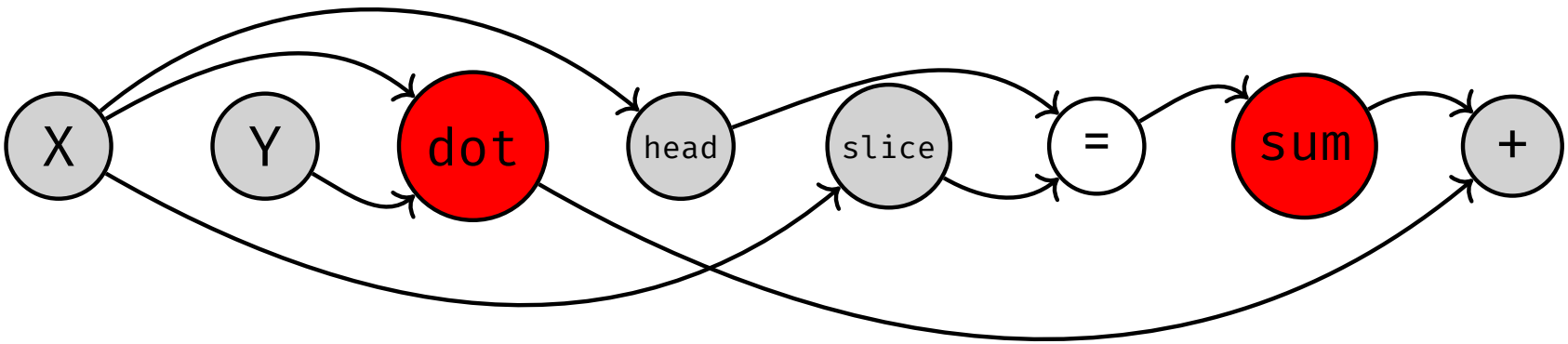
auto z = prod + sum(x);
```



..

Subset Assignment Becomes Very Hard

```
var<Vector<double>> x{{0, 1, 2, 3}};
x.slice(1, 3) = x.head(3);
```

Iter	X
0	$\{0, 0, 2, 3\}$
1	$\{0, 0, 0, 3\}$
2	$\{0, 0, 0, 0\}$

..

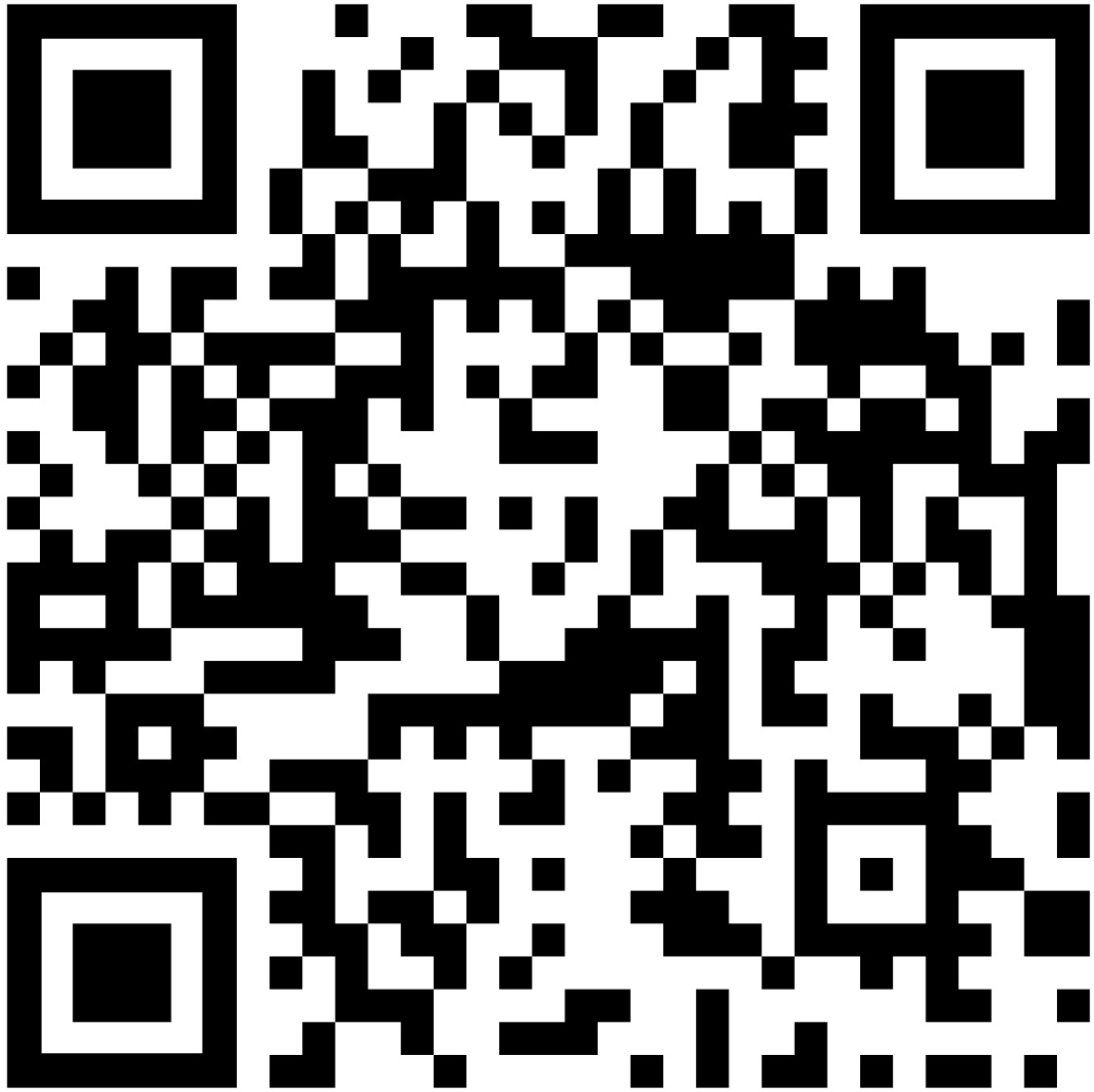
Subset Assignment Becomes Very Hard

```
tempalte <typename T>
struct var {
template <typename S>
require AssignableExpression<T, S>
inline var<T>& operator=(const var<S>& other) {
  arena_matrix<T> prev_val(vi_->val_.rows(),
  ↪  vi_->val_.cols());
  prev_val.deep_copy(vi_->val_);
  vi_->val_.deep_copy(other.val());
  g_tape.callback(
  [this_vi = this->vi_, other_vi = other.vi_,
  ↪  prev_val]() mutable {
    this_vi->val_.deep_copy(prev_val);
    prev_val.deep_copy(this_vi->adj_);
    this_vi->adj_.setZero();
    other_vi->adj_ += prev_val;
  });
  return *this;
}
}
```

..

Thanks!

Repository for benchmarks and slides



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