Computing the Singular Value Decomposition to High Relative Accuracy

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INTRODUCTION

- **High Relative Accuracy means computing the correct SIGN and LEADING DIGITS**
- **Singular Value Decomposition (SVD):**

$$A = U \Sigma V^T$$

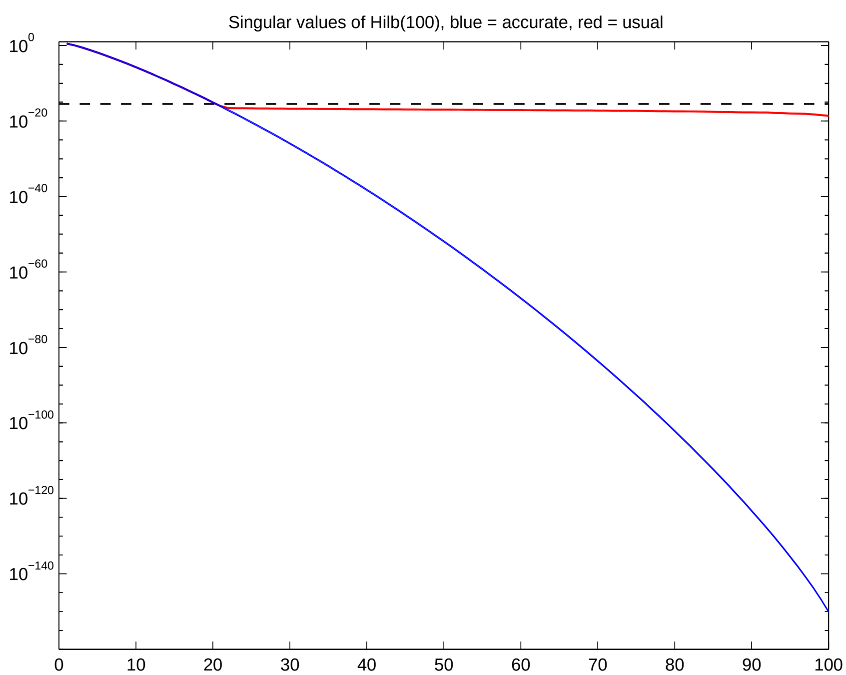
where U, V **are orthogonal,**

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} \quad \text{and} \quad \sigma_1 \geq \sigma_2 \geq \ldots \sigma_n \geq 0$$

- **GOAL: Compute all** σ_i **with high relative accuracy, even when** $\sigma_i \ll \sigma_1$
- **It all comes down to being able to compute determinants to high relative accuracy.**

Example: 100 by 100 Hilbert Matrix
$H(i,j) = 1/(i+j-1)$

- **Singular values range from 1 down to** 10^{-150}
- **Old algorithm, New Algorithm, both in 16 digits**



- $D = log(cond(A)) = log(\sigma_1/\sigma_n)$ **(here** $D = 150$**)**
- **Cost of Old algorithm =** $O(n^3 D^2)$

  - **Run in double, not bignums as in Mathematica**
  - **New hundreds of times faster than Old**
- **When does it work? Not for all matrices ...**
- **Why bother?**

Why do we want tiny singular values accurately?

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1. **When they are determined accurately by the data**
   - **Hilbert:** $H(i, j) = 1/(i + j - 1)$
   - **Cauchy:** $C(i, j) = 1/(x_i + y_j)$
2. **In some applications, tiny singular values matter most**
   - **Quantum mechanics: want lowest energy levels only**
   - **Elasticity: want lowest frequencies of vibration olny**
   - **Getting the sign of the determinant right**
   - **Always a good idea to get accurate results if we can do it at a similar cost**

Overview of Results

- **Being able to compute $|\det(A)| = \Pi_{i=1}^{n} \sigma_i$ to high relative accuracy is a necessary condition for accurate SVD.**
- **Well known similar sufficient condition for accurate A^{-1}: Enough to compute n^2+1 minors (Cramer's Rule)**
- **New: Similar sufficient condition for accurate SVD: Enough to compute $O(n^3)$ minors**
- **We have identified many matrix classes whose structure permits efficient ($O(n^3)$) accurate computation of these minors.**
  - **Sparse Matrices, depending on sparsity pattern**
  - **Cauchy, Vandermonde, Unit Displacement Rank Matrices**
  - **"Graded" matrices (diagonal · "nice" · diagonal)**
  - **Appropriately discretized ODEs, PDEs**

SVD Algorithm

A

$\downarrow$

Phase 1: compute Rank Revealing Decomp (RRD)

A = XDY^T

X, Y full column rank and "well-conditioned"
D diagonal

$\downarrow$

Phase 2: compute SVD of an RRD

A = UΣV^T

- **Examples of RRDs:**
  - $A = U\Sigma V^T$, **SVD itself**
  - $A = QDR$, **QR decomposition with pivoting**
  - $A = LDU$, **Gaussian Elimination with "complete" pivoting (GECP)**
- **Fact: Each entry of** L, D, U **is a quotient of minors**
- **Phase 1: GECP via (implicitly) computing accurate minors of** A
  - **Depends on structure of** A
- **Phase 2: Works for any RRD in** $O(n^3)$
  - **Independent of structure of** A
  - **Uses 1 or 2 one-sided Jacobis, matmuls**
- **Relative error in singular values bounded by** $O(macheps \cdot \max(\text{cond}(X)\ ,\ \text{cond}(Y)))$

How do we compute $A = L \cdot D \cdot U$ for a Hilbert (or Cauchy) Matrix?

- **How can we lose accuracy in computing in floating point?**
  - **OK to multiply, divide, add positive numbers**
  - **OK to subtract exact numbers (initial data)**
  - **Cancellation when subtracting approximate results dangerous:**

$$
\begin{array}{r}
.12345\text{xxx} \\
-\ \ .12345\text{yyy} \\
\hline
.00000\text{zzz}
\end{array}
$$

- **Cauchy:**

$$C(i,j) = \frac{1}{x_i + y_j}$$

-

$$\mathbf{det}(C) = \frac{\Pi_{i<j}(x_j - x_i)(y_j - y_i)}{\Pi_{i,j}(x_i + y_j)}$$

  - **No bad cancellation $\Rightarrow$ good to most digits**

- **Change inner loop of Gaussian Elimination from**

$$C(i,j) = C(i,j) - \frac{C(i,k)C(k,j)}{C(i,i)}$$

  to

$$C(i,j) = C(i,j)\frac{(x_i - x_k)(y_j - y_k)}{(x_k + y_j)(x_i + y_k)}$$

- **Each entry of L, D, U accurate to most digits!**

Vandermonde Matrices

- $V_{ij} = x_i^{j-1}$
- $\det(V) = \Pi_{1 \le i < j \le n}(x_i - x_j)$
  - **Computable to high relative accuracy**
- **For SVD use fact that** $V \cdot DFT = Cauchy$
  - **Extends to unit-displacement rank, but not higher**
- **Generalized Vandermonde Matrix** $G^{\mu}_{ij} = x_i^{\mu_j}, x_i > 0$
  - **Ex:** $\mu_j = j - 1$ **is usual Vandermonde**
  - G^{μ} **is a submatrix of a larger Vandermonde**
  - **Totally positive if** $0 < x_1 < \cdots < x_n$
  - **SVD determined to high relative accuracy; can we compute it?**
- **Let** $\lambda_j = \mu_j - j + 1$**,** $\lambda = (\lambda_1, \lambda_2, ..., \lambda_n)$**,** $|\lambda| = \Sigma_i \lambda_i$
- $\det(G^{\mu}) = \det(V) \cdot s_{\lambda}(x_1, ..., x_n)$
  - **Polynomial** s_{λ} **called** ***Schur Function***
  - **Widely studied in representation theory, combinatorics, ...**
  - **For usual Vandermonde,** $|\lambda| = 0$ **and** $s_{\lambda} = 1$
- **Theorem (Plamen Koev): Cost of computing** $\det(G^{\mu})$ **to high relative accuracy is** $n^{|\lambda|} + n^2$
- **Corollary: Cost of high relative accuracy for some minors of** V **can be exponential in** n**, alas**

When is High Accuracy Possible *Efficiently*?

- **When are all minors computable accurately?**
- **Depends on model of arithmetic**

  Model 1: $fl(a \odot b) = (a \odot b)(1 + \text{tiny})$

  Model 2: IEEE floating point

- **Model 1**
  - **Ok to multiply, divide, add positives, add or subtract initial data**
  - **Theorem 1. Can evaluate a polynomial accurately [in poly(n) time] if it factors into a product of [poly(n)] factors each of which is**
    - **initial data**
    - **sum or difference of initial data**
    - **sum of [poly(n)] positives**
  - **Covers many examples**
    - **Cauchy, real Vandermonde, graded, sparse, appropriately discretized ODEs and PDEs (so far)**
    - **Totally positive (eg generalized Vandermonde), but not in poly(n) time**
  - **Proposition (D,Kahan) Can't add three numbers accurately**
    - **Model 1 much weaker than Model 2**

Model 2 vs Model 1

- **How much stronger is Model 2 than Model 1?**

Cost (Big-Oh sense) of Accurate Evaluation of det(A) (Dekker, Kahan, Priest, Shewchuk)		
Form of $\det(A)$	**Model 1**	**Model 2**
$\Pi_{i=1}^{d} a_i$	d	d
$\Pi_{i=1}^{d}(a_i - b_i)$	d	d
$\Sigma_{i=1}^{t} a_i$, $a_i > 0$	t	t
$\Sigma_{i=1}^{t} a_i$	**imposs.**	$t \log t$
poly(a_i) (**t terms, degree** $\leq d$)	**imposs.**	$d^2 t \log t$

- **Idea: represent numbers** ***sparsely*****, not** ***densely***
- **Theorem 2. Can evaluate a polynomial accurately in poly(n) time if it factors into a produce of poly(n) factors each of which is has poly(n) terms of poly(n) degree**
- **Examples**
  - **All examples from Model 1**
  - **Complex Vandermonde**
  - **Substitute polynomials for input data in previous example**
    Ex: Cauchy with x_i, y_j replaced by $p(x_i)$, $q(y_j)$
  - **Inverse of a tridiagonal**
- **Open Problem: what is complexity of accurate determinant of a general floating point matrix?**

Conclusions and Future Work

- **We can compute the SVD much more accurately than via bidiagonalization for many matrix classes**
- **Some algorithms will appear in LAPACK**
- **We only solve accurately the problem as stored in the computer, i.e. the last link of the chain:**

  Real World

  $\longrightarrow$ Continuous Problem

  $\longrightarrow$ Discrete Problem

  $\longrightarrow$ Rounded Discrete Problem

  $\longrightarrow$ Solution

- **Many open problems remain to extend these algorithms to new problem classes, especially**
  - **finite element matrices, other PDE discretizations**
  - **totally positive matrices**
  - **higher displacement rank**
  - **sparse problems from these classes**

- Slides for this talk
  http://math.berkeley.edu/∼plamen/src99.ps
- Report on overall algorithm
  http://www.cs.berkeley.edu/∼demmel/DGESVD.ps.gz (to appear in Linear Algebra and its Applications).
- Report on Cauchy, Vandermonde
  http://www.cs.berkeley.edu/∼demmel/cauchy.ps.gz (to appear in SIAM J. Matrix Analysis and Applications)
- Report on Generalized Vandermonde Matrices and Schur Functions
  http://math.berkeley.edu/∼plamen/schur.ps