Sparser, better, faster, stronger

Automatic differentiation with a lot of zeros

Guillaume Dalle* – LVMT, École des Ponts (`gdalle.github.io`)

Laboratoire Jean Kuntzmann, 19.06.2025

*joint work with Adrian Hill, Alexis Montoison and Assefaw Gebremedhin

Agenda

Motivation

Newton's method

Root-finding

Solve $F(x) = 0$ by iterating

$$x_{t+1} = x_t - \underbrace{[\partial F(x_t)]}_{\text{Jacobian}}^{-1} F(x_t)$$

Optimization

Solve $\min_x f(x)$ by iterating

$$x_{t+1} = x_t - \underbrace{\left[\nabla^2 f(x_t)\right]}_{\text{Hessian}}^{-1} \nabla f(x_t)$$

Linear system involving a derivative matrix A.

Implicit differentiation

Differentiate $x \mapsto y(x)$ knowing **conditions** $c(x, y(x)) = 0$.

Applications: fixed-point iterations, optimization problems.

Implicit function theorem:

$$\frac{\partial}{\partial x} c(x, y(x)) + \frac{\partial}{\partial y} c(x, y(x)) \cdot \partial y(x) = 0$$

$$\partial y(x) = -\underbrace{\left[\frac{\partial}{\partial y} c(x, y(x))\right]^{-1}}_{\text{Jacobian}} \frac{\partial}{\partial x} c(x, y(x))$$

Linear system involving a derivative matrix A.

Linear systems of equations

How to solve $Au = v$?

Direct method (LU, Cholesky)

1. Decompose the matrix A.
2. Get an exact solution by substitution.

Requires storing A explicitly.

Iterative method (CG, GMRES)

1. Rephrase as $\min_u \|Au - v\|^2$.
2. Get an approximate solution.

Only requires matrix-vector products $u \mapsto Au$.

Conventional wisdom

- Jacobian and Hessian matrices are **too large** to compute or store
- We can only access linear maps $u \mapsto Au$ (JVPs, VJPs, HVPs)
- Linear systems $A^{-1}v$ must be solved with **iterative methods**
- Downsides: each iteration is expensive, convergence is tricky

The benefits of sparsity

- Jacobian and Hessian matrices have **mostly zero coefficients**
- We can compute and store A explicitly
- Linear systems $A^{-1}v$ can be solved with iterative **or direct** methods
- Upsides: faster iterations or exact solves, efficient linear algebra

Automatic differentiation

Differentiation

Given $f : \mathbb{R}^n \to \mathbb{R}^m$, its **differential** $\partial f(x)$ is the **linear map** which best approximates f around x:

$$f(x+u) = f(x) + \partial f(x)[u] + o(u)$$

It can be represented by the **Jacobian matrix**, which I will denote by $J = \partial_{\mathrm{mat}} f(x)$ instead.

Numeric differentiation

input	**output**
program computing the function $x \mapsto f(x)$	approximation of the differential with the same program $\partial f(x)[u] \approx \dfrac{f(x+\varepsilon u) - f(x)}{\varepsilon}$

Automatic / algorithmic differentiation

input	**output**
program computing the function $x \mapsto f(x)$	new program computing the exact differential $(x, u) \mapsto \partial f(x)[u]$ or $\partial f(x)^*[u]$

AD under the hood

Two ingredients only:

1. hardcode basic derivatives (+, ×, exp, log, ...)
2. handle composition $f = g \circ h$

Composition

For a function $f = g \circ h$, the **chain rule** gives its differential:

$$\begin{aligned} \text{standard} \qquad \partial f(x) &= \partial g(h(x)) \circ \partial h(x) \\ \text{adjoint} \qquad \partial f(x)^* &= \partial h(x)^* \circ \partial g(h(x))^* \end{aligned}$$

These linear maps apply as follows:

$$\begin{aligned} \text{forward} \qquad \partial f(x) &: u \xmapsto{\partial h(x)} v \xmapsto{\partial g(h(x))} w \\ \text{reverse} \qquad \partial f(x)^* &: u \;\underset{\partial h(x)^*}{\longleftarrow\!\shortmid}\; v \;\underset{\partial g(h(x))^*}{\longleftarrow\!\shortmid}\; w \end{aligned}$$

Why linear maps?

The chain rule has a matrix equivalent:

$$\partial_{\text{mat}}(g \circ h)(x) = \partial_{\text{mat}} g(h(x)) \cdot \partial_{\text{mat}} h(x)$$
$$\partial_{\text{mat}}(g \circ h)(x)^T = \partial_{\text{mat}} h(x)^T \cdot \partial_{\text{mat}} g(h(x))^T$$

Working with linear maps avoids allocation and manipulation of **intermediate Jacobian matrices**.

Essential for neural networks (scalar output but vector encodings)!

Two modes

Forward-mode AD computes Jacobian-Vector Products (**JVPs**) = "pushforward" of an **input perturbation**:

$$u \mapsto \partial f(x)[u] = J u \quad \text{with} \quad J = \partial_{\text{mat}} f(x)$$

Reverse-mode AD computes Vector-Jacobian Products (**VJPs**) = "pullback" of an **output sensitivity**:

$$v \mapsto \partial f(x)^*[v] = J^T v = v^T J \quad \text{with} \quad J = \partial_{\text{mat}} f(x)$$

Theorem (Baur-Strassen): cost of 1 JVP or VJP $\propto$ cost of 1 function evaluation

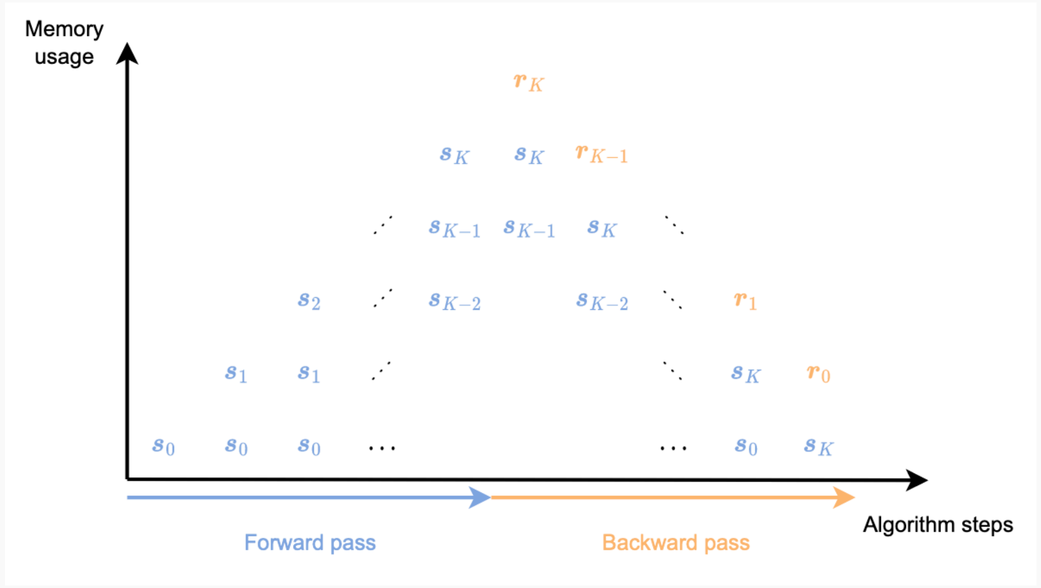
What about gradients?

Reverse mode computes **gradients for roughly the same cost** as the function itself:

$$\nabla f(x) = \partial f(x)^*[1]$$

Makes deep learning possible.

The devil is in the details: higher memory footprint.


Memory usage
Algorithm steps
Forward pass
Backward pass
s_0 s_1 s_2 s_{K-2} s_{K-1} s_K
r_K r_{K-1} r_1 r_0

Blondel & Roulet (2024)

What about second order?

The Hessian matrix is the Jacobian matrix of the gradient function.

A Hessian-Vector Product (HVP) can be computed as the JVP of a VJP, in **forward-over-reverse mode**[2]:

$$\nabla^2 f(x)[v] = \partial(\nabla f)(x)[v] = \partial(\partial^* f(x)[1])[v]$$

[2] Pearlmutter (1994)

Pocket AD

```
# Basic rules

using LinearAlgebra

A, b = rand(2, 3), rand(2)
residuals(x) = A * x - b
∂(::typeof(residuals)) = x → (u → A * u)  # ℝ³ → ℝ²
∂ᵀ(::typeof(residuals)) = x → (v → adjoint(A) * v)  # ℝ² → ℝ³

sqnorm(r) = sum(abs2, r)
∂(::typeof(sqnorm)) = r → (v → dot(2r, v))  # ℝ² → ℝ
∂ᵀ(::typeof(sqnorm)) = r → (w → 2r .* w)  # ℝ → ℝ²
```

Pocket AD

```
# Composition

function ∂(f::ComposedFunction)
    g, h = f.outer, f.inner
    return x → ∂(g)(h(x)) ∘ ∂(h)(x)
end

function ∂ᵀ(f::ComposedFunction)
    g, h = f.outer, f.inner
    return x → ∂ᵀ(h)(x) ∘ ∂ᵀ(g)(h(x))
end
```

Pocket AD

```
julia> import ForwardDiff as FD, Zygote

julia> f = sqnorm ∘ residuals;

julia> x, u = rand(3), [1, 0, 0];
```

```
julia> ∂(f)(x)(u)  # directional derivative
0.8691056836969242

julia> ∂ᵀ(f)(x)(1)  # gradient
3-element Vector{Float64}:
 0.8691056836969242
 0.9973491983376236
 0.5768822265195823
```

```
julia> FD.derivative(t -> f(x + t * u), 0)
0.8691056836969242

julia> Zygote.gradient(f, x)[1]
3-element Vector{Float64}:
 0.8691056836969242
 0.9973491983376236
 0.5768822265195823
```

Leveraging sparsity

From maps to matrices

To compute the Jacobian matrix J of a composition $f : \mathbb{R}^m \longrightarrow \mathbb{R}^n$:

- ~~product of intermediate Jacobian matrices~~
- reconstruction from several JVPs or VJPs

	forward mode	**reverse mode**
idea	1 JVP gives 1 column	1 VJP gives 1 row
formula	$J_{\cdot,j} = \partial f(x)[e_j]$	$J_{i,\cdot} = \partial f(x)^*[e_i]$
cost	n JVPs (input dimension)	m VJPs (output dimension)

Using fewer products

When the Jacobian is sparse, we can compute it faster[3].

If columns $j_1, \ldots, j_k$ of J are structurally **orthogonal** (their nonzeros never overlap), we deduce them all from a single JVP:

$$J_{j_1} + \ldots + J_{j_k} = \partial f(x)\left[e_{j_1} + \ldots + e_{j_k}\right]$$

Once we have grouped columns, sparse AD has two steps:

3. one JVP for each group $c = \{j_1, \ldots, j_k\}$
4. decompression into individual columns $j_1, \ldots, j_k$

[3] Curtis et al. (1974)

Two preliminary steps

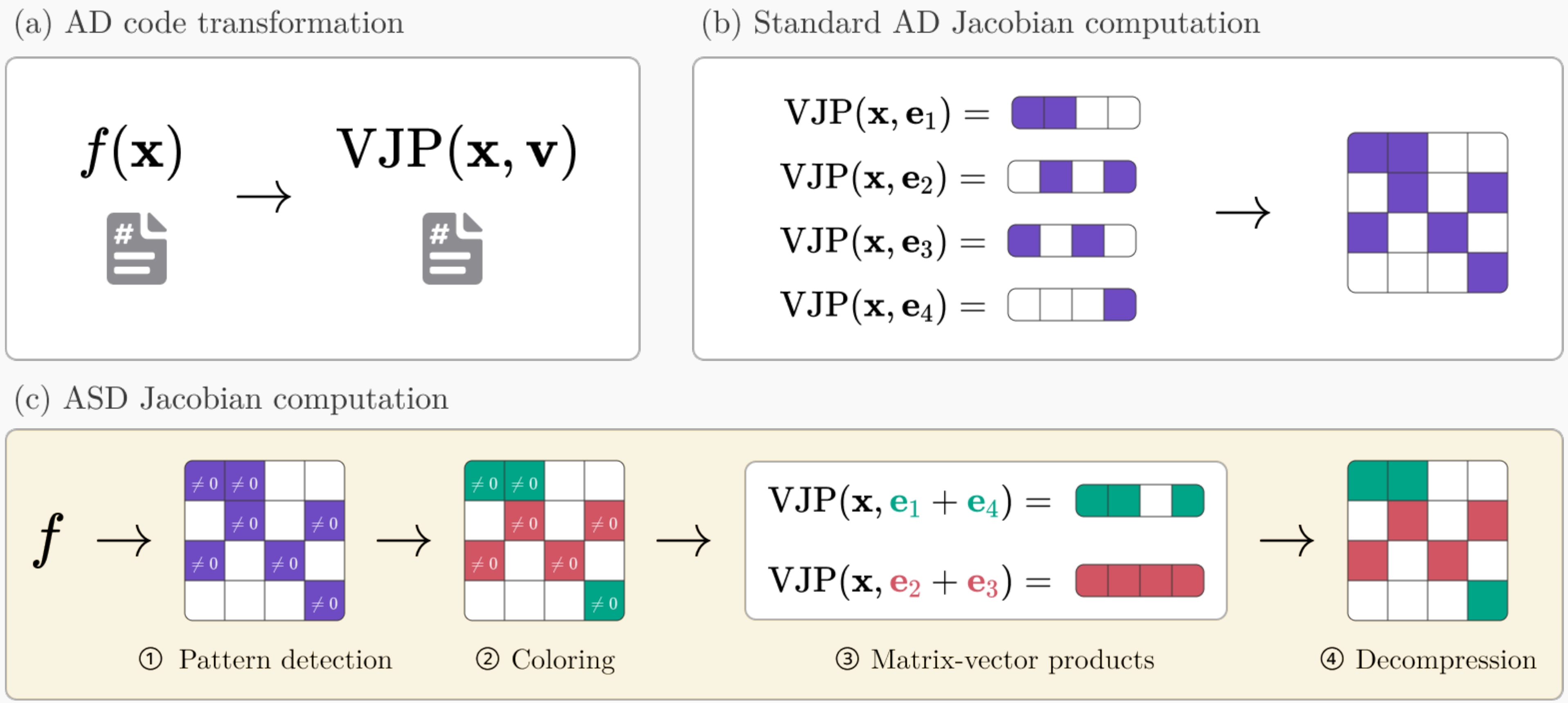
When grouping columns, we want to

- guarantee orthogonality (correctness) ⇒ pattern detection
- form the smallest number of groups (efficiency) ⇒ coloring

preparation	**execution**
1. pattern detection	3. matrix-vector products
2. coloring	4. decompression

The preparation phase can be **amortized** across several inputs.

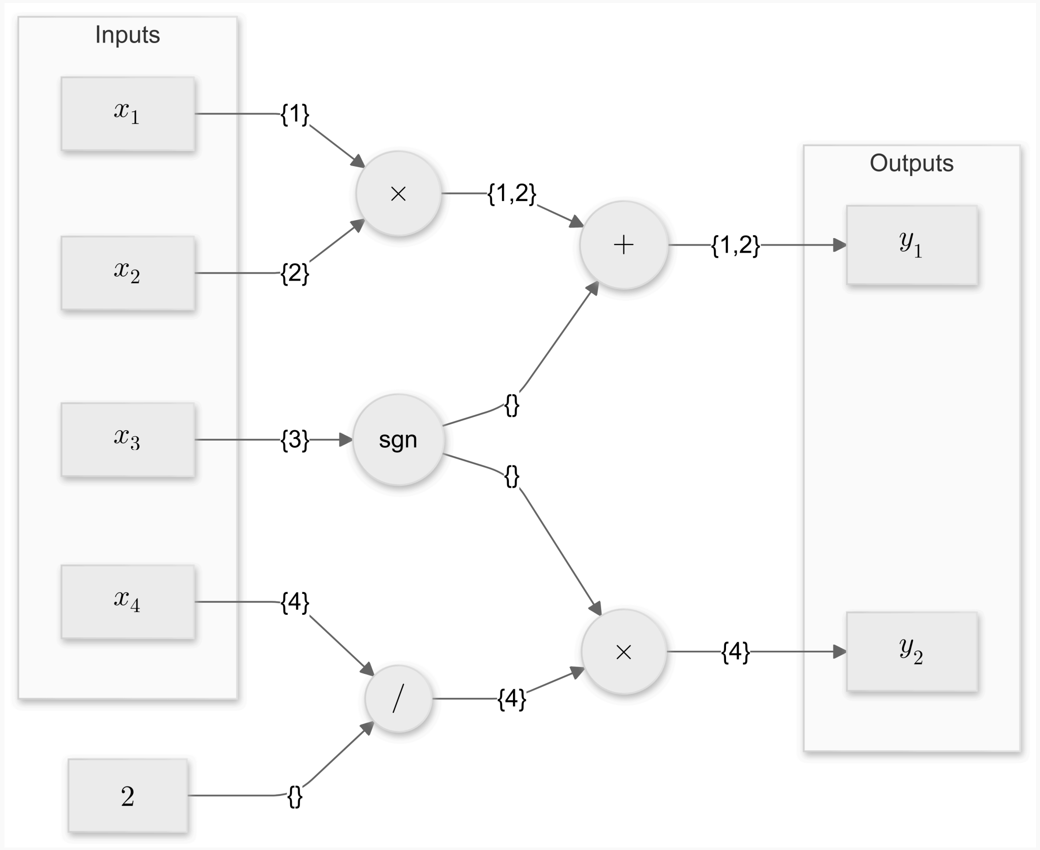
The gist in one slide



(a) AD code transformation
$f(\mathbf{x}) \rightarrow \mathrm{VJP}(\mathbf{x}, \mathbf{v})$
(b) Standard AD Jacobian computation
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_1) =$
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_2) =$
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_3) =$
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_4) =$
(c) ASD Jacobian computation
f
$\neq 0$
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_1 + \mathbf{e}_4) =$
$\mathrm{VJP}(\mathbf{x}, \mathbf{e}_2 + \mathbf{e}_3) =$
① Pattern detection
② Coloring
③ Matrix-vector products
④ Decompression

Hill & Dalle (2025)

Tracing dependencies in the computation graph



Hill et al. (2025)

Computation graph for

$$y_1 = x_1 x_2 + \operatorname{sign}(x_3)$$
$$y_2 = \operatorname{sign}(x_3) \times \left(\frac{x_4}{2}\right)$$

Its Jacobian matrix will have 3 nonzero coefficients:

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Pocket pattern detection

```julia
import Base: +, *, /, sign

struct Tracer
  indices::Set{Int}
end

Tracer() = Tracer(Set{Int}())

+(a::Tracer, b::Tracer) = Tracer(a.indices ∪ b.indices)
*(a::Tracer, b::Tracer) = Tracer(a.indices ∪ b.indices)
/(a::Tracer, b::Real) = Tracer(a.indices)
sign(a::Tracer) = Tracer()  # zero derivatives
```

Pocket pattern detection

```
julia> f(x) = [x[1] * x[2] * sign(x[3]), sign(x[3]) * x[4] / 2];

julia> x = Tracer.(Set.([1, 2, 3, 4]))
4-element Vector{Tracer}:
 Tracer(Set([1]))
 Tracer(Set([2]))
 Tracer(Set([3]))
 Tracer(Set([4]))

julia> f(x)
2-element Vector{Tracer}:
 Tracer(Set([2, 1]))
 Tracer(Set([4]))
```

Coloring for Jacobians

Matrix problem

Orthogonal partition of the columns of A.

If $A_{i j_1} \neq 0$ and $A_{i, j_2} \neq 0$, then columns j_1 and j_2 are in different groups $c(j_1) \neq c(j_2)$

Graph problem

Partial distance-2 coloring of a bipartite graph $\mathcal{G} = (\mathcal{I} \cup \mathcal{J}, \mathcal{E})$

If $(i, j_1) \in \mathcal{E}$ and $(i, j_2) \in \mathcal{E}$, then vertices j_1 and j_2 have different colors $c(j_1) \neq c(j_2)$.

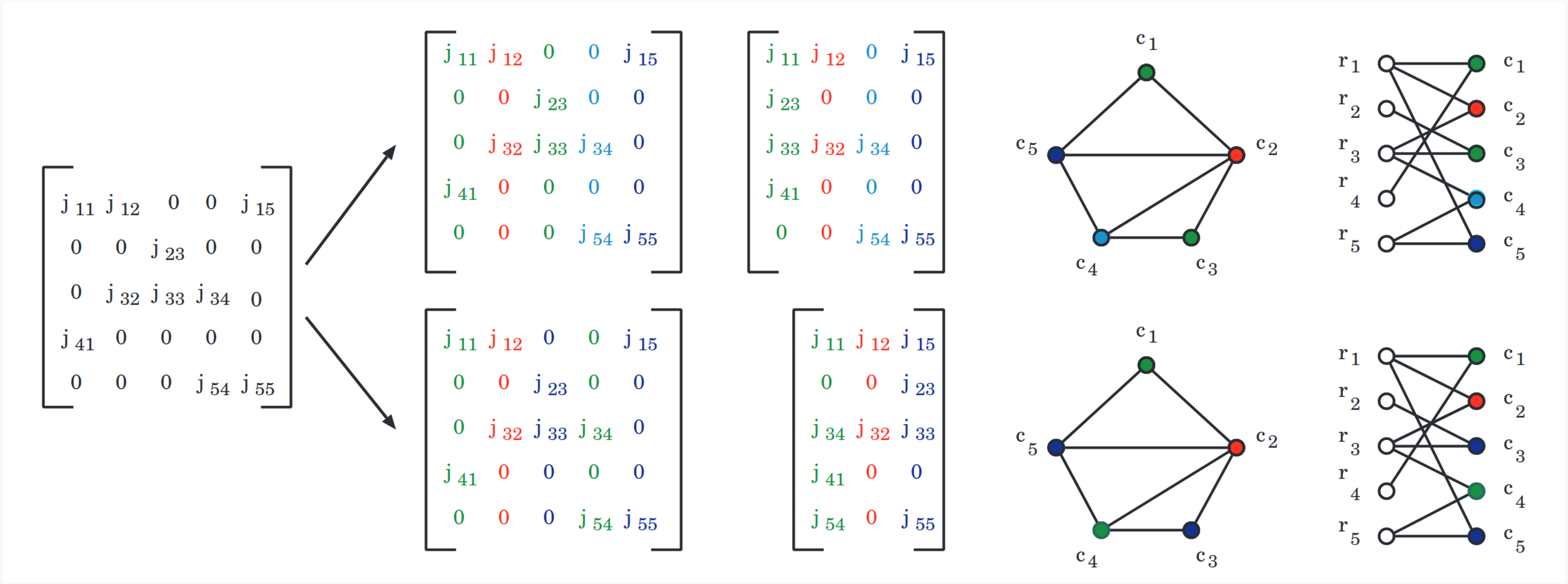
These are equivalent[4] if we define the graph representation

$$\mathcal{E} = \left\{(i, j) \in \mathcal{I} \times \mathcal{J} : A_{i,j} \neq 0\right\}$$

[4] Gebremedhin et al. (2005)

Coloring for Jacobians, illustrated

Coloring of intersection graph / distance-2 coloring of bipartite graph

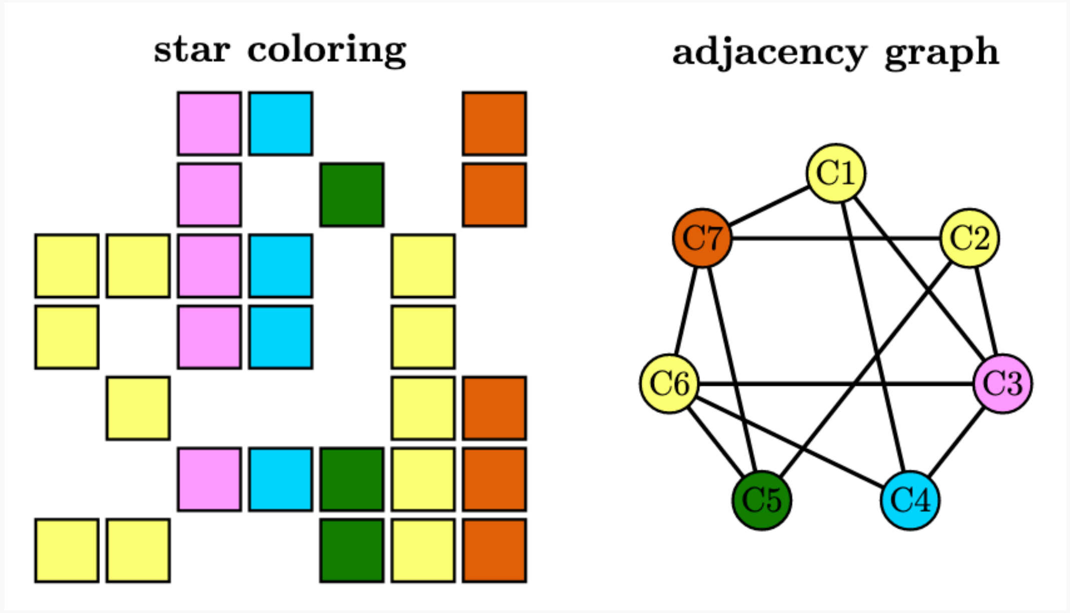


Gebremedhin et al. (2005)

Coloring for Hessians

What if our matrix has structure, like $A_{i,j} = A_{j,i}$?

We can compute a slightly different coloring[5] with fewer colors.

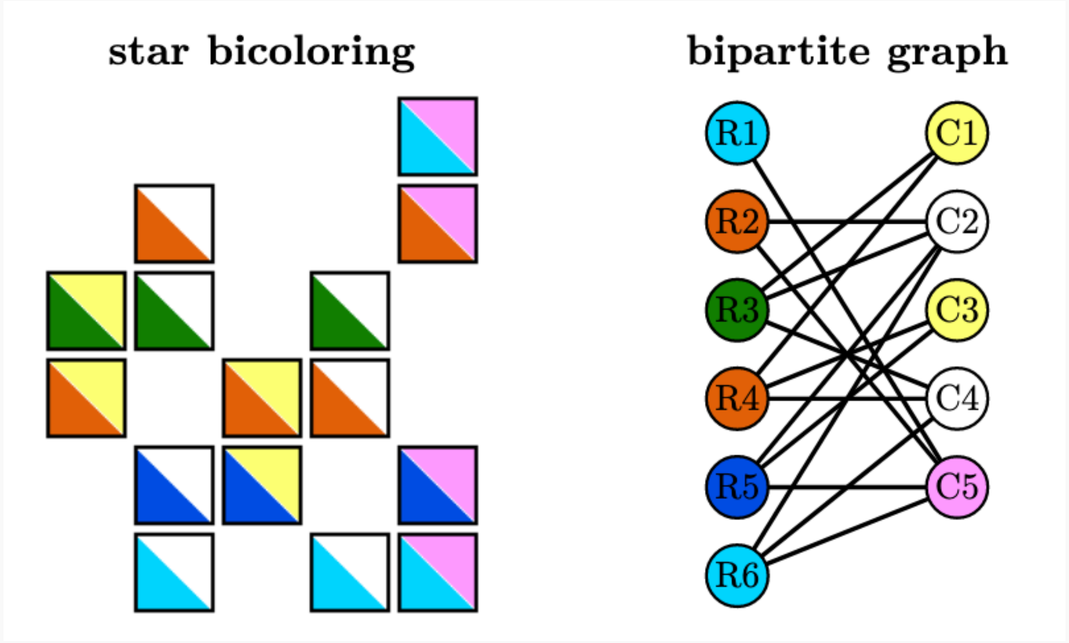


[5] Coleman & Moré (1984)

Coloring for bidirectional Jacobians

What if the columns are not orthogonal enough?

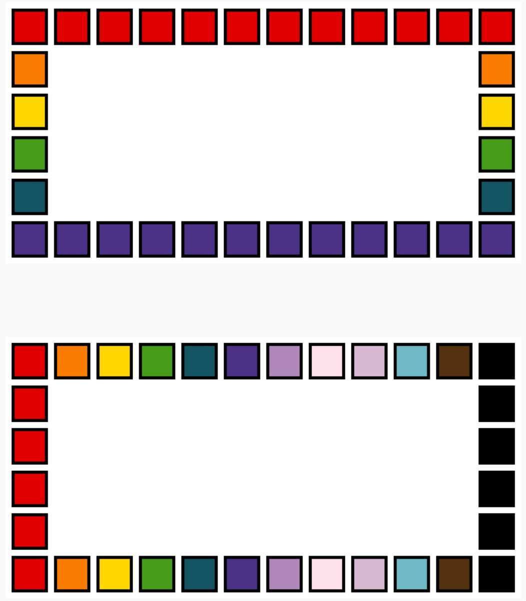
We can use both rows and columns[6] inside our coloring.

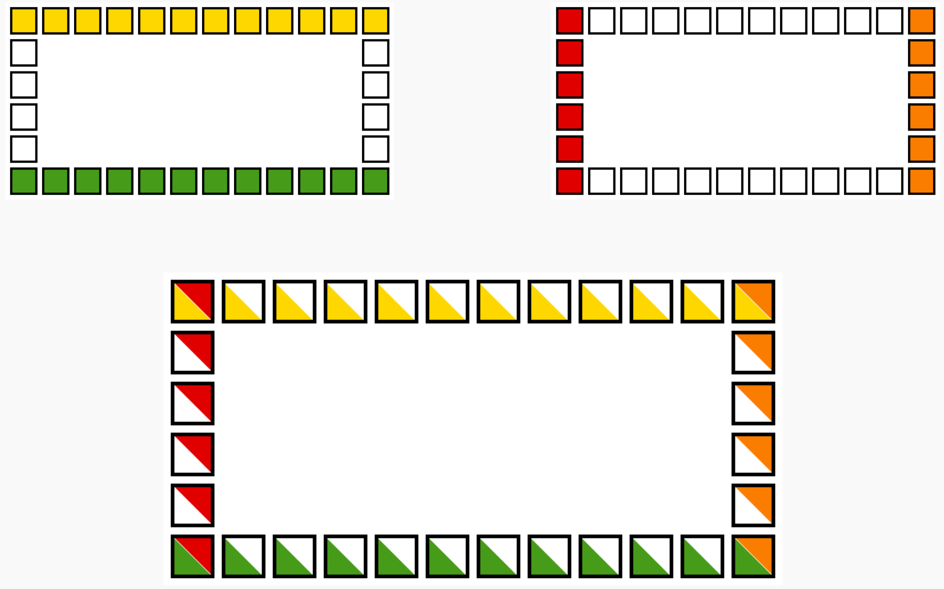


[6]Coleman & Verma (1998)

Benefits of bidirectional coloring

Compute Jacobians with a dense row **and** a dense column, using forward-mode AD + reverse-mode AD.


Unidirectional


Bidirectional

From bidirectional to symmetric [new]

To color the rows and columns of J, color the columns of $H = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}$

It sounds simple, but:

- Some colors may be redundant
- Detecting these is tightly linked to the two-colored structures
- Efficient decompression requires lots of preprocessing

Explanations and benchmarks in Montoison et al. (2025)

The sharp bits

Pattern detection

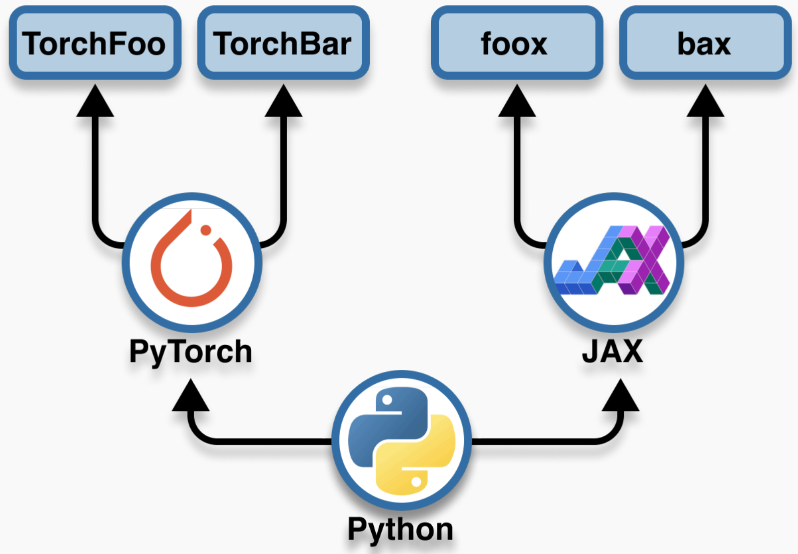
- Local versus global sparsity
- Control flow
- Linear and nonlinear interactions

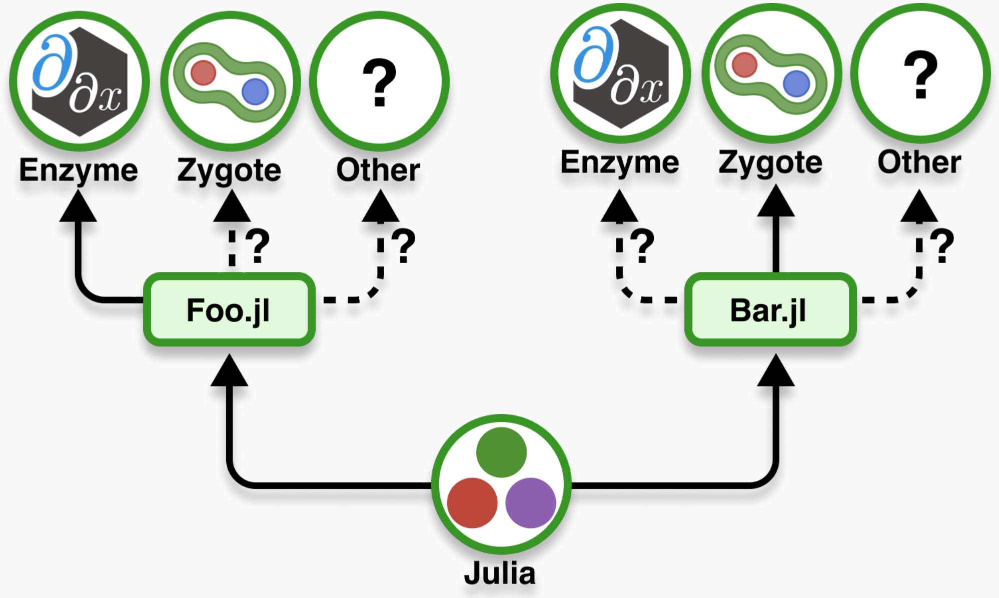
Coloring

- Only heuristic algorithms
- Vertex ordering matters a lot

Implementation

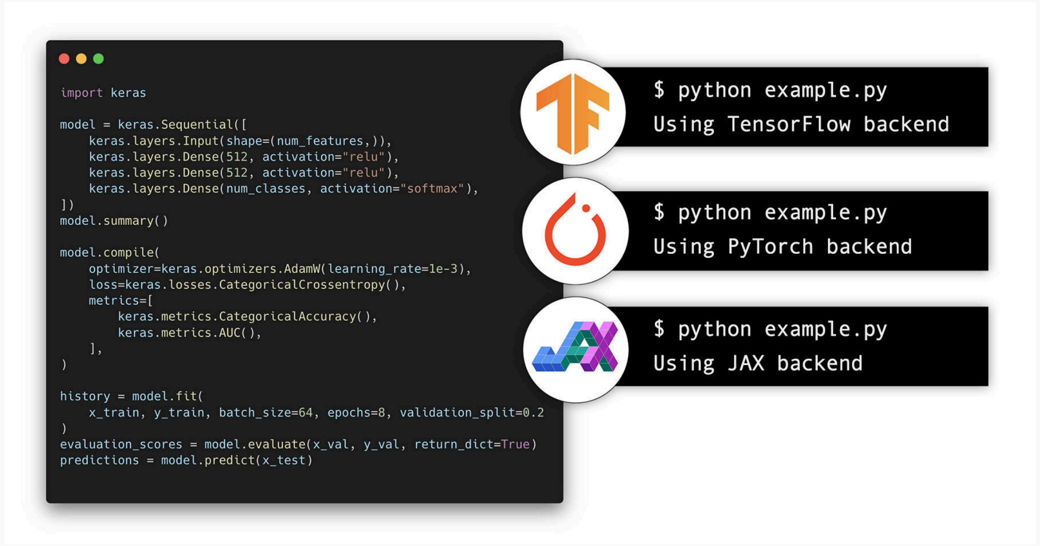
AD in Python & Julia





Interfaces for experimenting [new]

Once we have a common syntax, we can do more!



```python
import keras

model = keras.Sequential([
    keras.layers.Input(shape=(num_features,)),
    keras.layers.Dense(512, activation="relu"),
    keras.layers.Dense(512, activation="relu"),
    keras.layers.Dense(num_classes, activation="softmax"),
])
model.summary()

model.compile(
    optimizer=keras.optimizers.AdamW(learning_rate=1e-3),
    loss=keras.losses.CategoricalCrossentropy(),
    metrics=[
        keras.metrics.CategoricalAccuracy(),
        keras.metrics.AUC(),
    ],
)

history = model.fit(
    x_train, y_train, batch_size=64, epochs=8, validation_split=0.2
)
evaluation_scores = model.evaluate(x_val, y_val, return_dict=True)
predictions = model.predict(x_test)
```

```
$ python example.py
Using TensorFlow backend
```

```
$ python example.py
Using PyTorch backend
```

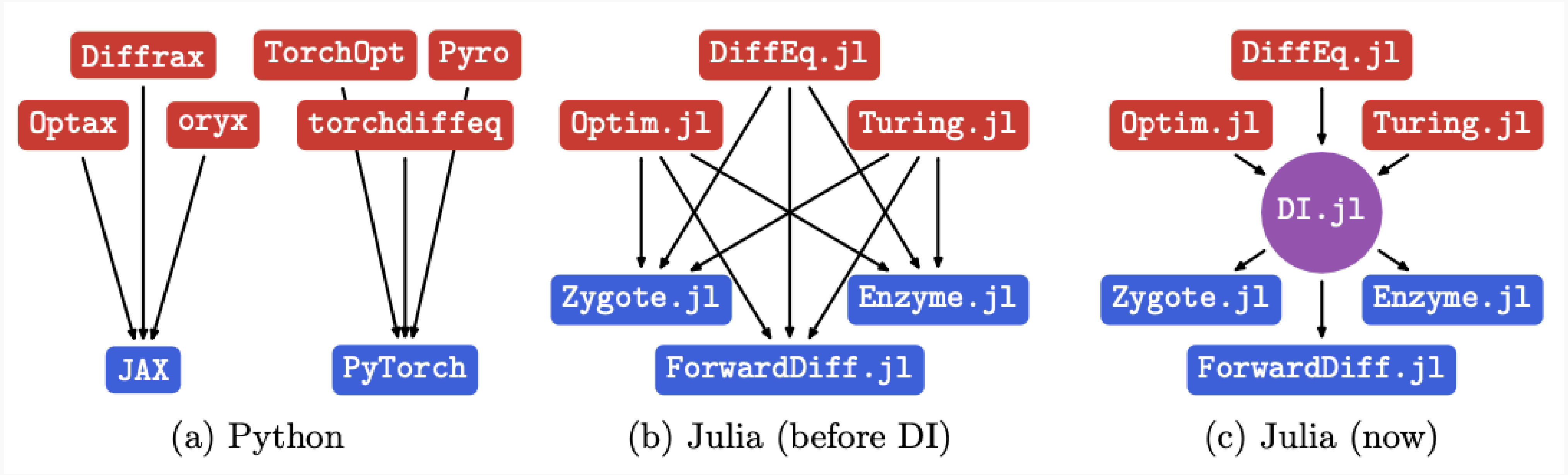
```
$ python example.py
Using JAX backend
```

In Python, `Keras` supports Tensorflow, PyTorch and JAX.

In Julia, 14 AD backends inside `Differentiationterface.jl`

One API to rule them all

Decouple the scientific libraries from the AD underneath.



Dalle & Hill (2025)

Previous implementations of sparse AD

- In low-level programming languages (C, Fortran)
- In closed-source languages (Matlab)
- In domain-specific languages (AMPL, CasADi)

Basically nothing in Python (either in JAX or PyTorch).

First drafts in Julia for scientific machine learning, but severely limited: single-backend, slow.

A modern sparse AD ecosystem [new]

Independent packages working together:

- **Step 1:** `SparseConnectivityTracer.jl` (Hill & Dalle, 2025)
- **Steps 2 & 4:** `SparseMatrixColorings.jl` (Montoison et al., 2025)
- **Step 3:** `Differentiationterface.jl` (Dalle & Hill, 2025)

	`SCT.jl`	`SMC.jl`	`DI.jl`
lines of code	5202	5184	19980
indirect dependents	461	487	896
downloads / month	7.8k	9.7k	33k

Compatible with generic code!

Impact

Users already include...

- Scientific computing: `SciML` (Julia's `scipy`)
  - Differential equations
  - Nonlinear solvers
  - Optimization
- Probabilistic programming: `Turing.jl`
- Symbolic regression: `PySR`

Python bindings in construction:

- `pysparsematrixcolorings`
- `sparsediffax`

Live demo

This is the part where things go sideways.

Perspectives

- GPU-compatible pattern detection and coloring
- Pattern detection in JAX with program transformations
- New, unsuspected applications “just because we can”

Going further

On general AD:

- Baydin et al. (2018)
- Margossian (2019)
- Blondel & Roulet (2024)

On sparse AD:

- Gebremedhin et al. (2005)
- Griewank & Walther (2008)
- Hill et al. (2025)

Bibliography

Baydin, A. G., Pearlmutter, B. A., Radul, A. A., & Siskind, J. M. (2018). Automatic Differentiation in Machine Learning: A Survey. *Journal of Machine Learning Research*, *18*(153), 1–43. http://jmlr.org/papers/v18/17-468.html

Blondel, M., & Roulet, V. (2024, July). *The Elements of Differentiable Programming*. arXiv. https://doi.org/10.48550/arXiv.2403.14606

Coleman, T. F., & Moré, J. J. (1984). Estimation of Sparse Hessian Matrices and Graph Coloring Problems. *Mathematical Programming*, *28*(3), 243–270. https://doi.org/10.1007/BF02612334

Coleman, T. F., & Verma, A. (1998). The Efficient Computation of Sparse Jacobian Matrices Using Automatic Differentiation. *SIAM Journal on Scientific Computing*, *19*(4), 1210–1233. https://doi.org/10.1137/S1064827595295349

Curtis, A. R., Powell, M. J. D., & Reid, J. K. (1974). On the Estimation of Sparse Jacobian Matrices. *IMA Journal of Applied Mathematics*, *13*(1), 117–119. https://doi.org/10.1093/imamat/13.1.117

Dalle, G., & Hill, A. (2025, May). *A Common Interface for Automatic Differentiation*. arXiv. https://doi.org/10.48550/arXiv.2505.05542

Gebremedhin, A. H., Manne, F., & Pothen, A. (2005). What Color Is Your Jacobian? Graph Coloring for Computing Derivatives. *SIAM Review*, *47*(4), 629–705. https://doi.org/10/cmwds4

Griewank, A., & Walther, A. (2008). *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation* (2nd ed). Society for Industrial and Applied Mathematics. https://epubs.siam.org/doi/book/10.1137/1.9780898717761

Hill, A., & Dalle, G. (2025). Sparser, Better, Faster, Stronger: Sparsity Detection for Efficient Automatic Differentiation. *Transactions on Machine Learning Research*. https://openreview.net/forum?id=GtXSN52nIW

Hill, A., Dalle, G., & Montoison, A. (2025, April). An Illustrated Guide to Automatic Sparse Differentiation. *ICLR Blogposts 2025*. https://iclr-blogposts.github.io/2025/blog/sparse-autodiff/

Margossian, C. C. (2019). A Review of Automatic Differentiation and Its Efficient Implementation. *Wires Data Mining and Knowledge Discovery*, *9*(4), e1305. https://doi.org/10.1002/widm.1305

Montoison, A., Dalle, G., & Gebremedhin, A. (2025, May). *Revisiting Sparse Matrix Coloring and Bicoloring*. arXiv. https://doi.org/10.48550/arXiv.2505.07308

Pearlmutter, B. A. (1994). Fast Exact Multiplication by the Hessian. *Neural Computation*, *6*(1), 147–160. https://doi.org/10.1162/neco.1994.6.1.147