Multiple Precision Arithmetic Versions of SDP solvers; SDPA-GMP, SDPA-QD and SDPA-DD

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Collaborators

The SDPA project members in alphabetic order with WAKI, Hayato

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- FUKUDA, Mituhiro
- FUTAKATA, Yoshiaki
- KOBAYASHI, Kazuhiro
- KOJIMA, Masakazu
- NAKATA, Kazuhide
- (NAKATA, Maho)
- YAMASHITA, Makoto

Outline

1. Introduction
   - Abstract
   - What is number?
   - Semidefinite programming
   - Necessity of accurate solver
   - Origins of accuracy loss
2. Development of SDPA-GMP, SDPA-QD, DD, and MPACK
3. Results

Outline

Abstract

- I just want to solve SDP very very accurately!
- Problems from chemistry can be solved via SDP solvers: [Nakata-Nakatsuji-Ehara-Fukuda-Nakata-Fujisawa, J. Chem. Phys. 114, 8282 (2001)]
- Such problems require very high accuracy to SDP; relative gap $< 1.0 \times 10^{-8}$
- There are some inaccurate results.
- Multiple precision arithmetic version of SDPA; SDPA-GMP, SDPA-QD, SDPA-DD: http://sdpa.indsys.chuo-u.ac.jp/sdpa/.
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Do not think seriously. Take it easy!

Keep it sweet and simple

JUST ADD PRECISION

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Outline

What is number?

There are several kinds of numbers.

- Natural number: $0, 1, 2, 3, 4, \cdots$
- Integer: $\cdots, -3, -2, -1, 0, 1, 2, 3, 4, \cdots$
- Rational number: a/b, where a, b are relatively prime
- Real number: convergence of Cauchy series. $\{x_n : x_n \in \mathbb{Q}\}_{n=0,1\cdots}$ s.t. $\forall \epsilon > 0, \exists N, \forall n, m > N \rightarrow |x_n - x_m| < \epsilon$ defines a real number x.
- Complex number: $z = a + bi$: two real numbers with i.
- floating point number: designed for computers, subset of rational numbers.

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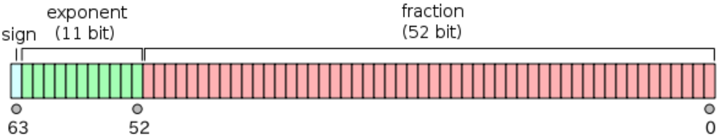
IEEE 754: Standard for Binary Floating-Point Arithmetic

- The IEEE Standard for Floating-Point Arithmetic (IEEE 754) is the most widely-used standard for floating-point computation.
- Very well designed we feel as if we treat real numbers.
- IEEE 754 double is expressed in 64-bit (= 8 bytes)



- $a = \pm\left(\frac{1}{2} + \frac{d_2}{2^2} + \frac{d_3}{2^3} + \cdots + \frac{d_{52}}{2^{52}}\right) \times 2^e$, $d = 0$ or 1, $e = -1022 \sim 1023$
- about 16 significant digits ($\log_{10} 2^{53} = 15.955$).
- Implemented for popular CPUs.

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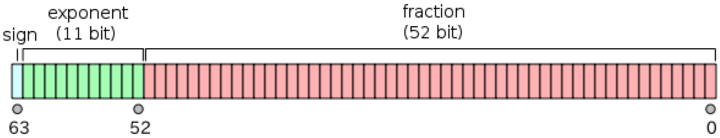

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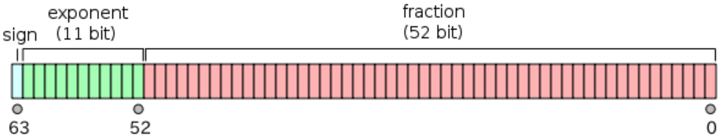

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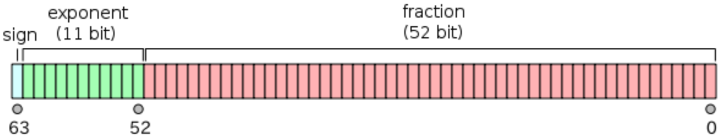

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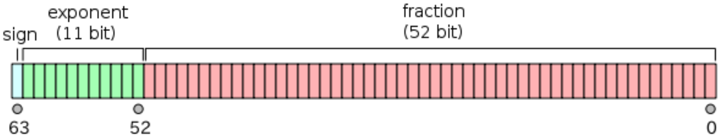

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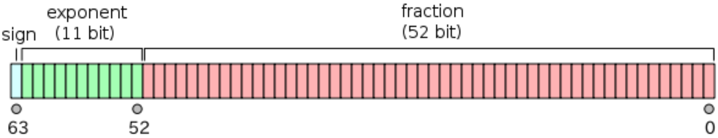

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$$A \oplus B \neq A + B$$

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Semidefinite programming

$$
\begin{cases}
\text{primal} & \text{minimize:} & A_0 \bullet X & \\
 & \text{s.t.:} & A_i \bullet X = b_i & (i = 1, 2, \cdots, m) \\
 & & X \succeq 0 & \\
\text{dual} & \text{maximize:} & \sum_{i=1}^{m} b_i z_i & \\
 & \text{s.t.:} & \sum_{i=1}^{m} A_i z_i + Y = A_0 & \\
 & & Y \succeq 0 &
\end{cases}
$$

A_i is $n \times n$ real symmetric matrices, X $n \times n$ real symmetric variable matrix, b_i are constant vectors of m-dimension, Y is $n \times n$ a real symmetric variable matrix, $X \bullet Y := \sum X_{ij} Y_{ij}$. $X \succeq 0$ means X is positive semidefinite.

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Do we need to solve SDP problems *accurately?*

There are some questions for SDP results.

- Some SDPs are hard to solve. The results may have large gaps, not feasible.
- Simply we may not trust the results: “Strange Behaviors of Interior-point Methods for Solving Semidefinite Programming Problems in Polynomial Optimization” [Waki-Nakata-Muramatsu submitted]
- Users seldom care about the input file: try to solve ill-posed SDPs.

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Sources of the evil (I)

- IEEE 754 double arithmetic: done in 16 significant digits. accuracy losses in manipulations

$$1 \oplus 1.0 \times 10^{-17} = 1$$

- Condition number of matrix A; $||A||||A^{-1}||$. when it becomes 10^{16}, solution to the linear equation is inaccurate with IEEE 754 double.
- $X \bullet Y = 0$ at the optimum (complementarity slackness theorem for SDP)
  variable matrix becomes singular at the optimum; condition number becomes infinite!

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Sources of the evil (II)

- Z^{-1}: Primal-dual interior point method calculates Z^{-1}; *"It is seldom necessary to compute the inverts of matrix explicitly, and it is certainly not recommended as a means of solving linear systems."* by LAPACK Users' Guide Third Edition, p.14.
- Human factor: users try to solve SDPs which do not satisfy Slater's condition, i.e., *no interior points* etc, NO GUARANTEE! DO NOT BLAME SOLVERS!

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A brute force method for accurate SDP solutions

- Use multiple precision arithmetic; GMP, QD rather than IEEE 754 double.
- Simple answer to obtain high accuracy.
- Do not solve all the problems, but many!

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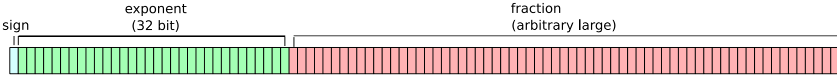
What is GMP?

- GMP is a free library for arbitrary precision arithmetic, operating on signed integers, rational numbers, and floating point numbers.
- significant digits: arbitrary (I usually use $60 \sim 72$ digits)



Strategy and features

- Using existing multiple precision libraries.
- Based on SDPA; http://sdpa.indsys.chuo-u.ac.jp/sdpa/
- No changes in algorithm.
- Changes from SDPA should be minimal to reduce the maintenance cost.
- Matrix-vector manipulations and eigenvalues etc. → Multiple precision version of LAPACK and BLAS.
  - 49 routines from MPACK; Rpotrf (dpotrf.f; cholesky), Rsyev (dsyev.f eigenvalue), Rsterf, Rsteqr (dsterf.f, dsteqr.f) etc..
- Introduction of “precision” parameter; controls number of significant bits used in the calculations.
- Actually I did was replacing “double” to “mpf_class” carefully.

Another MP library: Quad-Double library

- Usually quadruple or octuple precision are enough.
- Double-Double and Quad-Double Arithmetic; by Y. Hida, Xiaoye S. Li, David H Bailey, and faster than GMP.
- Four/two unevaluated IEEE 754 double $\sim$ approx octuple/quadruple precision.

$$A = (a_0, a_1, a_2, a_3)$$

- Utilize exact transformations [Dekker, Knuth, Priest, Shewcheck].

$$a = x \oplus y, b = x + y - (x \oplus y)$$

  Error by IEEE754 add $x \oplus y$ can be *exactly* evaluated.
- Replace “mpf_class” to “dd_real” and “qd_real” $\rightarrow$ SDPA-QD, SDPA-DD.

What is MPACK?

- MPACK is a multiple precision version of BLAS and LAPACK. http://mplapack.sourceforge.net/
- What is the BLAS? The BLAS (Basic Linear Algebra Subprograms) are routines that provide standard building blocks for performing basic vector and matrix operations.
- What is LAPACK? This provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems.
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MBLAS Rgemm.cpp and BLAS dgemm.f

Rgemm.cpp

```
//Start the operations.
if (notb) {
    if (nota) {
        //Form C := alpha*A*B + beta*C.
        for (int j = 0; j < n; j++) {
            if (beta == Zero) {
                for (int i = 0; i < m; i++) {
                    C[i + j * ldc] = Zero;
                }
            } else if (beta != One) {
                for (int i = 0; i < m; i++) {
                    C[i + j * ldc] = beta * C[i + j * ldc];
                }
            }
            for (int l = 0; l < k; l++) {
                if (B[l + j * ldb] != Zero) {
                    temp = alpha * B[l + j * ldb];
                    for (int i = 0; i < m; i++) {
                        C[i + j * ldc] =
                            C[i + j * ldc] + temp * A[i + l * lda];
                    }
                }
            }
        }
    } else {
//Form  C := alpha*A'*B + beta*C.
```

dgemm.f

```
*
*     Start the operations.
*
      IF (NOTB) THEN
          IF (NOTA) THEN
*
*           Form  C := alpha*A*B + beta*C.
*
              DO 90 J = 1,N
                  IF (BETA.EQ.ZERO) THEN
                      DO 50 I = 1,M
                          C(I,J) = ZERO
   50                 CONTINUE
                  ELSE IF (BETA.NE.ONE) THEN
                      DO 60 I = 1,M
                          C(I,J) = BETA*C(I,J)
   60                 CONTINUE
                  END IF
                  DO 80 L = 1,K
                      IF (B(L,J).NE.ZERO) THEN
                          TEMP = ALPHA*B(L,J)
                          DO 70 I = 1,M
                              C(I,J) = C(I,J) + TEMP*A(I,L)
   70                     CONTINUE
                      END IF
   80             CONTINUE
   90         CONTINUE
          ELSE
*
*           Form  C := alpha*A'*B + beta*C
```

How MBLAS is used in SDPA-GMP?

From sdpa_linear.cpp from SDPA-GMP 7.1.2.

```
    if (scalar==NULL) {
      scalar = &MONE;
      // scalar is local variable
    }
    // The Point is the first argument is "Transpose".
    Rgemm("Transpose","NoTranspose",retMat.nRow,retMat.nCol,aMat.nCol,
           *scalar,aMat.de_ele,aMat.nCol,bMat.de_ele,bMat.nRow,
           0.0,retMat.de_ele,retMat.nRow);
    break;
  case DenseMatrix::COMPLETION:
    rError("no support for COMPLETION");
    break;
  }

  return _SUCCESS;
```

Results (I)

Some results from SDPLIB, on Opteron 250 (2.4GHz), 16G Mem, FreeBSD 7/amd64.
"precision" is 250 for GMP.

instance	arch8(GMP)	arch8(QD)	arch8(DD)	arch8(double)
iter	47	47	37	25
rel. gap	$3.57e-31$	$3.58e-31$	$3.80e-21$	$1.65e-08$
p feas. error	$3.11e-76$	$1.02e-61$	$5.05e-29$	$1.14e-12$
d feas. error	$5.66e-72$	$9.01e-52$	$4.85e-21$	$1.10e-07$
time (s)	634.766	497.289	55.445	9.35

instance	mcp500-4(GMP)	mcp500-4(QD)	mcp500-4(DD)	mcp500-4(double)
iter	38	38	28	15
rel. gap	$1.36e-31$	$1.36e-31$	$1.36e-21$	$1.16e-08$
p feas. error	$1.28e-76$	$6.08e-64$	$6.41e-31$	$4.88e-15$
d feas. error	$1.67e-75$	$7.72e-59$	$1.68e-28$	$1.02e-13$
time (s)	5711.6	4678.1	455.0	10.2

instance	maxG32(GMP)	maxG32(QD)	maxG32(DD)	maxG32(double)
iter	40	40	30	17
rel. gap	$2.07e-31$	$2.07e-31$	$2.04e-21$	$1.65e-08$
p feas. error	$1.74e-76$	$1.09e-64$	$1.23e-31$	$1.14e-12$
d feas. error	$1.90e-72$	$2.47e-53$	$8.53e-25$	$1.10e-07$
time (s)	348564.8	315969.5	30472.0	9.35

Results (II) 1D-Hubbard model

1D Hubbard model Strong correlation limit: $|U/t| \to \infty$:[Nakata et al. JCP 2008]; with SDPA-GMP 6.

Ground state energy of 1D Hubbard model

PBC, # of sites:4, # of electrons: 4, spin 0

U/t	SDPA (16 digits)	SDPA-GMP (60 digits)	fullCI
10000.0	0	$-1.1999998800000251 \times 10^{-3}$	$-1.199999880 \times 10^{-3}$
1000.0	-1.2×10^{-2}	$-1.1999880002507934 \times 10^{-2}$	$-1.1999880002 \times 10^{-2}$
100.0	-1.1991×10^{-1}	$-1.1988025013717993 \times 10^{-1}$	$-1.19880248946 \times 10^{-1}$
10.0	-1.1000	-1.0999400441222934	-1.099877772750
1.0	-3.3417	-3.3416748070259956	-3.340847617248

PBC, # of sites:6, # of electrons: 6, spin 0

U/t	SDPA (16 digits)	SDPA-GMP (60 digits)	fullCI
10000.0	0	$-1.7249951195749525 \times 10^{-3}$	$-1.721110121 \times 10^{-3}$
1000.0	-1×10^{-2}	$-1.7255360310431304 \times 10^{-2}$	$-1.7211034713 \times 10^{-2}$
100.0	-1.730×10^{-1}	$-1.7302157140594339 \times 10^{-1}$	$-1.72043338097 \times 10^{-1}$
10.0	-1.6954	-1.6953843276854447	-1.664362733287
1.0	-6.6012	-6.6012042217806286	-6.601158293375

Results (III) Kissing number

Kissing number from A New Library of Structured Semidefinite Programming Instances; the optimal values *were* uncertain or only known with low accuracy. Powered by Fujisawa-san (2008/12/21); precision is 128bit for GMP.

instance	opt (double)	opt (GMP)
kissing_3_10_10	-11.4385	-11.43814328
kissing_4_10_10	-23.14	-23.13553364
kissing_5_10_10	-44.15	-44.158868754
kissing_6_10_10	-77.9	-77.912852357
kissing_7_10_10	-134.3	-134.32853967
kissing_8_10_10	-238.929	-238.99981527
kissing_9_10_10	-365	-365.21946909
kissing_10_10_10	-562.9	-562.89594739
kissing_11_10_10	-889.74	-889.74203646
kissing_12_10_10	-1369.485	-1369.5287720

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Summary

- We developed multiple precision version of SDP solver. SDPA-GMP, SDPA-QD and SDPA-DD.
- Can solve SDPs very accurately.
- MPACK 0.0.9: Multiple precision version of LAPACK/BLAS: development ongoing.

- Outlook
  - Faster SDPA-GMP, QD, DD and MPACK, parallel and multicore versions.
  - More routines for MPACK.
  - Higher accuracy to SDPA; minimal use of multiple precision arithmetic.