Exploiting Intermediate Sparsity in Computing Derivatives for a Leapfrog Scheme

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Outline

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1. What is Leapfrog
2. Black-Box Approach
3. Intermediate Sparsity (IS) Approach, Compressed Jacobian
4. 2d-Example Shallow Water
   - Simple Update
   - Complex Update
5. Conclusion

What is Leapfrog

Target: Calculate $Z(T)$ from $Z(0)$ (initial value) and W (parameter)

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Leapfrog Scheme (LS)

Initialize $Z(0)$ and W

Compute $Z(1)$

for $t = 1$ **to** $T - 1$ **do**

$$Z(t+1) = H(Z(t), Z(t-1), W)$$

end do

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Calculate Derivatives

Let X be a subset of s elements from the $n + p$ sized $[Z(0), W]$.

We want:

$$\frac{dZ(T)}{dX}$$

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Black-Box Approach (BB)

Initialize $[Z(0), \frac{dZ(0)}{dX}]$ and $[W, \frac{dW}{dX}]$

Compute $[Z(1), \frac{dZ(1)}{dX}]$

for $t = 1$ **to** $T-1$ **do**

$$\left[Z(t+1), \frac{dZ(t+1)}{dX}\right] = \hat{H}\left(Z(t), \frac{dZ(t)}{dX}, Z(t-1), \frac{dZ(t-1)}{dX}, W, \frac{dW}{dX}\right)$$

end do

Complexity of BB

Operations:

- Computation of H takes f_H flops

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- $Z \in \mathbb{R}^n$, $W \in \mathbb{R}^p$
  therefore computation of H takes $O(2n + p)$ words of storage

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Differentiate w.r.t. X:

$$\frac{dZ(t+1)}{dX} = \frac{\partial H}{\partial Z(t)} \cdot \frac{dZ(t)}{dX} + \frac{\partial H}{\partial Z(t-1)} \cdot \frac{dZ(t-1)}{dX} + \frac{\partial H}{\partial W} \cdot \frac{dW}{dX}$$

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Fact

$$\frac{\partial H}{\partial \ldots} \textit{ is sparse for PDE problems}$$

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Fact

$$\frac{\partial H}{\partial \ldots} \text{ *is sparse for PDE problems*}$$

Exploit this fact with cheap "sparse matrix – matrix" multiplications

Why is the matrix sparse

H typically comes from a stencil, which depends only on a few, neighbored cells

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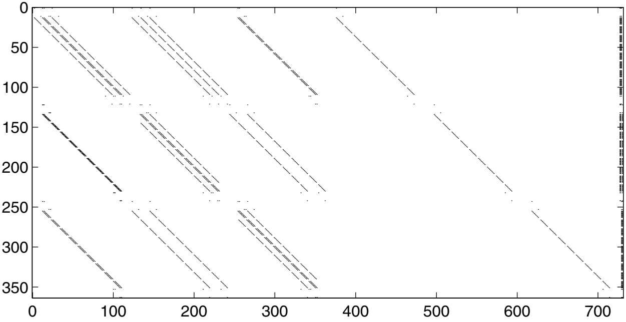
In forthcoming example:
max. 13 non-zero entries of $[\frac{\partial H}{\partial Z(t)}, \frac{\partial H}{\partial Z(t-1)}, \frac{\partial H}{\partial W}]$



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Compute $[Z(1), \frac{dZ(1)}{dX}]$.

for $t = 1$ **to** $T - 1$ **do**

  Step 1: Compute $Z(t+1)$ and $\frac{\partial H}{\partial Z(t)}, \frac{\partial H}{\partial Z(t-1)}, \frac{\partial H}{\partial W}$

  Step 2: Compute* $\frac{dZ(t+1)}{dX}$ via matrix-matrix multiplication

end do

* via $$\frac{dZ(t+1)}{dX} = \frac{\partial H}{\partial Z(t)} \cdot \frac{dZ(t)}{dX} + \frac{\partial H}{\partial Z(t-1)} \cdot \frac{dZ(t-1)}{dX} + \frac{\partial H}{\partial W} \cdot \frac{dW}{dX}$$

Complexity for IS-SL

Assume: "matrix-matrix" multiplications are optimized for sparse matrices: sparse linear algebra (SL)

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Another way: Compressed Jacobians (IS-CJ)

Let S^1, S^2 be suitable chosen seed matrices with λ_1, λ_2 columns for $\frac{dZ(t)}{dX}$ and $\frac{dZ(t-1)}{dX}$

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Complexity: $(\lambda = \lambda_1 + \lambda_2 + p)$

- Computation: $O(\lambda f_H T) + O(snT)$
- Memory: $O(\lambda(2n + p)) + O(sn)$

Complexity overview

	BB	IS–SL	IS–CJ
Computation	$O(sf_H T)$	$O(\kappa f_H T) + O(snT)$	$O(\lambda f_H T) + O(snT)$
Storage	$O(s(2n+p))$	$O(\kappa(2n+p)) + O(sn)$	$O(\lambda(2n+p)) + O(sn)$

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Assume: $\kappa, \lambda \ll s$

IS is faster then BB if $O(\kappa f_H T) \gg O(snT)$

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Example Shallow Water in 2d

Shallow Water used to simulate water flow, where vertical dimension is much smaller than horizontal (shallow).

E.g. rivers, lakes, costal flow

Variables: water height, x-momentum, y-momentum (2d)

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We calculate $s = n + p$ derivatives

Grid size	n	p	$s = n + p$
11×11	$3 \cdot 11 \cdot 11 = 363$	4	367
16×16	$3 \cdot 16 \cdot 16 = 768$	4	772
21×21	$3 \cdot 21 \cdot 21 = 1323$	4	1327

Memory & . . .

Grid size	IS–SL	IS–CJ	BB
11×11	3.72	3.85	4.70
16×16	13.61	13.84	18.82
21×21	37.82	38.16	53.31

Memory requirements in megabytes

. . . & Runtime

Grid size (platform)	SL	CJ	MM	IS–SL	IS–CJ	BB
11×11 (IBM)	4.90	1.93	8.03	12.93	9.96	4.24
16×16 (IBM)	17.77	8.70	38.66	56.43	47.36	36.68
21×21 (IBM)	42.98	21.51	119.32	162.30	140.83	71.98
11×11 (Sun)	12.26	6.55	19.24	31.50	25.79	26.63

Runtime in seconds

- SL: calculate sparse Jacobians
- CJ: calculate compressed Jacobians
- MM: matrix-matrix multiplications
- SL+MM = IS-SL, CJ+MM = IS-CJ

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Expensive Update

Lets evaluate H not only one time, but up to 16 times to emulate a function H, which is more expensive to calculate

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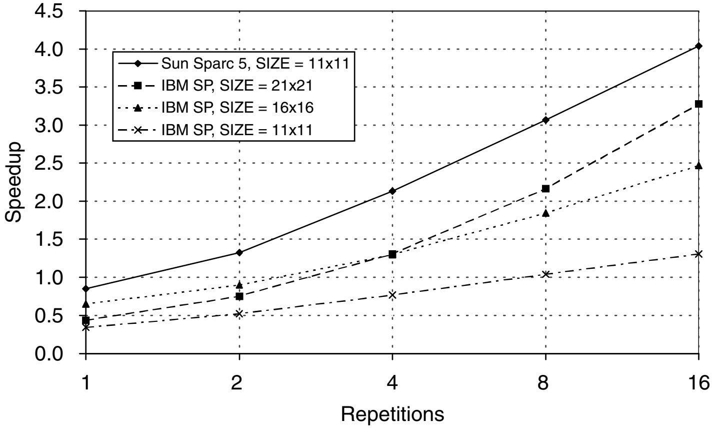
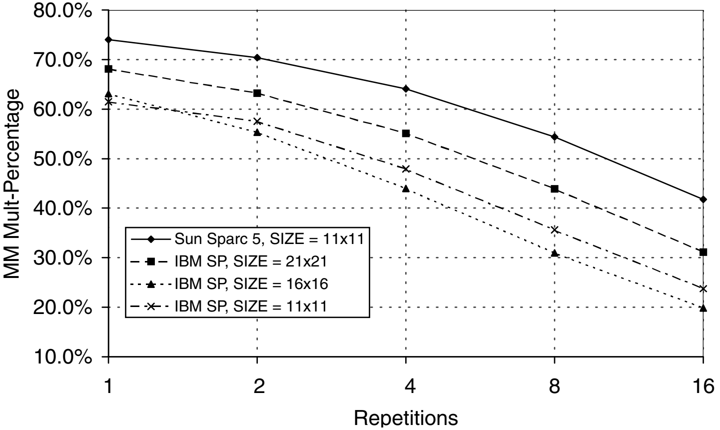


MM Multiplication Percentage



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Lit.: C. Bischof, M. Bücker, P. Wu:
Exploiting Intermediate Sparsity in Computing Derivatives for a Leapfrog Scheme,
Comp. Opt. Appl. 24, 117–133, 2003