

On Stability of Newton Schulz Iterations in an Approximate Algebra

Matt Challacombe* and Nicolas Bock†

Theoretical Division, Los Alamos National Laboratory

I. INTRODUCTION

Decay principles, often very sparse but very ill-conditioned problems.

A. Incomplete Schemes

Incompleteness -i sparse approximations dense problems, uses conventional sparse infrastructure, second order errors in matrix multiplication. Often adhoc.

$$\tilde{\mathbf{a}} = \mathbf{a} + \delta \mathbf{a}$$

$$\tilde{\mathbf{a}} \cdot \tilde{\mathbf{b}} = \mathbf{a} \cdot \mathbf{b} + \delta \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \cdot \delta \mathbf{b} + \delta \mathbf{a} \cdot \delta \mathbf{b}$$

The variations do not express in the overall context of the product. Because the error in the incomplete case is additive, the

For example, \mathbf{a} may be small, but $\delta \mathbf{a} \cdot \mathbf{b}$ large, leading extra work. Also, once a truncation error is committed, it is encountered in all subsequent steps; it becomes difficult to impossible to manage error flows of differing magnitude in complex maps.

B. On “Variational” and “non-Variational” Iteration

Gradients lack convergence properties Iteration without orig drives away from basis NS has both. Difference

*Electronic address: matt.challacombe@freeon.org; URL: <http://www.freeon.org>

†Electronic address: nicolasbock@freeon.org; URL: <http://www.freeon.org>

between scalar iteration, Higham page 92.

C. Methods that accumulate incompleteness (purification, and Krylov subspace):

D. “Variational” Methods Stay Close to the Basis (LNV Gradients, RQI and Newton Schulz)

E. Approximation with Incompleteness and Iteration: Corruption of the Eigen Basis

F. Approximate Algebras as N-Body Problem

SpAMM is the recursive Cauchy-Schwarz occlusion product \otimes_τ on matrix quadrees

$$\mathbf{a}^i = \begin{bmatrix} \mathbf{a}_{00}^{i+1} & \mathbf{a}_{01}^{i+1} \\ \mathbf{a}_{10}^{i+1} & \mathbf{a}_{11}^{i+1} \end{bmatrix} \quad (1)$$

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$$\mathbf{a}^i \otimes_\tau \mathbf{b}^i = \begin{cases} \emptyset & \text{if } \|\mathbf{a}^i\| \|\mathbf{b}^i\| < \tau \\ \mathbf{a}^i \cdot \mathbf{b}^i & \text{if (i = leaf)} \\ \begin{bmatrix} \mathbf{a}_{00}^{i+1} \otimes_\tau \mathbf{b}_{00}^{i+1} + \mathbf{a}_{01}^{i+1} \otimes_\tau \mathbf{b}_{10}^{i+1}, & \mathbf{a}_{00}^{i+1} \otimes_\tau \mathbf{b}_{01}^{i+1} + \mathbf{a}_{01}^{i+1} \otimes_\tau \mathbf{b}_{11}^{i+1} \\ \mathbf{a}_{10}^{i+1} \otimes_\tau \mathbf{b}_{00}^{i+1} + \mathbf{a}_{11}^{i+1} \otimes_\tau \mathbf{b}_{10}^{i+1}, & \mathbf{a}_{10}^{i+1} \otimes_\tau \mathbf{b}_{01}^{i+1} + \mathbf{a}_{11}^{i+1} \otimes_\tau \mathbf{b}_{11}^{i+1} \end{bmatrix} & \text{else} \end{cases} \quad (2)$$

database orientation, Cauchy sch Approximate Algebra, SpAMM Cauchy Schwarz occlusion, n-body approach to numerical linear algebra, first order errors in matrix multiplication. Based on Cauchy Schwarz inequality.

error accumulation may be better than row-col single programing model. generacity. communication optimality and strong scaling.

G. Incomplete Algorithms and Approximate Algebras

Incompleteness -i sparse approximations dense problems, uses conventional sparse infrastructure, second order errors in matrix multiplication. Often adhoc.

Philosophy: Don’t know which elements to drop, because only make sense in context. It is very difficult to

incorporate this context in a dropping strategies.

Approximate Algebra, SpAMM Cauchy Schwarz occlusion, n-body approach to numerical linear algebra, first order errors in matrix multiplication. Based on Cauchy Schwarz inequality.

We show that this first order error in algebraic context follows the functional analysis, and enables the consideration *and separate treatment* of first order error flows in the analysis of complex maps.

$$\mathbf{a} \otimes_{\tau} \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + \Delta_{\tau}^{a \cdot b} \quad (3)$$

where $\Delta_{\tau}^{a \cdot b}$ is a deterministic first order variation cooresponding to the branch pattern set by Cauchy-Schwarz culling, with length $\|\Delta_{\tau}^{a \cdot b}\| \leq \tau \|\mathbf{a}\| \|\mathbf{b}\|$.

For a vector space S with $\mathbf{a}, \mathbf{b} \in S$, the operator \otimes_{τ} leads to a non-associative algebra with Lie bracket

$$[\mathbf{a}, \mathbf{b}]_{\tau} = \mathbf{a} \otimes_{\tau} \mathbf{b} - \mathbf{b} \otimes_{\tau} \mathbf{a} = \Delta_{\tau}^{a \cdot b} - \Delta_{\tau}^{b \cdot a}, \quad (4)$$

determined by the occlusion field. Our challenge is to master the error flows of these occlusion fields under iteration, for ill-conditioned problems and with permissive values of τ .

II. NEWTON SHULZ ITERATION

A. Idempotence

B. The Scaled Map

C. Alternative Formulations

dual, stabilized and naive

III. OCCLUSION FLOWS

$\delta \mathbf{x}_k$ and $\delta \mathbf{z}_k$ arrize from itteration with \otimes_{τ} , and are deterministic flows away from the manifold of \mathbf{s} determined by sensitivity of the NS iteration to these numerical in-sults.

$$\delta \mathbf{x}_k^{\text{naiv}} = \delta \tilde{\mathbf{z}}_k \cdot \mathbf{s} \cdot \tilde{\mathbf{z}}_k + \tilde{\mathbf{z}}_k \cdot \mathbf{s} \cdot \delta \tilde{\mathbf{z}}_k \quad (5)$$

$$\delta \mathbf{x}_k^{\text{dual}} = \delta \tilde{\mathbf{y}}_k \cdot \tilde{\mathbf{z}}_k + \tilde{\mathbf{y}}_k \cdot \delta \tilde{\mathbf{z}}_k \quad (6)$$

$$\begin{aligned} \tilde{\mathbf{x}}_k &= f[\tilde{\mathbf{z}}_{k-1}, \tilde{\mathbf{x}}_{k-1}] \\ &= \mathfrak{m}[\tilde{\mathbf{x}}_{k-1}] \cdot \tilde{\mathbf{z}}_{k-1}^{\dagger} \cdot \mathbf{s} \cdot \tilde{\mathbf{z}}_{k-1} \cdot \mathfrak{m}[\tilde{\mathbf{x}}_{k-1}] \end{aligned} \quad (7)$$

$$\delta \mathbf{x}_k = f_{\delta \mathbf{z}_{k-1}} \|\delta \mathbf{z}_{k-1}\| + f_{\delta \mathbf{x}_{k-1}} \|\delta \mathbf{x}_{k-1}\| + \mathcal{O}(\tau^2) \quad (8)$$

generalized Gateaux differential

$$\begin{aligned} f_{\delta \mathbf{z}_{k-1}} &= \lim_{\tau \rightarrow 0} \frac{f[\mathbf{z}_{k-1} + \tau \delta \tilde{\mathbf{z}}_{k-1}, \tilde{\mathbf{x}}_{k-1}] - f[\mathbf{z}_{k-1}, \tilde{\mathbf{x}}_{k-1}]}{\tau} \\ &= L_{\tilde{\mathbf{x}}_k}(\tilde{\mathbf{z}}_k, \delta \tilde{\mathbf{z}}_{k-1}) \end{aligned} \quad (9)$$

$$\begin{aligned} f_{\delta \mathbf{x}_{k-1}} &= \lim_{\tau \rightarrow 0} \frac{f[\tilde{\mathbf{z}}_{k-1}, \mathbf{x}_{k-1} + \tau \delta \tilde{\mathbf{x}}_{k-1}] - f[\tilde{\mathbf{z}}_{k-1}, \mathbf{x}_{k-1}]}{\tau} \\ &= L_{\tilde{\mathbf{x}}_k}(\tilde{\mathbf{z}}_k, \delta \tilde{\mathbf{x}}_{k-1}) \end{aligned} \quad (10)$$

$$\begin{aligned} L_{\tilde{\mathbf{x}}_k}(\tilde{\mathbf{z}}_k, \delta \tilde{\mathbf{x}}_{k-1}) &= \delta \tilde{\mathbf{x}}_{k-1}^{\dagger} \cdot \mathfrak{m}'[\mathbf{x}_{k-1}] \cdot \{\tilde{\mathbf{z}}_{k-1}^{\dagger} \cdot \mathbf{s} \cdot \tilde{\mathbf{z}}_k\} \\ &\quad + \{\tilde{\mathbf{z}}_k^{\dagger} \cdot \mathbf{s} \cdot \tilde{\mathbf{z}}_{k-1}\} \cdot \mathfrak{m}'[\mathbf{x}_{k-1}] \cdot \delta \tilde{\mathbf{x}}_{k-1} \end{aligned} \quad (11)$$

$$\begin{aligned} L_{\tilde{\mathbf{x}}_k}(\tilde{\mathbf{z}}_k, \delta \tilde{\mathbf{z}}_{k-1}) &= \{\mathfrak{m}[\mathbf{x}_{k-1}] \cdot \delta \tilde{\mathbf{z}}_{k-1}^{\dagger} \cdot \mathbf{s}\} \cdot \tilde{\mathbf{z}}_k \\ &\quad + \tilde{\mathbf{z}}_k^{\dagger} \cdot \{\mathbf{s} \cdot \delta \tilde{\mathbf{z}}_{k-1} \cdot \mathfrak{m}[\mathbf{x}_{k-1}]\} \end{aligned} \quad (12)$$

$$\{\tilde{\mathbf{z}}_k^{\dagger} \cdot \mathbf{s} \cdot \tilde{\mathbf{z}}_{k-1}\} \rightarrow \mathbf{p}_+[\mathbf{s}] \quad (13)$$

$$\{\mathbf{s} \cdot \delta \tilde{\mathbf{z}}_{k-1} \cdot \mathfrak{m}[\mathbf{x}_{k-1}]\} \rightarrow \mathbf{n}[\mathbf{s}] \quad (14)$$

IV. BASIS SET ILL-CONDITIONING IN ELECTRONIC STRUCTURE

A. 3,3 carbon nanotube with diffuse sp -function

double exponential (Fig.)

B. Water with triple zeta and double polarization

Here's looking at you Jurg...

V. IMPLEMENTATION

A. Methods

FP, F08, OpenMP 4.0

B. A Modified NS Map

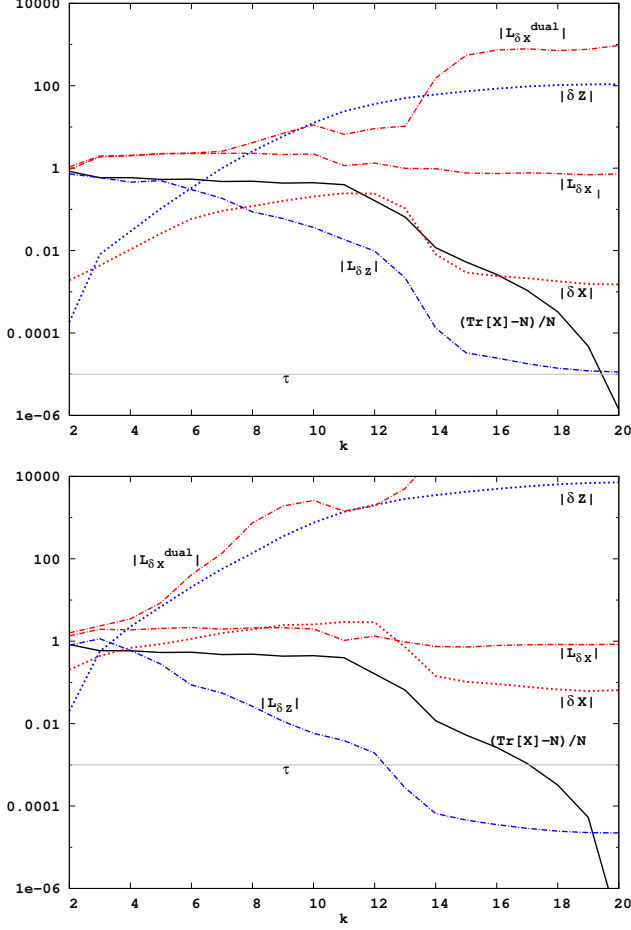
C. $\delta \mathbf{x}_k$ and $\delta \mathbf{x}_k$ channels

tau= Figure showing channels etc.

VI. EXPERIMENTS

A. Occlusion Flows

FIG. 1: equation...



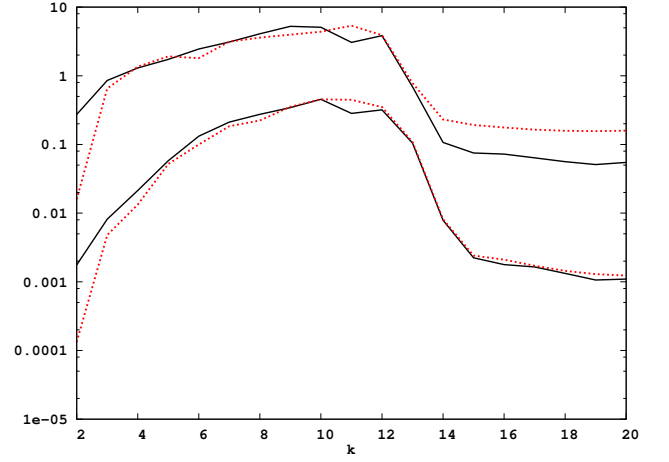
B. Comments

$$\delta z_{k-1} \approx \Delta_{\tau}^{\tilde{z}_{k-2} \cdot m[\tilde{x}_{k-2}]} + z_{k-2} \cdot m'[\tilde{x}_{k-2}] \cdot \delta x_{k-2} + \delta z_{k-2} \cdot m[\tilde{x}_{k-2}] \quad (15)$$

$$\|\delta z_{k-1}\| \lesssim \|z_{k-2}\| \left(\tau \|m[\tilde{x}_{k-2}]\| + \|\delta x_{k-2}\| \|m'[\tilde{x}_{k-2}]\| \right) \quad (16)$$

$$\|z_k\| \rightarrow \sqrt{\kappa(s)} \quad (17)$$

FIG. 2: equation...



C. Scaling

D. Comments

Pictures of the spamm structure

VII. CONCLUSION