SDPB 2.2.0

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1 Introduction

SDPB is an arbitrary-precision semidefinite program solver, specialized for "polynomial matrix programs" (defined below). This document describes SDPB's usage and input/output. Much more detail about its design is given in [1]. The reader is encouraged to look there for a better understanding of SDPB's parameters and internal operation.

1.1 Installation and Requirements

See Install.md for up-to-date instructions on getting pre-made binaries or building from source.

2 Polynomial Matrix Programs

SDPB solves the following type of problem, which we call a *polynomial matrix program* (PMP). Consider a collection of symmetric polynomial matrices

$$M_{j}^{n}(x) = \begin{pmatrix} P_{j,11}^{n}(x) & \dots & P_{j,1m_{j}}^{n}(x) \\ \vdots & \ddots & \vdots \\ P_{j,m_{j}1}^{n}(x) & \dots & P_{j,m_{j}m_{j}}^{n}(x) \end{pmatrix}$$
(2.1)

labeled by $0 \le n \le N$ and $1 \le j \le J$, where each element $P_{j,rs}^n(x)$ is a polynomial in x. Given $b \in \mathbb{R}^N$, we would like to

maximize
$$b_0 + b \cdot y$$
 over $y \in \mathbb{R}^N$,
such that $M_j^0(x) + \sum_{n=1}^N y_n M_j^n(x) \succeq 0$ for all $x \geq 0$ and $1 \leq j \leq J$. (2.2)

The notation $M \succeq 0$ means "M is positive semidefinite."

3 Input to SDPB

SDPB takes the following input:

- for each $j = 1, \ldots, J$:
 - polynomial matrices $M_j^0(x), \ldots, M_j^N(x)$ of maximum degree d_j ,
 - bilinear bases $q_m^{(j)}(x)$ $(m = 0, \dots, \lfloor d_i/2 \rfloor)$,
 - sample points $x_k^{(j)}$ $(k = 0, \dots, d_j),$
 - sample scalings $s_k^{(j)}$ $(k = 0, \dots, d_j),$
- an objective function $b_0 \in \mathbb{R}$ and $b \in \mathbb{R}^N$.

A bilinear basis is a collection of polynomials $q_m^{(j)}(x)$ such that $\deg q_m^{(j)} = m$, for example monomials $q_m^{(j)}(x) = x^m$. (A better choice for numerical stability is usually orthogonal polynomials on the positive real line.) The sample points and sample scalings determine how the PMP is represented internally as an SDP. In principle, they do not affect the solution of the PMP, but in practice they can affect numerical stability. The constant b_0 is completely irrelevant to the solution algorithm, but is included for convenience. See [1] for details.

3.1 Input Format

SDPB reads the data above in the following XML format.

Listing 1: XML input format for SDPB

```
input\ to\ \mathit{SDPB}\ \equiv
  <sdp>
      \langle xml \ for \ objective \rangle
      \langle xml \ for \ polynomial \ vector \ matrices \rangle
  </sdp>
xml for objective \equiv
  <objective>
      <elt>b_0</elt>
      <elt>b_N < /elt>
  </objective>
xml\ for\ polynomial\ vector\ matrices\ \equiv
  <polynomialVectorMatrices>
      \langle xml\ for\ polynomial\ vector\ matrix\ M_1^n(x)\rangle
      \langle xml \ for \ polynomial \ vector \ matrix \ M_J^n(x) \rangle
  </polynomialVectorMatrices>
xml for polynomial vector matrix M_i^n(x) \equiv
  <polynomialVectorMatrix>
      < rows > m_j < / rows >
      <cols>m_j</cols>
      <elements>
         \langle xml \ for \ polynomial \ vector \ P_{i,11}^n(x) \rangle
         \langle xml \ for \ polynomial \ vector \ P^n_{i,m,i}(x) \rangle
         \langle xml\ for\ polynomial\ vector\ P^n_{i,1m_i}(x)\rangle
         \langle xml \ for \ polynomial \ vector \ P^n_{j,m_jm_j}(x) \rangle
      </elements>
      <samplePoints>
         \langle \text{elt} \rangle x_0^{(j)} \langle /\text{elt} \rangle
         <elt>x_{d_j}^{(j)}</elt>
      </samplePoints>
     <sampleScalings>
         \stackrel{\text{-}}{<\!\!\!\text{elt}}\!\!>\!\!s_0^{(j)}\!\!<\!\!/\!\!\!\text{elt}\!\!>
```

```
<elt>s_{d_j}^{(j)}</elt>
     </sampleScalings>
     <br/>
<br/>
dilinearBasis>
        \langle xml \ for \ polynomial \ q_0^{(j)}(x) \rangle
        \langle xml \ for \ polynomial \ q_{|d_i/2|}^{(j)}(x) \rangle
     </bilinearBasis>
  </polynomialVectorMatrix>
xml\ for\ polynomial\ vector\ P^n_{i,rs}(x) \equiv
  <polynomialVector>
     \langle xml \ for \ polynomial \ P_{j,rs}^0(x) \rangle
  \langle xml\ for\ polynomial\ P^N_{j,rs}(x) \rangle 
xml for polynomial a_0 + a_1x + \dots a_dx^d \equiv
  <polynomial>
     <coeff>a_0</coeff>
     <coeff>a_d</coeff>
  </polynomial>
```

The data can be spread over multiple files. In such cases the different input files should all follow the above format except that $\langle xml \ for \ objective \rangle$ should be omitted from all but one file. The parser will combine the constraints from all the polynomial vector matrices specified in the different files.

Several aspects of the input format are inefficient. Because the matrices are symmetric, rows and cols are redundant, and most elements are listed twice. Also, XML is extremely verbose.

To improve performance for large inputs, the XML files must first be preprocessed into a more efficient format. Instructions on how to preprocess the input and run SDPB are in docs/Usage.md.

3.2 Mathematica Interface

The program sdp2input generates preprocessed input files from Mathematica data. It automatically makes sensible choices for the bilinear bases $q_m^{(j)}(x)$, the sample points $x_k^{(j)}$ and the sample scalings $s_k^{(j)}$. If you wish to experiment with these choices, there is also an included Mathematica notebook SDPB.m.

The Mathematica definition of a PMP is slightly different but trivially equivalent to

(2.2). It is:

maximize
$$a \cdot z$$
 over $z \in \mathbb{R}^{N+1}$,
such that $\sum_{n=0}^{N} z_n W_j^n(x) \succeq 0$ for all $x \geq 0$ and $1 \leq j \leq J$, $n \cdot z = 1$. (3.1)

where $W_j^n(x)$ are matrix polynomials. The normalization condition $n \cdot z = 1$ can be used to solve for one of the components of z in terms of the others. Calling the remaining components $y \in \mathbb{R}^N$, we arrive at (2.2), where $M_j^n(x)$ are linear combinations of $W_j^n(x)$ and b_0, b_n are linear combinations of the a_n . This difference in convention is for convenient use in the conformal bootstrap.

SDPB.m defines a function WriteBootstrapSDP[file, sdp], where file is the XML file to be written to, and sdp has the following form, where the polynomials $Q_{j,rs}^n(x)$ are the elements of $W_j^n(x)$.

Listing 2: Usage of WriteBootstrapSDP in SDPB.m

```
function \ call \equiv WriteBootstrapSDP[file, \langle sdp \rangle]
sdp \equiv SDP[\langle objective \rangle, \langle normalization \rangle, \langle positive matrices with prefactors \rangle]
objective \equiv \{a_0, \ldots, a_N\}
normalization \equiv \{n_0, \ldots, n_N\}
positive matrices with prefactors \equiv \{
      \langle positive\ matrix\ with\ prefactor\ 1 \rangle,
      \langle positive\ matrix\ with\ prefactor\ J \rangle,
  }
positive matrix with prefactor j \equiv
  PositiveMatrixWithPrefactor [\langle prefactor \rangle,
      {
           \{Q_{j,11}^0(x)\text{, }\ldots\text{, }Q_{j,11}^N(x)\}\text{, }\ldots\text{, }\{Q_{j,m_j1}^0(x)\text{, }\ldots\text{, }Q_{j,m_j1}^N(x)\}
         },
           \{Q_{j,1m_j}^0(x), \ldots, Q_{j,1m_j}^N(x)\}, \ldots, \{Q_{j,m_jm_j}^0(x), \ldots, Q_{j,m_jm_j}^N(x)\}
      }
  ]
prefactor \equiv
      DampedRational[c, {p_1, \ldots, p_k}, b, x]
```

```
or const
```

The prefactor in PositiveMatrixWithPrefactor is used for constructing bilinear bases and sample scalings. Specifically, if the prefactor is $\chi(x)$, the bilinear basis is a set of orthogonal polynomials with respect to measure $\chi(x)dx$ on the positive real line, and sample scalings are $\chi(x_k)$, where the x_k are sample points. The notebook SDPB.m only deals with damped-rational prefactors because these are relevant to the conformal bootstrap. These stand for

DampedRational[
$$c$$
, $\{p_1, \dots, p_k\}$, b , x] $\rightarrow c \frac{b^x}{\prod_{i=1}^k (x-p_i)}$. (3.2)

We do not use an exponential-times-rational Mathematica function directly because the DampedRational data structure makes it easier to extract information needed to construct a bilinear basis. The notebook SDPB.m makes a choice of sample points that are reasonable for conformal bootstrap applications.

As an example bootstrap application, the included notebook Bootstrap2dExample.m computes a single-correlator dimension bound for 2d CFTs with a \mathbb{Z}_2 symmetry, as in [2].

3.3 An Example

Let's look at an example. Consider the following problem: maximize -y such that

$$1 + x^4 + y\left(\frac{x^4}{12} + x^2\right) \ge 0 \quad \text{for all } x \ge 0$$
 (3.3)

This is an PMP with 1×1 positive-semidefiniteness constraints. We will arbitrarily choose a prefactor of $e^{-x} = \mathtt{DampedRational[1,\{\}, 1/E,x]}$, so that the bilinear basis consists of Laguerre polynomials. The Mathematica code for this example is

Listing 3: Mathematica input for the example (3.3)

It produces the following XML file

Listing 4: XML file test.xml produced by listing 3. Decimals are truncated at 12 digits.

```
<sdp>
 <objective><elt>0</elt><elt>-1</elt></objective>
 <polynomialVectorMatrices>
   <polynomialVectorMatrix>
     <rows>1</rows>
     <cols>1</cols>
     <elements>
       <polynomialVector>
         <polynomial>
           <coeff>1</coeff><coeff>0</coeff><coeff>0</coeff>
           <coeff>0</coeff><coeff>1</coeff>
         </polynomial>
         <polynomial>
           <coeff>0</coeff><coeff><coeff>1</coeff>
           <coeff>0</coeff><coeff>0.0833333333333</coeff>
         </polynomial>
       </polynomialVector>
     </elements>
     <samplePoints>
       <elt>0.017496844815</elt><elt>0.157471603340</elt><elt>0.857345395967</elt>
       <elt>2.117118222694</elt><elt>3.936790083523</elt>
     </samplePoints>
     <sampleScalings>
       <elt>0.982655336118</elt><elt>0.854301072560</elt><elt>0.424286902403</elt>
       <elt>0.120378031823</elt><elt>0.019510742190</elt>
     </sampleScalings>
     <br/>
<br/>
dilinearBasis>
       <polynomial><coeff>1</coeff></polynomial>
       <polynomial><coeff>-1</coeff><coeff>1</coeff></polynomial>
       <polynomial><coeff>1</coeff><coeff>-2</coeff><coeff>0.5</coeff></polynomial>
     </bilinearBasis>
   </polynomialVectorMatrix>
 </polynomialVectorMatrices>
</sdp>
```

4 Internal SDP

To understand the output of SDPB, we need a rough understanding of its internal representation of the above PMP as a semidefinite program (SDP). Much more detail is given in [1]. The PMP (2.2) is translated into a dual pair of SDPs of the following form:

$$\mathcal{D}$$
: maximize $\operatorname{Tr}(CY) + b_0 + b \cdot y$ over $y \in \mathbb{R}^N$, $Y \in \mathcal{S}^K$, such that $\operatorname{Tr}(A_*Y) + By = c$, and $Y \succeq 0$. (4.1)

$$\mathcal{P}$$
: minimize $b_0 + c \cdot x$ over $x \in \mathbb{R}^P$, $X \in \mathcal{S}^K$,
such that $X = \sum_{p=1}^P A_p x_p - C$,
 $B^T x = b$,
 $X \succeq 0$, (4.2)

where " \succeq 0" means "is positive-semidefinite" and

$$c \in \mathbb{R}^{P},$$

$$B \in \mathbb{R}^{P \times N},$$

$$A_{1}, \dots, A_{P}, C \in \mathcal{S}^{K}.$$

$$(4.3)$$

Here, \mathcal{S}^K is the space of $K \times K$ symmetric real matrices, and $\text{Tr}(A_*Y)$ denotes the vector $(\text{Tr}(A_1Y), \ldots, \text{Tr}(A_PY)) \in \mathbb{R}^P$. An optimal solution to (4.1) and (4.2) is characterized by XY = 0 and also equality of the primal and dual objective functions $\text{Tr}(CY) + b_0 + b \cdot y = b_0 + c \cdot x$.

The residues

$$P \equiv \sum_{i} A_{i}x_{i} - X - C,$$

$$p \equiv b - B^{T}x,$$

$$d \equiv c - \text{Tr}(A_{*}Y) - By,$$

$$(4.4)$$

measure the failure of x, X, y, Y to satisfy their constraints. We say a point q = (x, X, y, Y) is "primal feasible" or "dual feasible" if the residues are sufficiently small,

primal feasible: primalError
$$\equiv \max_{i,j}\{|p_i|,|P_{ij}|\} < \text{primalErrorThreshold};$$
 dual feasible: dualError $\equiv \max_i\{|d_i|\} < \text{dualErrorThreshold},$

where primalErrorThreshold $\ll 1$ and dualErrorThreshold $\ll 1$ are parameters chosen by the user.

An optimal point should be both primal and dual feasible, and have (nearly) equal primal and dual objective values. Specifically, let us define dualityGap as the normalized difference between the primal and dual objective functions

$$\begin{array}{lll} \mbox{dualityGap} & \equiv & \frac{|\mbox{primalObjective} - \mbox{dualObjective}|}{\max\{1, |\mbox{primalObjective} + \mbox{dualObjective}|\}}, \\ \mbox{primalObjective} & \equiv & b_0 + c \cdot x, \\ \mbox{dualObjective} & \equiv & \mathrm{Tr}(CY) + b_0 + b \cdot y. \end{array} \tag{4.5}$$

A point is considered "optimal" if

$$dualityGap < dualityGapThreshold,$$
 (4.6)

where dualityGapThreshold $\ll 1$ is chosen by the user.

5 Output of SDPB

5.1 Terminal Output

Listing 5: Output of SDPB for the input file in listing 4

```
$ ./build/sdpb -s test/test --noFinalCheckpoint --dualityGapThreshold=1e-10 --procsPerNode=1
SDPB started at 2019-May-31 16:02:24
SDP directory : "test/test"
out directory
             : "test/test_out'
checkpoint in : "test/test.ck"
checkpoint out : "test/test.ck"
Parameters:
maxIterations
                          = 500
maxRuntime
                          = 86400
                          = 3600
checkpointInterval
noFinalCheckpoint
                         = true
writeMatrices
                         = false
findPrimalFeasible
                         = false
findDualFeasible
                          = false
detectPrimalFeasibleJump
                         = false
detectDualFeasibleJump
                         = false
                         = 400(448)
precision(actual)
dualityGapThreshold
                         = 1e-10
                         = 1e-30
primalErrorThreshold
dualErrorThreshold
                         = 1e-30
initialMatrixScalePrimal
                         = 1e+20
                         = 1e+20
initialMatrixScaleDual
feasibleCenteringParameter = 0.1
infeasibleCenteringParameter = 0.3
stepLengthReduction
                         = 0.7
maxComplementarity
                         = 1e+100
                         = 1
procsPerNode
procsGranularity
                         = 1
verbosity
                          = 1
Block Grid Mapping
Node Num Procs
                     Cost
                                    Block List
\{(0,5)\}
       1
                     1
```

	time mu	P-obj	D-obj	gap	P-err	p-err	D-err	P-step	D-step	beta
1	0 1.0e+4	00.00	+0.00	0.00	+1.00e+20	+1.00	+2.88e+20	0.631	0.647	0.300
2	0 5.0e+3	9 +9.49e+19	-1.64e+20	1.00	+3.69e+19	+0.369	+1.02e+20	0.653	0.639	0.300
3	0 2.5e+3	9 +1.04e+20	-2.92e+20	1.00	+1.28e+19	+0.128	+3.68e+19	0.660	0.639	0.300
119	0 2.4e-0	9 +1.84	+1.84	3.24e-09	+5.99e-136	+9.64e-137	+4.11e-127	0.777	0.777	0.100
120	0 7.2e-1	+1.84	+1.84	9.73e-10	+2.26e-136	+2.06e-136	+9.14e-128	0.778	0.778	0.100
121	0 2.2e-1	+1.84	+1.84	2.92e-10	+8.56e-136	+3.81e-136	+2.03e-128	0.778	0.778	0.100
fou	nd primal-dua	l optimal sol	ution							

Saving solution to : "test/test_out"

The output from running SDPB on the example problem in section 3.3 is in listing 5. The

input, output, and checkpoint files are listed first, followed by various parameters. After each iteration, SDPB prints the following:

time: The current solver runtime in seconds.

mu: The value of the complementarity Tr(XY)/K.

P-obj: The primal objective value $b_0 + c \cdot x$.

D-obj: The dual objective value $Tr(CY) + b_0 + b \cdot y$.

gap: The value of dualityGap.

P-err: The primal error $\max_{i,j} \{|P_{ij}|\}.$

p-err: The primal error $\max_i \{|p_i||\}.$

D-err: The dual error $\max_i \{|d_i|\}.$

P-step: The primal step length $\alpha_{\mathcal{P}}$ described in [1].

D-step: The dual step length $\alpha_{\mathcal{D}}$ described in [1].

beta: The corrector centering parameter β_c described in [1].

If an optimal solution exists, the primal and dual error will decrease until the problem becomes primal and dual feasible. Then the primal and dual objective functions start to converge, and the complementarity μ decreases until the duality gap becomes smaller than dualityGapThreshold.

The terminal output ends with the final values of the primal/dual objectives, primal/dual errors and duality gap.

5.2 Termination

The possible termination reasons for SDPB are as follows

found primal-dual optimal solution

Found a solution for x, X, y, Y that is simultaneously primal feasible, dual feasible, and optimal.

found primal feasible solution

Found a solution for x, X that is primal feasible. SDPB will only terminate with this result if the option --findPrimalFeasible is specified.

found dual feasible solution

Found a solution for y, Y that is dual feasible. SDPB will only terminate with this result if the option --findDualFeasible is specified.

primal feasible jump detected

A Newton step with primal step length $\alpha_{\mathcal{P}}$ just occurred, without resulting in a primal feasible solution. (Usually this means one should increase precision.)

dual feasible jump detected

A Newton step with dual step length $\alpha_{\mathcal{D}}$ just occurred, without resulting in a dual feasible solution. (Usually this means one should increase precision.)

maxIterations exceeded

SDPB has run for more iterations than specified by the option --maxIterations.

maxRuntime exceeded

SDPB has run for longer than specified by the option --maxRuntime.

maxComplementarity exceeded

 $\mu = \text{Tr}(XY)/\dim(X)$ exceeded the value specified by --maxComplementarity. This might indicate that the problem is unbounded and no optimal solution will be found.

When using SDPB to determine primal or dual feasibility, one can specify the options --findPrimalFeasible or --findDualFeasible. This will cause the solver to terminate immediately once the primal or dual errors are sufficiently small. This often occurs immediately after the primal or dual step lengths become equal to 1. A step length of 1 means that the solver has found a Newton step that exactly solves the primal or dual constraints, while preserving positive-semidefiniteness of X,Y. Sometimes a step length of 1 does not result in sufficiently small primal/dual errors. This is indicative of numerical instabilities and usually means precision should be increased. The options --detectPrimalFeasibleJump and --detectPrimalFeasibleJump cause SDPB to terminate if a step length of 1 occurs without resulting in primal/dual feasibility. If desired, one can then restart the solver with a higher value of precision.

5.3 Output File

Listing 6: Contents of the output file test_out/out.txt corresponding to listing 4. Decimal expansions have been truncated for brevity. Mathematica uses *^ instead of the character e for scientific notation. Thus, the output format is not quite suitable for import into Mathematica without modification. This could be changed in future versions.

```
terminateReason = "found primal-dual optimal solution";
primalObjective = 1.8402657633256563167214658396501869910056150833758753686...;
dualObjective = 1.8402657630028082077820253928104073320607351655204857599...;
dualityGap = 8.7717794734256614842509900260886197501683175194215210809...e-11;
primalError = 7.5108955634818106482332674480361038465586804606828026812...e-136;
dualError = 4.5214060425644592084868012680871048751928431201688166507...e-129;
Solver runtime = 0;
```

The output file test_out/out.txt corresponding to listing 4 is shown in listing 6. It includes the reason for termination, the final primal/dual objective values, the final



Figure 1: A plot of $1 + x^4 + y\left(\frac{x^4}{12} + x^2\right)$ with y = -1.840265763084 equal to its optimal value. The zero near x = 1 shows that -y cannot be further increased without violating the positivity constraint.

duality gap, the final primal/dual errors, and the total runtime. The vector y is saved in test_out/y.txt, and the two blocks of the x vector are saved in test_out/x_0.txt and test_out/x_1.txt. To include the matrices X and Y, add the option --writeMatrices.

The value of y gives the solution to our optimization problem. The function

$$1 + x^4 + (-1.840265763084) \left(\frac{x^4}{12} + x^2\right) \tag{5.1}$$

is plotted in figure 1. The zero near x=1 shows that y is optimal.

5.4 Checkpoints

Every checkpointInterval, SDPB saves a new checkpoint in a directory with the .ck extension. SDPB also saves a checkpoint after termination, provided the option --noFinalCheckpoint is not specified.

A checkpoint file encodes the values of x, X, y, Y. If SDPB detects an existing checkpoint file on startup, it will use those values of x, X, y, Y as initial conditions in the solver. Thus, SDPB can be stopped and started at will without losing progress.

A typical workflow for long-running computations on shared machines is to specify a moderate checkpointInterval (e.g. one hour) and a somewhat larger maxRuntime (e.g. 12 hours). SDPB will terminate after 12 hours and can then be restarted without losing progress. If SDPB is killed prematurely, then at most 1 hour of progress will be lost. This

pattern of restarting gives other users chances to run their processes. It can be sustained indefinitely, allowing extremely long computations.

Checkpoints are written in binary format to conserve space and speed up loading and unloading. If you specify the --writeMatrices option, the output directory can also be used to restart a computation with the -i option. It will not be bitwise identical to restarting from a binary checkpoint, but it should be very, very, very close.

Text checkpoints can be useful if you want to solve a different system by starting closer to previously solved system. You can also use it to continue a calculation with a different number of cores, or even on a different machine. Using the previous input as an example,

```
$ ./build/sdpb -s test/test --noFinalCheckpoint --dualityGapThreshold=1e-10 --procsPerNode=1 --writeMatrices
$ ./build/sdpb -s test/test --noFinalCheckpoint --dualityGapThreshold=1e-10 --procsPerNode=1 -i test/test\_out
```

the second calculation will start from the end of the first calculation.

6 Attribution

If you use SDPB in work that results in publication, please cite [1]. Depending on how SDPB is used, the following sources might also be relevant:

- The first use of semidefinite programming in the bootstrap [3].
- The generalization of semidefinite programming methods to arbitrary spacetime dimension [4].
- The generalization of semidefinite programming methods to arbitrary systems of correlation functions [5].

7 Acknowledgements

SDPB makes extensive use of the parallel linear algebra library Elemental [11], the Boost C++ libraries [9], the library [10], and the multiprecision libraries GMP [12], and MPFR [13].

SDPB was partially based on the solvers SDPA and SDPA-GMP [6-8], which were essential sources of inspiration and examples.

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