Distributed Matrix Exponentiation in R

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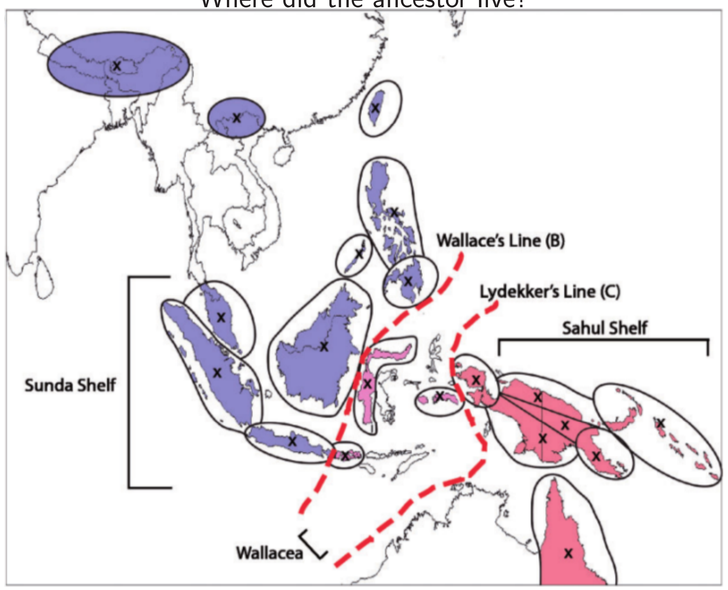
NIMBioS

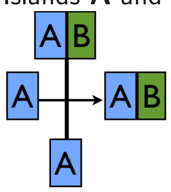
Motivation: Biogeography

Where did the ancestor live?



Modeling anagenic events requires matrix exponentiation.

2 Islands **A** and **B**



Problems:

- n areas $\implies$ 2^n ranges $\implies$ exponential of $2^n \times 2^n$ matrix.
- Matrix exponentiation is very slow!
- Needed for every branch, at every step of ML search.

Matrix Exponentiation

For a square matrix $\mathbf{X}$ (Laguerre 1867):

$$e^{\mathbf{X}} := \mathbf{I} + \frac{1}{1!}\mathbf{X} + \frac{1}{2!}\mathbf{X}^2 + \frac{1}{3!}\mathbf{X}^3 + \dots$$

Scaling-and-squaring techniques with Padé approximations are typical [1] and exploit these two relationships:

$$e^{\mathbf{X}} := \text{expm}(\mathbf{X}) = \text{expm}\left(\frac{1}{2^j}\mathbf{X}\right)^{2^j} \text{ and } e^{\mathbf{X}} \approx P_p(\mathbf{X})Q_p(\mathbf{X})^{-1}$$

with $p = 6$ typical, and j bounded by $\|A\|_1$.

This approach is:

- Computationally expensive.
- An approximation.
- (Relatively) Numerically stable.
- Needs $\left(p + j + \frac{1}{3}\right) n^3$ float ops.

Improvements to the Algorithm

- Need j large enough for accurate estimations . . . but no larger.
- Larger j $\implies$ more matrix multiplications.
- More mults $\implies$ longer run times and worse numerical precision.
- Al-Mohy and Higham [2] significantly improved the bound on j.

`expm()` in the pbdDMAT Package

- Uses Al-Mohy and Higham's improved method.
- Serial and distributed versions (same syntax!) [3].
- Each easily linked with parallel BLAS.

```
library(pbdDMAT)

x <- matrix(rnorm(100), 10, 10)
expm(x)

dx <- as.ddmatrix(x)
expm(dx)
```

Benchmark Configuration

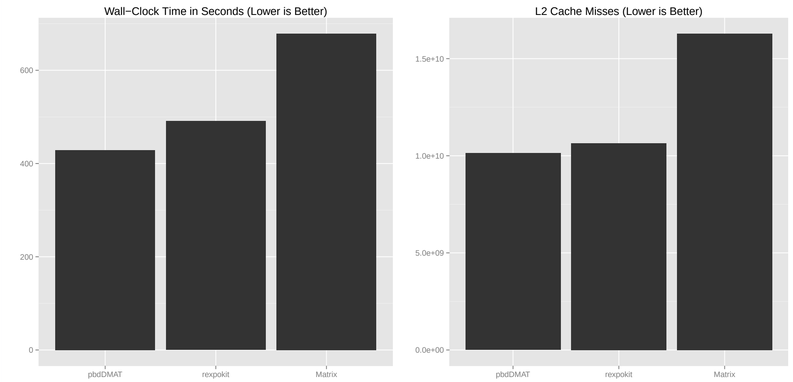
We compared different implementations on **Darter**, a 250 Tflops Cray supercomputer at the University of Tennessee. It has 748 compute nodes, each with 2 2.6 GHz Intel 8-core Sandy Bridge XEON's, 2 GiB RAM per core, and connected with a Cray Aries router (8GB/s bandwidth).

Problem:	Matrix exponential of 5000×5000 matrix.
R:	3.1.0
Packages:	Matrix 1.1-2, rexpokit 0.25, pbdDMAT 0.3-0
Libraries:	Cray LibSci 12 and MPT 6, NETLIB ScaLAPACK
Compilers:	gnu 4.8.2
Configuration:	1 thread == 1 MPI rank == 1 physical core

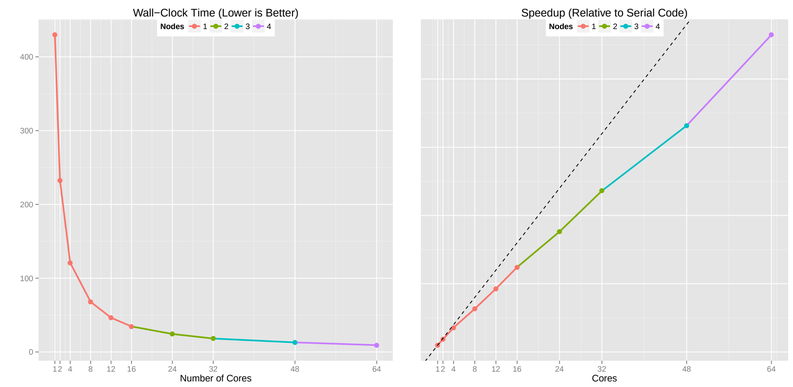
pbdR
Programming with Big Data in R

Performance Benchmarking

Serial Matrix Exponentiation Comparison



Parallel Matrix Exponentiation Scalability Study



References

[1] Al-Mohy, A. H. and N. J. Higham (2009). A New Scaling and Squaring Algorithm for the Matrix Exponential.

[2] Moler, C. and C. Van Loan (2003). Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later. *SIAM Review 45*(1), 3–49.

[3] Schmidt, D., W.-C. Chen, G. Ostrouchov, and P. Patel (2012). pbdDMAT: Distributed Matrix Algebra Computation. R package.

Acknowledgements

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