The Big Bang Theory
In High Accuracy Computations

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DMML

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Outline

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1. The Big Bang
2. Two immediate “after bangs"
3. Aftermath – Summary
4. Case Study
   - Inverse of M-Matrix
   - M-matrix algebraic Riccati equation
5. Conclusions

Ultimate Goal in Numerical Computation

An unknown number x, waiting to be computed.

Best approximation $\widetilde{x}$, differing from x within half unit in the last place (ulp):

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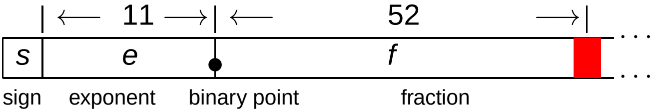

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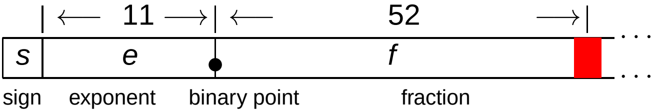

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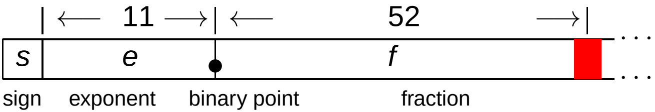

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Key Result – Perturbation Theorem

$$B = \text{bidiag}\begin{pmatrix} a_1 & & a_2 & & a_3 & \cdots & a_{n-1} & & a_n \\ & b_1 & & b_2 & & \cdots & & b_{n-1} & \end{pmatrix}$$

perturbed to bidiagonal $\widetilde{B}$:

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Let $\gamma = \Pi_{i,j} \max\{|\alpha_i|, |\alpha_i|^{-1}\} \max\{|\beta_j|, |\beta_j|^{-1}\}$. Then

$$\frac{\sigma_i(B)}{\gamma} \leq \sigma_i(\widetilde{B}) \leq \gamma\sigma_i(B).$$

It is asymptotically sharp.

Key Result – Perturbation Theorem

In particular, if $1 - \epsilon \leq |\alpha_i|, |\beta_j| \leq 1 + \epsilon$, where $\epsilon > 0$, then

$$1-(2n-1)\epsilon \approx (1-\epsilon)^{2n-1} \leq \gamma^{-1} \leq \gamma \leq (1-\epsilon)^{-(2n-1)} \approx 1+(2n-1)\epsilon.$$

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Favorably compared with classical result:

$$\frac{|\sigma_i(B) - \sigma_i(\widetilde{B})|}{\sigma_i(B)} \leq \frac{\sigma_1(B)}{\sigma_i(B)} 2|\gamma' - 1|, \quad \gamma' = \max_{i,j}\{|\alpha_i|, |\beta_j|\}.$$

Key Result – Convergence Criteria

Need two simple recursions:

- $\lambda_n = |a_n|$, and $\lambda_j = |a_j|[\lambda_{j+1}/(\lambda_{j+1} + |b_j|)]$;
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Convergence Criterion 2. Setting b_{n-1} to 0 will change all $\sigma_i(B)$ relatively by no more than $n\epsilon$, provided $|b_{n-1}|^2 \leq .5\epsilon[\delta^2 - |a_n|^2]$, where $\delta = \sigma_{\min}(B_{(1:n-1,1:n-1)})$.

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Both cheap to implement.

Key Result – Numerical Method

Zero-shift QR will deliver computed σ_i all bits accurately, except last few bits.

Previously, up to an error $O(\epsilon\,\sigma_1)$. Thus for σ_i relatively so tiny such that

$$\sigma_1/\sigma_i = O(1/\epsilon),$$

no bits are guaranteed to be correct.

Key Result – Singular Vectors

Conjecture. Singular vectors are also well-determined and accurately computed in the sense that committed errors is inversely proportional to relative singular value gaps:

$$\sin\theta(v_i, \widetilde{v}_i) \leq \frac{O(\gamma)}{\text{RelGap}_i}, \quad \text{RelGap}_i := \min_{j \neq i} \frac{|\sigma_i - \sigma_j|}{\sigma_i}.$$

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Example. Singular values: 1.5, $2.0 \times 10^{-16}, 1.0 \times 10^{-16}$. Then

$$\text{AbsGap}_3 = \min_{j \ne 3} |\sigma_3 - \sigma_j| = 10^{-16}, \quad \text{RelGap}_3 \approx 1.$$

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Scaled Diagonally Dominant Matrices

$H = DAD$ perturbed to $\widetilde{H} = D\widetilde{A}D$, both γ-s.d.d.;
H's eigenvalues: λ_i in decreasing order, and eigenvector v_i;
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Classical results (convention $\delta X := \widetilde{X} - X$)

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New results (sample): if $\epsilon := \|\delta A\|_2 < (1-\gamma)/n$, then

$$\frac{|\delta\lambda_i|}{|\lambda_i|} \leq \frac{n\epsilon}{1-\gamma} + O(\epsilon^2).$$

Roughly speaking, first $-\log_2(n\epsilon/(1-\gamma))$ significant bits of $\widetilde{\lambda}_i$ are good. Also

$$\sin(v_i, \widetilde{v}_i) \leq O(\frac{n\epsilon}{(1-\gamma)\,\text{RelGap}_i}).$$

Scaled Diagonally Dominant Matrices

Numerical methods:

- via bidiagonal singular value problem
- bisection via stable inertia computation
- inverse iteration for eigenvectors

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The numerical method – Jacobi’s.

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Aftermath (disclaimer: not-intended-to-be-complete)

- SVD for matrices with acyclic graphs (Demmel & Gragg, 1993)
- (Entrywise) perturbations of Hermitian matrices (Veselić & Slapničar, 1993; Truhar & Slapničar, 1999; Dopico, Moro, & Molera, 2000)
- dqds for bidiagonal SVD (Fernando & Parlett, 1994); implementation of dqds on positive definite tridiagonal matrices (Parlett & Marques, 2000);
- Accurate EVD for symmetric tridiagonals, MRRR (Parlett & Dhillon, 2000 & 2003; Dhillon, Parlett, & Vömel, 2006; ...)
- SVD for Cauchy, Vandermonde matrices, and related unit-displacement-rank matrices (Demmel 1999); polynomial Vandermonde matrices (Demmel & Koev, 2006)
- SVD for XDY^T with $D =$ diag, well-conditioned X and Y (D.G.E.S.V.D, 1999); As stage 1 for EVP (Dopico, Molera, & Moro, 2003)
- SVD for $B^T C$ (Drmač, 1998); SVD via fast Jacobi (Drmač & Veselić, 2008)
- EVD for XDX^T with $D =$ diag, well-conditioned X (Dopico, Koev, Molera, 2009)
- Polar decomposition (Li, 1997 & 2005)
- Multiplicative perturbation (Eisenstat & Ipsen, 1995; Li, 1993-2000; C. Li & Mathias, 1999; Li & Stewart, 2000; Truhar & Li, 2003)
- Deflations preserving relative accuracy (Kahan, work-in-progress)
- M-matrix – smallest eigenvalue, inverses (Xue & Jiang, 1995; Alfa, Xue, & Ye, 2002); M-matrix Algebraic Riccati equation (Guo, Lin, & Xu, 1996; Xue, Xu, & Li, 2002; Wang, Wang, & Li, 2012)
- Diagonally dominant matrices – SVD, LU (Demmel & Koev, 2004; Ye, 2008-2009; Koev & Dopico, 2011; Dailey, Dopico, & Ye, 2014)
- Matrix exponential for essentially non-negative matrices (Zhu, Xue,& Gao, 2008; Xue & Ye, 2008-2013; Shao, Gao, & Xue, 2014)

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Outline

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If needed, can recover D_A by $D_A u = v + N_A u$ without subtraction.

Inverse of M-Matrix

[Alfa, Xue, & Ye, 2002]

Nonsingular M-matrix $A = \{N_A, u, v\}$ perturbed to $\widetilde{A} = \{N_{\widetilde{A}}, u, \widetilde{v}\}$ satisfying

$$|N_{\widetilde{A}} - N_A| \leq \epsilon N_A, \quad |\widetilde{v} - v| \leq \epsilon v.$$

Then $\widetilde{A}$ is also an nonsingular M-matrix, and

$$\frac{(1-\epsilon)^{n-1}}{(1+\epsilon)^n} A^{-1} \leq \widetilde{A}^{-1} \leq \frac{(1+\epsilon)^{n-1}}{(1-\epsilon)^n} A^{-1}.$$

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[Alfa, Xue, & Ye, 2002] GTH-like algorithm, a version of *Gaussian elimination without pivoting*, working on $\{N_A, u, v\}$ but not A will compute A^{-1} this accurate.

ARE: Algebraic Riccati Equation

ARE: $XDX - AX - XB + C = 0$, $X_{n \times m}$, $\begin{array}{c} \\ m \\ n \end{array} \begin{array}{c} \begin{array}{cc} m & n \end{array} \\ \left[\begin{array}{cc} B & D \\ C & A \end{array} \right] \end{array}$.

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Frequently appear in Optimal Control Theory, Well-studied.

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M-Matrix Algebraic Riccati Equation (MARE)

It is an MARE: $XDX - AX - XB + C = 0$ if

$$W = \begin{bmatrix} B & -D \\ -C & A \end{bmatrix} \text{ is a nonsingular or an irreducible singular } M\text{-matrix.} \tag{1}$$

Arise in applied probability, transportation theory, stochastic fluid models.

MARE has a unique minimal nonnegative solution Φ, i.e.,

$$0 \le \Phi \le X \quad \text{for any other nonnegative solution } X.$$

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Not so much of practical importance, but theoretically interesting nonetheless.

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Relative perturbation:
$|\widetilde{A} - A| \leq \epsilon|A|$, $|\widetilde{B} - B| \leq \epsilon|B|$, $|\widetilde{C} - C| \leq \epsilon C$, $|\widetilde{D} - D| \leq \epsilon D$, $0 \leq \epsilon < 1$.

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Proposition (Xue, Xu, Li, 2012)

$\widetilde{\Phi}_{(i,j)} = 0$ if and only if $\Phi_{(i,j)} = 0$.

Thus make sense to study entrywise relative accuracy.

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Theorem (Xue, Xu, Li, 2012)

If not in the critical case, then

$$|\Phi - \widetilde{\Phi}| \le \left[2\gamma\epsilon\,\mathbf{1}_{n,m} + O\left(\epsilon^2\right)\right]\Phi, \qquad \text{where}$$

$$(A - \Phi D)\Upsilon + \Upsilon(B - D\Phi) = D_1\Phi + \Phi D_2, \quad \gamma = \max_{i,j} \frac{\Upsilon_{(i,j)}}{\Phi_{(i,j)}} < \infty.$$

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$$A = D_1 - N_1, \quad D_1 = \mathrm{diag}(A), \qquad B = D_2 - N_2, \quad D_2 = \mathrm{diag}(B),$$
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Theorem 2 (Xue, Xu, Li, 2012).

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- for singular M-matrix W, $\chi = 2 \times \begin{cases} \dfrac{1 + \lambda_1 + 2\tau_1^{-1}}{1 - \lambda_1}, & \text{if } x_1^T y_1 > x_2^T y_2, \\ \dfrac{1 + \lambda_2 + 2\tau_2^{-1}}{1 - \lambda_2}, & \text{if } x_1^T y_1 < x_2^T y_2. \end{cases}$

Relative perturbation: $|\widetilde{A} - A| \le \epsilon|A|$, $|\widetilde{B} - B| \le \epsilon|B|$, $|\widetilde{C} - C| \le \epsilon C$, $|\widetilde{D} - D| \le \epsilon D$, $0 \le \epsilon < 1$.

$$\begin{aligned}
&A = D_1 - N_1, \quad D_1 = \mathrm{diag}(A), \qquad B = D_2 - N_2, \quad D_2 = \mathrm{diag}(B),\\
&A - \Phi D = D_1 - N_1 - \Phi D, \qquad B - D\Phi = D_2 - N_2 - D\Phi,\\
&\lambda_1 = \rho(D_1^{-1}(N_1 + \Phi D)), \quad \lambda_2 = \rho(D_2^{-1}(N_2 + D\Phi)), \quad \lambda = \max\{\lambda_1, \lambda_2\},\\
&\tau_1 = \frac{\min_i A_{(i,i)}}{\max_j B_{(j,j)}}, \qquad \tau_2 = \frac{\min_j B_{(j,j)}}{\max_i A_{(i,i)}}.
\end{aligned}$$

Theorem 2 (Xue, Xu, Li, 2012).

If not in the critical case, then

$$|\Phi - \widetilde{\Phi}| \le \left[2mn\,\kappa\chi\,\epsilon + O\left(\epsilon^2\right)\right]\Phi,$$

where $(A - \Phi D)\Phi_1 + \Phi_1(B - D\Phi) = C$, $\kappa = \max_{i,j}(\Phi_1)_{(i,j)}/\Phi_{(i,j)} < \infty$, and

- for nonsingular M-matrix W,

$$\chi = \max\left\{\frac{1 + \lambda_1 + (1+\lambda_2)\tau_1^{-1}}{1 - \lambda_1 + (1-\lambda_2)\tau_1^{-1}}, \frac{1 + \lambda_2 + (1+\lambda_1)\tau_2^{-1}}{1 - \lambda_2 + (1-\lambda_1)\tau_2^{-1}}\right\} \le \frac{1+\lambda}{1-\lambda},$$

- for singular M-matrix W, $\chi = 2 \times \begin{cases} \dfrac{1 + \lambda_1 + 2\tau_1^{-1}}{1 - \lambda_1}, & \text{if } x_1^T y_1 > x_2^T y_2,\\ \dfrac{1 + \lambda_2 + 2\tau_2^{-1}}{1 - \lambda_2}, & \text{if } x_1^T y_1 < x_2^T y_2. \end{cases}$

MARE: Numerical Methods

- Newton method: naturally, after all it is a nonlinear equation – Guo, Higham, Laub, etc.
- Fixed point iterations [C. Guo, 2001]
- Doubling algorithms – SDA [X. Guo, Lin, & Xu, 2006], SDA-ss [Bini, Meini, and Poloni, 2010], and, *optimal of all*, ADDA [Wang, Wang, & Li, 2012]
- Cyclic reduction on equivalent unilateral quadratic matrix equation $B_2Z^2 + B_1Z + B_0 = 0$ [Bini, Meini, and Poloni, 2010]

  Some of them are doubling algorithms in disguise!

MARE: ADDA [Wang, Wang, & Li, 2012]

$\alpha = \left[\max_{1 \le i \le m} A_{(i,i)} \right]^{-1}$, $\beta = \left[\max_{1 \le j \le n} B_{(j,j)} \right]^{-1}$, $k = 0$;

$k = 0$ and compute

$$\begin{bmatrix} E_0 & Y_0 \\ X_0 & F_0 \end{bmatrix} = \begin{bmatrix} \alpha B + I_m & -\beta D \\ -\alpha C & \beta A + I_n \end{bmatrix}^{-1} \begin{bmatrix} I_m - \beta B & \alpha D \\ \beta C & I_n - \alpha A \end{bmatrix}; \tag{3}$$

repeat

  compute

$$E_{k+1} = E_k (I - Y_k X_k)^{-1} E_k, \tag{4a}$$

$$F_{k+1} = F_k (I - X_k Y_k)^{-1} F_k, \tag{4b}$$

$$Y_{k+1} = Y_k + E_k (I - Y_k X_k)^{-1} Y_k F_k, \tag{4c}$$

$$X_{k+1} = X_k + F_k (I - X_k Y_k)^{-1} X_k E_k; \tag{4d}$$

  $k = k + 1$;

until convergence;

return the last X_k as approximations to Φ.

MARE: accurate implementation of ADDA

If a triplet representation of

$$W = \begin{bmatrix} B & -D \\ -C & A \end{bmatrix}$$

is known to begin with, then there is a way to implement ADDA without any substraction
[Xue & Li, *work-in-progress*].

An Example

$$B = \begin{bmatrix} 3 & -1 & & \\ & 3 & \ddots & \\ & & \ddots & -1 \\ -1 & & & 3 \end{bmatrix} \in \mathbb{R}^{n\times n}, \; C = 2I_n, \; A = \xi B, \; D = \xi C,$$

where $\xi > 0$ is a parameter. W is an irreducible singular M-matrix:

$$W \begin{bmatrix} \mathbf{1}_n \\ \xi^{-1}\mathbf{1}_n \end{bmatrix} = 0, \quad \mathbf{1}_{2n}^T W = 0.$$

It is in the critical case if $\xi = 1$ and not in the critical case otherwise.

An Example

$$B = \begin{bmatrix} 3 & -1 & & \\ & 3 & \ddots & \\ & & \ddots & -1 \\ -1 & & & 3 \end{bmatrix} \in \mathbb{R}^{n\times n},\ C = 2I_n,\ A = \xi B,\ D = \xi C,$$

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It is in the critical case if $\xi = 1$ and not in the critical case otherwise.

The "exact" solutions Φ:

$$\begin{aligned} 7.4339 \cdot 10^{-4} &\le \Phi_{(i,j)} \le 3.8270 \cdot 10^{-1}, \quad \text{for } \xi = 1, \\ 1.3336 \cdot 10^{-35} &\le \Phi_{(i,j)} \le 4.0231 \cdot 10^{-2}, \quad \text{for } \xi = 2^4. \end{aligned}$$

Error Measures for Computed $\widehat{\Phi}$

Normalized Residual (NRes) – (readily available):

$$\text{NRes} = \frac{\|\widehat{\Phi}D\widehat{\Phi} - A\widehat{\Phi} - \widehat{\Phi}B + C\|}{\|\widehat{\Phi}\|(\|\widehat{\Phi}\|\|D\| + \|A\| + \|B\|) + \|C\|}.$$

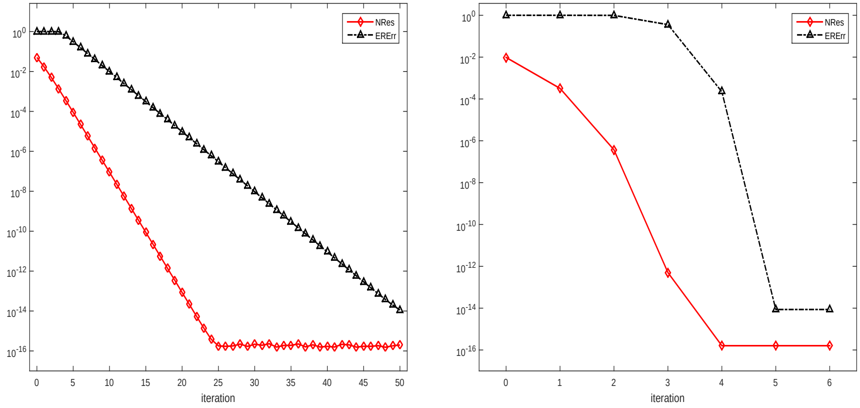
Will use $\|\cdot\| = \|\cdot\|_1$ for convenience.

Entrywise Relative Error (ERErr) – (not readily available):

$$\text{ERErr} = \max_{i,j} \frac{|(\widehat{\Phi} - \Phi)_{(i,j)}|}{\Phi_{(i,j)}}.$$

Made available for testing purpose.

Convergence History



$$7.4339 \cdot 10^{-4} \leq \Phi_{(i,j)} \leq 3.8270 \cdot 10^{-1}, \quad \text{for } \xi = 1 \text{ (left plot)},$$
$$1.3336 \cdot 10^{-35} \leq \Phi_{(i,j)} \leq 4.0231 \cdot 10^{-2}, \quad \text{for } \xi = 2^4 \text{ (right plot)}.$$

Outline

Conclusions

- Numerous “stars" formed after the “big bang"
- “Universe" is expanding

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Happy 60th Birthday, Jim!