FAST JACOBIANS AND HESSIANS BY LEVERAGING SPARSITY

An Illustrated Guide to Automatic Sparse Differentiation

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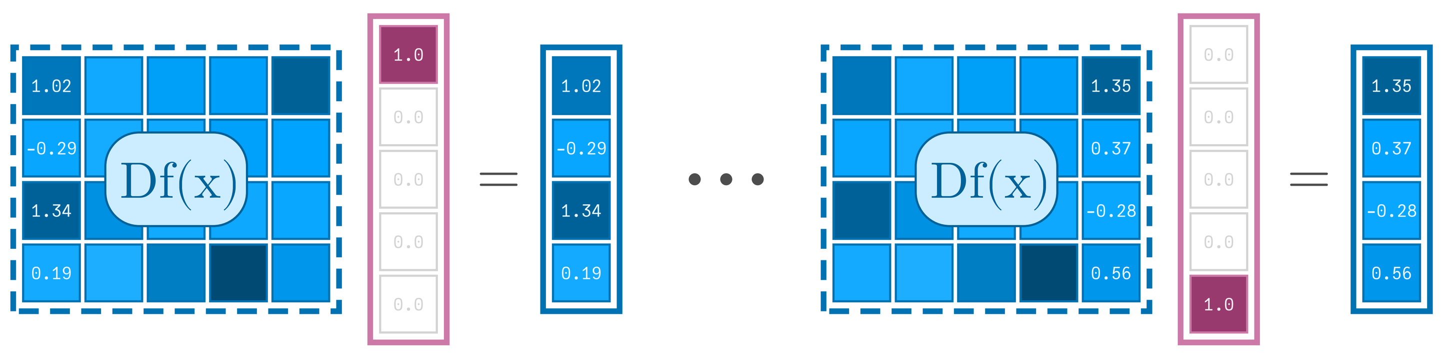
BLOG & CODE

Recap: Automatic Differentiation (AD)

The use of AD in deep learning is ubiquitous: Instead having to compute gradients and Jacobians by hand, AD automatically computes them for given PyTorch, JAX or Julia code.

Matrix-free Jacobian operators (dashed) lie at the core of AD. While we illustrate them as matrices to provide intuition, they are best thought of as **black-box functions** with unknown structure.
To turn such Jacobian operators into **Jacobian matrices** (solid), they are evaluated with all standard basis vectors.

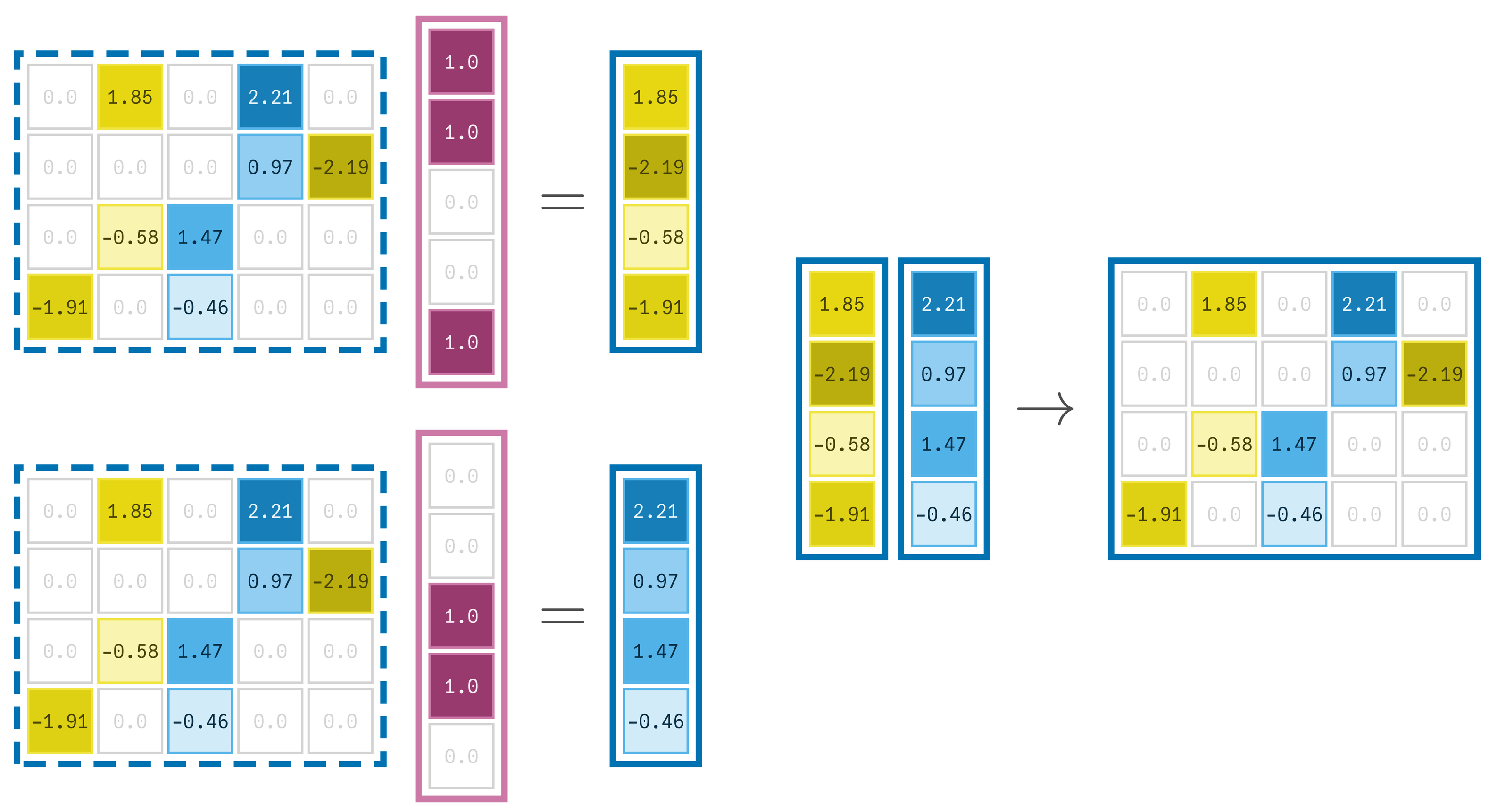


This constructs Jacobian matrices column-by-column[1] or row-by-row[2].

[1] Forward mode, computing as many JVPs as there are inputs (pictured).
[2] Reverse mode, computing as many VJPs as there are outputs.

Idea: Automatic Sparse Differentiation (ASD)

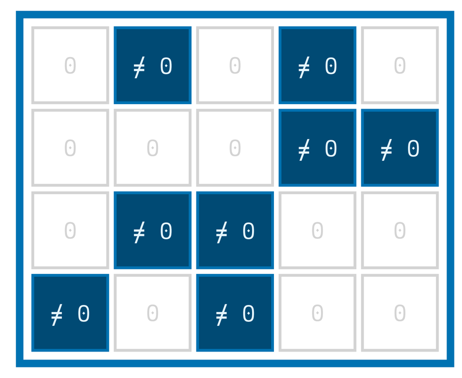
Since Jacobian operators are linear maps, we can **simultaneously compute the values of multiple orthogonal columns** (or rows) and decompress the resulting vectors into the Jacobian matrix [1, 2].



To do this, ASD requires knowledge of the structure of the resulting Jacobian matrix. Since Jacobian operators have unknown structure, two preliminary steps are required.

Step 1: Sparsity Pattern Detection

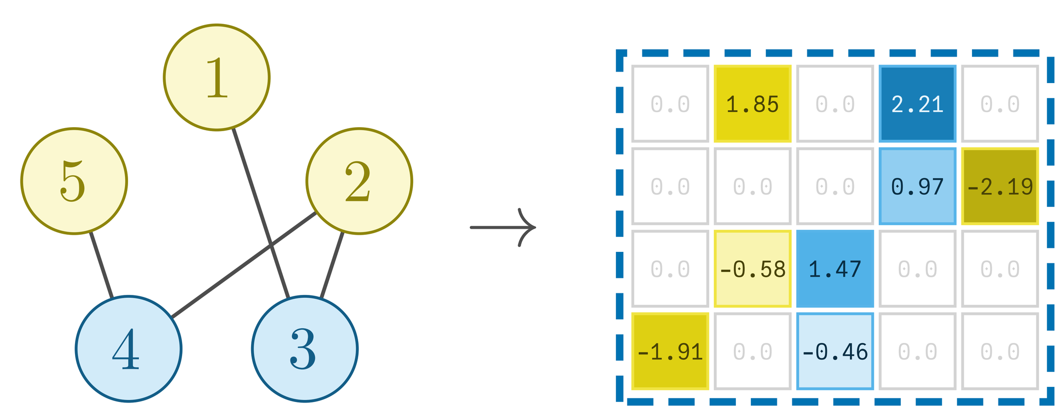
To find orthogonal colomns, the pattern of non-zero values in the Jacobian matrix has to be computed. This requires a binary AD system.



Mirroring the multitude of approaches to AD, many viable approaches to pattern detection exist [3–5].

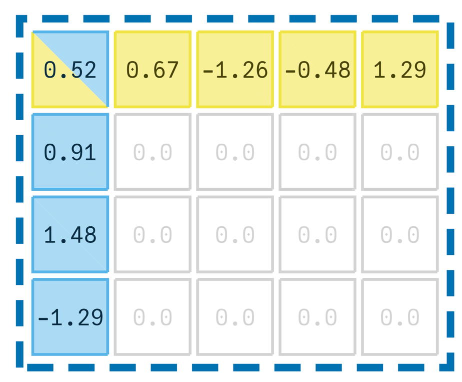
Step 2: Coloring

Graph coloring algorithms are applied to the sparsity pattern to detect orthogonal columns/rows [2].



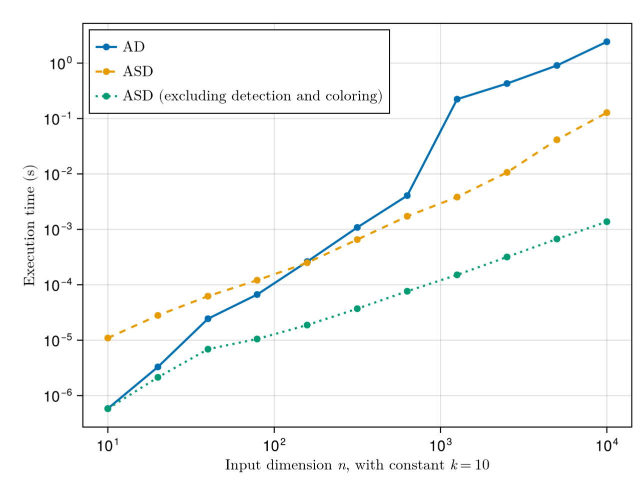
Bicoloring

ASD can be accelerated even further by coloring both rows and columns and combining forward and reverse modes [6, 7].



Benchmarks

ASD can drastically outperform AD. The performance depends on the sparsity of the Jacobian matrix: savings of fewer matrix-vector products have to outweigh the cost of sparsity pattern detection and coloring.



Benchmark: k iterations of difference operator on input of length n.

References

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