

Seed Matrices

Ludger Paehler
Jan Hückelheim
Sri Hari Krishna Narayanan

SIAM CSE 2023



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Seed Matrices: Theory

Recall:

Forward mode computes

$$JS$$

at cost proportional to number of columns in S .

Reverse mode computes

$$W^T J$$

at cost proportional to number of columns in W .

Seed Matrices: Practice

In reality, it is rarely that simple.

- ▶ data structure pragmatics
- ▶ multiple output variables
- ▶ multiple input variables
- ▶ Jacobian compression

Seed Matrices: data structure pragmatics

Depending on

- ▶ programming language (row-major vs. column-major arrays)
- ▶ choice of AD tool

the J , S , W matrices might be stored in a transposed layout or as part of a struct and the derivative dimension might be flattened.

Consequently, what is logically \dot{X}_{ij} might be stored as $dX(j,i)$ or $x[i].grad[j]$.

Seed Matrices: multiple scalar outputs, scalar input

- Consider function `foo(in:x,out:f,out:g)`
- Then, forward mode AD computes

$$\dot{f} = \frac{\partial f}{\partial x} \dot{x} \quad \text{and} \quad \dot{g} = \frac{\partial g}{\partial x} \dot{x}$$

- Initializing $\dot{x} = 1$ yields the full (logical) Jacobian, split over two data structures.

$$J = \begin{bmatrix} \dot{f} \\ \dot{g} \end{bmatrix}$$

Seed Matrices: multiple scalar outputs, vector input

- Consider function `foo(in:x(N), out:f, out:g)`
- That is, x is now a vector of length N .
- Then, vector forward mode AD computes

$$\dot{f} = \frac{\partial f}{\partial x} \dot{x} \quad \text{and} \quad \dot{g} = \frac{\partial g}{\partial x} \dot{x}$$

- Initializing \dot{x} to the identity matrix yields the full Jacobian, at a cost proportional to N .
- Alternatively, one could loop over $\dot{x} = e_i$, computing one column of the Jacobian at a time.

Seed Matrices: multiple scalar outputs, vector input

- Consider function `foo(in:x(N),out:f,out:g)`
- Then, reverse mode AD computes

$$\bar{x} = \bar{f} \frac{\partial f}{\partial x} + \bar{g} \frac{\partial g}{\partial x}$$

- Initializing $\bar{f} = 1$ and $\bar{g} = 0$ yields $\bar{x} = \frac{\partial f}{\partial x}$
- Initializing $\bar{f} = 0$ and $\bar{g} = 1$ yields $\bar{x} = \frac{\partial g}{\partial x}$

Seed Matrices: multiple scalar outputs, vector input

- Initializing $\bar{f} = 1$ and $\bar{g} = 0$ yields $\bar{x} = \frac{\partial f}{\partial x}$
- Initializing $\bar{f} = 0$ and $\bar{g} = 1$ yields $\bar{x} = \frac{\partial g}{\partial x}$
- Thus, we are computing $W^T J$ for each of

$$W = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad W = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- In vector reverse mode, we can let $\bar{f} = [1 \ 0]$ and $\bar{g} = [0 \ 1]$ and compute the full Jacobian all at once, using $W = I$.

Seed Matrices: multiple scalar inputs, scalar output

- Now, consider function `foo(in:x,in:y,out:f)`
- Then, reverse mode AD computes

$$\bar{x} = \bar{f} \frac{\partial f}{\partial x} \quad \text{and} \quad \bar{y} = \bar{f} \frac{\partial f}{\partial y}$$

- Initializing $\bar{f} = 1$ yields the full Jacobian, or gradient, split over two data structures.

$$J = \begin{bmatrix} \bar{x} & \bar{y} \end{bmatrix}$$

Seed Matrices: multiple scalar inputs, scalar output

- Consider function `foo(in:x,in:y,out:f)`
- Then, forward mode AD computes

$$\dot{f} = \frac{\partial f}{\partial x} \dot{x} + \frac{\partial f}{\partial y} \dot{y}$$

- Initializing $\dot{x} = 1$ and $\dot{y} = 0$ yields $\dot{f} = \frac{\partial f}{\partial x}$
- Initializing $\dot{x} = 0$ and $\dot{y} = 1$ yields $\dot{f} = \frac{\partial f}{\partial y}$

Seed Matrices: multiple scalar inputs, scalar output

- Initializing $\dot{x} = 1$ and $\dot{y} = 0$ yields $\dot{f} = \frac{\partial f}{\partial x}$
- Initializing $\dot{x} = 0$ and $\dot{y} = 1$ yields $\dot{f} = \frac{\partial f}{\partial y}$
- Thus, we are computing JS for each of

$$S = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad S = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

- In vector forward mode, we can let $\dot{x} = [1 \ 0]$ and $\dot{y} = [0 \ 1]$ and compute the full Jacobian all at once, using $S = I$.

Seed Matrices: multiple vector inputs

- Consider `foo(in:x(3),in:y(3),out:f)`
- Then, to compute the full Jacobian using vector forward mode AD, we must initialize

$$\dot{x} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

and

$$\dot{y} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Seed Matrices: Jv and $J^T v$ products

- ▶ Numerical algorithms may only need Jv and/or $J^T v$ products
- ▶ Can initialize S or W to v and compute this product at a small multiple of function cost
- ▶ AD tool may not support vector forward or vector reverse mode
- ▶ Can iterate through columns of S or W