FAST JACOBIANS AND HESSIANS BY LEVERAGING SPARSITY

An Illustrated Guide to Automatic Sparse Differentiation

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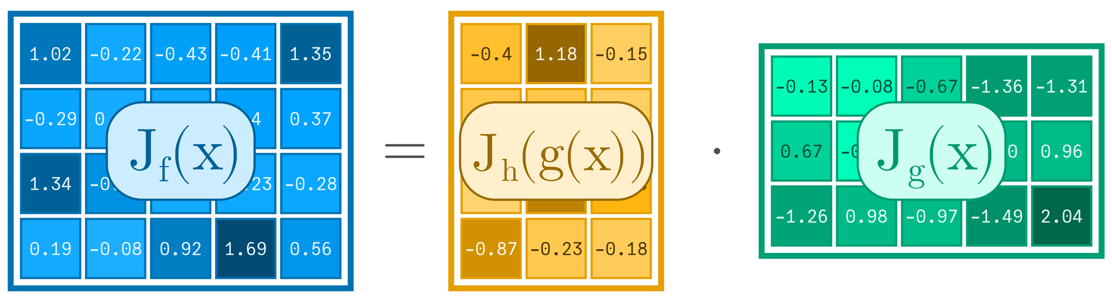
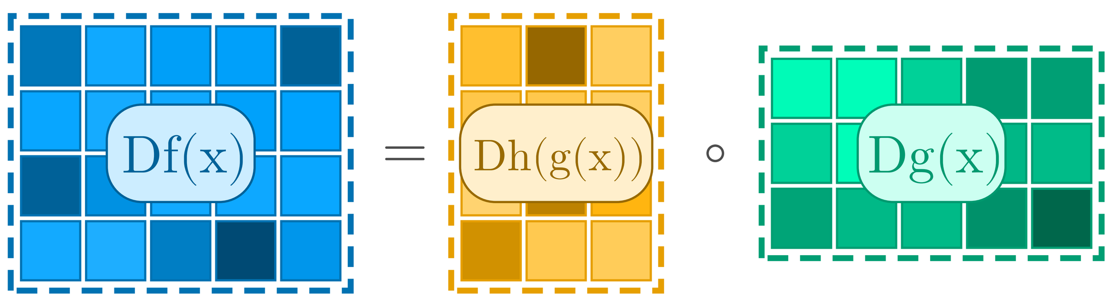
Recap: Automatic Differentiation (AD)

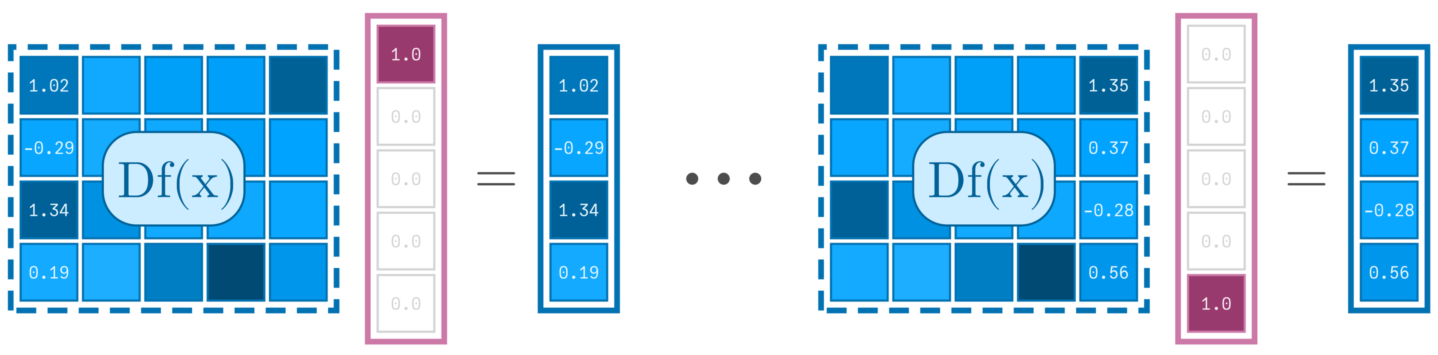
The chain rule tells us that the Jacobian of a composed function $f = h \circ g$ is obtained by multiplying the **Jacobian matrices** (solid) of h and g.



However, AD doesn't use Jacobian matrices, instead opting for matrix-free **Jacobian operators** (dashed). The chain rule now corresponds to a composition of operators.



To turn such (composed) **Jacobian operators** into **Jacobian matrices**, they are evaluated with all standard basis vectors.

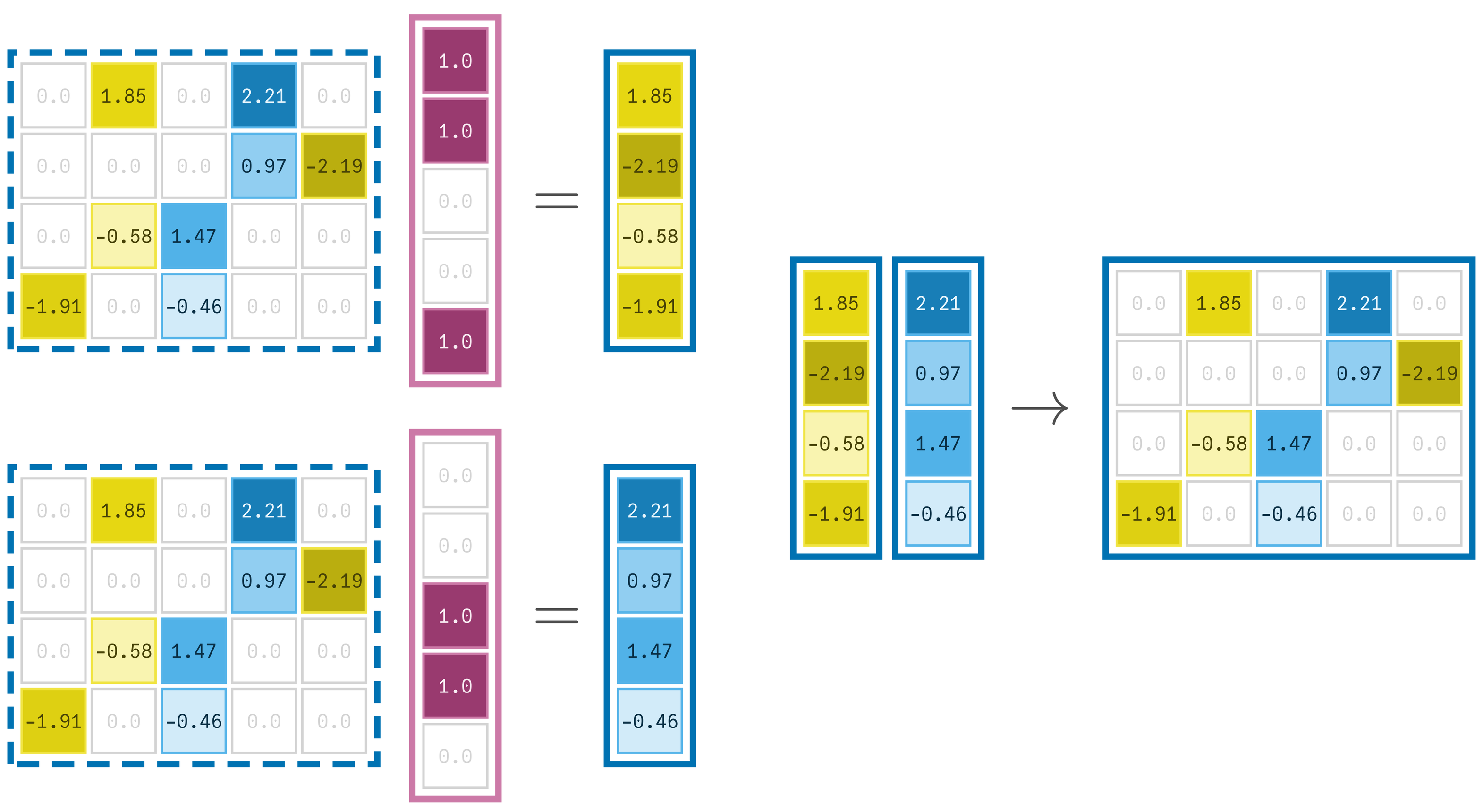


This either constructs matrices column-by-column (forward mode, computing as many JVPs as there are inputs) or row-by-row (reverse mode, computing as many VJPs as there are outputs) .

Idea: Automatic Sparse Differentiation (ASD)

Since Jacobian operators are linear maps, we can:

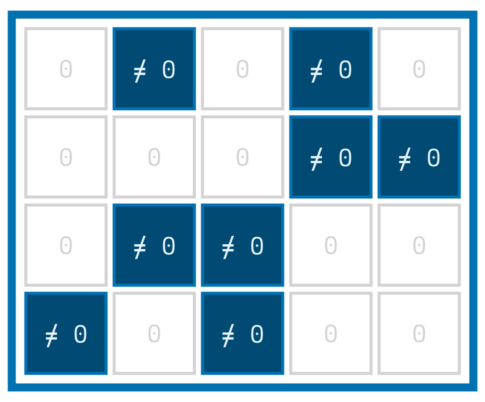
1. simultaneously compute the values of orthogonal columns/rows
2. decompress the resulting vectors into the Jacobian matrix.



Unfortunately, contrary to our illustrations, Jacobian operators (dashed) are black-box functions with unknown structure. Two preliminary steps are therefore required to determine orthogonal columns/rows.

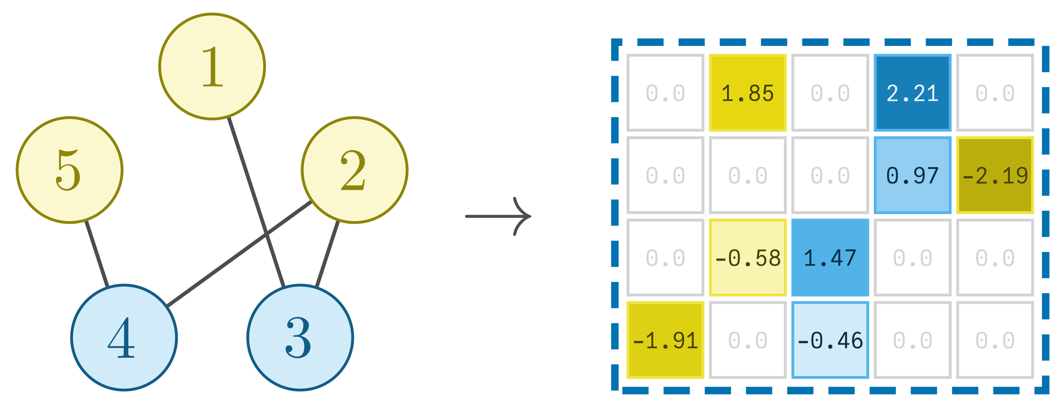
Step 1: Pattern Detection

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



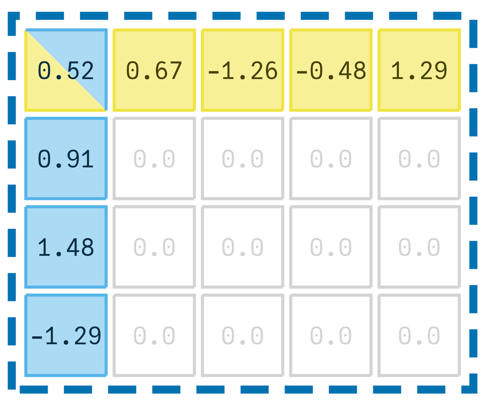
Step 2: Coloring

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



Bicoloring

ASD can be accelerated even further by coloring both rows and columns and combining forward and reverse modes.



Demonstration

```julia
using DifferentiationInterface
using SparseConnectivityTracer, SparseMatrixColorings
import ForwardDiff

ad_backend = AutoForwardDiff()
asd_backend = AutoSparse(
    ad_backend;
    TracerSparsityDetector(),
    GreedyColoringAlgorithm()
)

jacobian(f, ad_backend,  x) # dense
jacobian(f, asd_backend, x) # sparse
```

References

Bibliography goes here

Check out our ICLR blog post for more information!