Kodiak, a C++ Library for Rigorous Branch and Bound Computation

Kodiak is a C++ library that implements a generic branch and bound algorithm for rigorous numerical approximations. Particular instances of the branch and bound algorithm allow the user to refine and isolate solutions to systems of nonlinear equations and inequalities, global optimization problems, and bifurcation sets for systems of ODEs. Kodiak utilizes interval arithmetic (via the filib++ library) and Bernstein enclosure (for polynomials and rational functions) as self-validating enclosure methods. Symbolic operations support procedures such as automatic partial differentiation.

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Documentation

Currently, the main documentation is contained in this file. Publications concerning the library and associated algorithms are in preparation. There are also numerous comments in the source code.

Support and Contribution

See the instructions in this file and the linked resources. For further assistance, or to report problems and bugs, please contact the authors. Contributions to the library are welcomed.

Obtaining *Kodiak*

The repository is located at: https://github.com/nasa/Kodiak/

License

The Kodiak C++ Library is released under NASA's Open Source Agreement. See the file LICENSE.pdf; see also the copyright notice at the end of this file.

Installation and Usage Options

Kodiak can either be installed from the source code, or, if available, a pre-built executable may be used instead.

The software can then be run in one of the following ways:

- Use the provided run-time interface, either interactively, or from an input file (either installation option)
- Encode a problem in a C++ program file, then compile and run it (only for installation from source code)

The following section assumes that you are installing the software from the source code; if you already have a pre-built or compiled executable, you can skip ahead to the section on using the software.

Installation

1. Prerequisites

It is recommended to run *Kodiak* on a Linux or Mac computer with the GNU C++ compiler; so far it has been successfully tested on Ubuntu Linux and Mac OS X. Use of Windows is not supported, although it ought to be feasible, and the authors would welcome any report of successfully running the software on Windows or any other system.

The following software should firstly be installed, if not already present (please follow the links for instructions and support):

- Boost libraries (required):
 http://www.boost.org/users/download/
 In addition to the headers, you need at least the library serialization.
 This library can be installed using ./bootstrap.sh --with-libraries=serialization and then sudo ./b2 install. Finally, you need to define the environment variable BOOST_ROOT to point to the directory where Boost's include and lib directories were installed, e.g., /usr/local.
- filib++ interval library (required): http://www2.math.uni-wuppertal.de/~xsc/software/filib.html

This library should be configured with the following options before making and installing it:

- ./configure CFLAGS=-fPIC CPPFLAGS=-fPIC CXXFLAGS=-fPIC
- Python language (recommended, necessary for the interface): http://www.python.org/ There is a good chance that Python is already installed.
- Cython, a Python to C translator (recommended, necessary for the interface): http://cython.org/#download
- PyInstaller package utility (optional, necessary to build a standalone executable)
 http://www.pyinstaller.org/
- gnuplot plotting software (optional, necessary for graphical output) http://www.gnuplot.info/

2. Build Library and Examples

If necessary, unzip the zip file in order to extract the files. The following files and directories should be present:

- In the working directory: this readme file (in various formats), the license, and a makefile
- src: source code for the library
- python: code for the Python interface
- examples: example C++ files (.cpp) containing several problems
- kdks: example text files (.kdk) for use with the interface

If any of the prerequisite libraries were installed in non-standard directories, then the files src/Makefile and python/Makefile should be modified accordingly.

Type make lib to compile the library. The lib directory and a static library file are created.

Type make examples to compile the examples. An executable for each example is created in the examples directory.

3. Build Interface (Recommended)

Type make python to build the interface.

The program and interface can be run with the command: python python/kodiak.py

4. Build Standalone Executable (Optional)

Type make kodiak to build a self-contained executable. The bin directory and a binary file are created.

It can be run with the command: bin/kodiak

Using the Interface

Starting the Interface

The program and interface can be run with the command: python python/kodiak.py

If using the standalone executable, instead type: bin/kodiak

You are now presented with a prompt and may issue commands (see below).

Exiting the Interface

To quit type quit or press ctrl+c.

Program Arguments

If not using the standalone executable, substitute python kodiak.py <arguments> for bin/kodiak <arguments> in the following:

The program can be called with a file or files as $\operatorname{argument}(s)$:

bin/kodiak <file>

It will process each file and print the output.

Files can be specified with an absolute or a relative path, e.g., to solve a problem contained in a file bar.kdk which is in the /home/foo/ directory:

bin/kodiak /home/foo/bar.kdk

Files must have a .kdk file extension.

To pass multiple files as arguments:

bin/kodiak <file> <file> ...

You can add as many as you like.

An output file can be specified; if the file already exists, results are appended to it:

bin/kodiak -o <output_file>

```
To read files and write the output to a different file: bin/kodiak -o <output_file> <file> ...

To switch on unsafe input mode (permits floating-point approximations to real numbers):
```

bin/kodiak -u

To save the (syntactically correct) session input to a file: bin/kodiak -s <save_file>

To run in quiet mode, with no output to console: bin/kodiak -q

To continue the session after processing input files: bin/kodiak <file> ... -c

To start *Kodiak* in debug mode:

bin/kodiak -d

For more help on the command line arguments:

bin/kodiak -h

All the aforementioned flags can be combined, e.g.: bin/kodiak -o foo -d -s bar -u -c foobar.kdk

Using Input Files

Input files can be created with a text editor; as noted, the filename extension must be .kdk. There are numerous examples in the kdks directory.

Anything after # on a line is a comment and is ignored by the program:

```
# this is a comment
file test.kdk # this is also a comment
```

```
Each expression must be followed by a semicolon, e.g.: var x in [0,1]; var y in [1,5];
```

To read an input file (either from the prompt or from another input file), the filename can contain a relative path or an absolute path to the file: file <file>

Commands in Input Files and Interactive Mode

The commands listed below can equivalently be used either interactively, from the command prompt, or else (if followed by a semicolon) in an input file.

Paving Problems (Systems of Equations and Inequalities)

Variables and their ranges can be declared with the var keyword, e.g.: var <var_name> in [13, 42]

The lower and upper bounds can be any integer in the range [-2147483648, 2147483647] on a 64-bit machine.

The bounds can also be set to either precise or approximate representations of floating-point numbers. Precise bounds can be set using one the following commands, where a and b are integers:

rat(a,b), to input rational numbers dec(a,b), to input decimal numbers

Numbers in the hexadecimal floating-point format are also accepted. The format follows the rules for the C definition of hex floats, e.g., 0x1ap-2 specifies the number 6.5.

Approximate representations of numbers in usual floating-point format can be entered using the approx(a) command, but this is discouraged and to do this the safe mode of *Kodiak* has to be set to false.

Constants, declared with the const keyword, and global definitions, with the def keyword, are also supported. The difference between them is that constants can only contain a single number, whereas definitions can hold entire equations.

Pavings without any constraints are not very interesting. Constraints (either equality or inequality) can be added to the problem with the cnstr command, e.g.:

```
cnstr x^2 + y < x
```

A list of mathematical operations which can be used in formulae can be found later in this document.

There are three possible options for the paving mode:

- first: this produces the first sub-box found which is feasible
- std: this paves the entirety of the feasible set
- full: this paves both the feasible and infeasible sets

The paving mode can be set as follows: set paving mode = <mode>

For further options to control the search space, see **Settings**, later in this guide.

Finally, to solve the paving problem, after it and the settings have been declared, use the pave command.

Bifurcation Problems (Bifurcation Analysis of ODEs)

Variables and their ranges can be declared as above, e.g.: var <var_name> in [13, 42]

Bifurcation problems also take parameters, which can be declared similarly using the param keyword, e.g.:

```
param <param_name> in [-42, 42]
```

One or more ordinary differential equations are required. An ODE in the form <expr>=0 can be declared with dfeq <expr>, e.g.: dfeq x+sqrt(y)

Constraints can be declared as above, e.g.:

```
cnstr x^2 + y < x
```

To pave the equilibrium manifold, use the command equilibrium; to pave the bifurcation manifold (limit point and Hopf bifurcations), which is a subset thereof, use the command bifurcation.

Minimization and Maximization Problems (Global Optimization)

For optimization problems, variables, constants, definitions, and constraints can be declared, as above. In addition, an objective function is needed; it is declared with the objfn keyword, e.g., objfn sin(x)+2*y

The solve commands min, max, and minmax are used to find an enclosure for the minimum, the maximum, and both the minimum and maximum, respectively.

Plotting

Both paving and bifurcation problems support graphical output using the *gnuplot* software. The projection of a paving into the space of selected variables is depicted. To plot the last solved problem in 2D or 3D, issue the plot command with two or three variables, e.g.:

```
plot x y z
```

To avoid having to redo calculations each time you start *Kodiak*, you can save the most recently produced paving with the save paving command. For example, save paving foo will save the paving to the file foo.pav in the current directory.

A paving can be loaded into *Kodiak* using the load paving command, e.g., load paving foo loads the paving in the file foo.pav.

Settings

To set the name of the problem: set name = <name>

To print out extra diagnostic information when solving problems: set debug = true|false (default: false)

To switch off safe input: set safe input = true|false (default: true). When safe input is on, approximate (i.e. floating-point) input values are not permitted.

To set the solver to use Bernstein enclosure in place of interval arithmetic where possible: set bp = true|false (default: false)

To set a resolution for all variables: set resolution = <real_number> As a termination criterion, the resolution is a non-negative number that specifies the smallest range (box width) where a bisection is considered for that variable.

To set a resolution for a specific variable: set resolution <var_name> = <real_number>

To set a precision for all variables: set precision = <integer>. If the precision (typically a small negative integer) is set to n, then the tolerance for the "almost certainly true" category of boxes is set to 10^n. It is not required to use this setting and this category of boxes, although doing so can speed up some problems.

To set the variable selection mode for branch and bound subdivision: set selectvar = 0|1|2 (default: 1). This option is only used for minimization/maximization problems. If 0, round-robin is used to select a subdivision variable; if 1, a heuristic is applied to the objective function; if 2, a heuristic is applied to the constraint system.

To set the maximum depth (in the search tree) for the branch and bound algorithm: set depth = <natural_number>

To print the output of the solver to a file: set output = <file>

To clean the program state, so that new problems can be entered: reset

If output was set using the $\neg o$ flag or the $\verb"set"$ output command, to reset output back to the console: $\verb"reset"$ output

Declaration and Expression Types

```
Numerical values: <num_val> = <integer> | approx(<real>) |
rat(<integer>, <integer>) | dec(<integer>, <natural_number>) |
<hex_constant>

Variable declarations: var <name> in [<num_val>, <num_val>]

Parameter declarations: param <name> in [<num_val>, <num_val>]

Constant declarations: const <name> = <num_val>

Mathematical expressions: <math_expr> = <num_val> | <var> |
<param> | <const> | <unary_operator>(<math_expr>) |
```

```
<math_expr> <binary_operator> <math_expr> |
let <name> = <math_expr> in <math_expr> |
let <name> = <math_expr>, <name> = <math_expr>, ... in
<math_expr>

Example: sin(approx(-1.1)*y)*sqrt(rat(3,2))^3-x

Objective function (optimization problems): objfn <math_expr>
Differential equation of the form <math_expr> = 0 (bifurcation problems):
dfeq <math_expr>
Constraint: cnstr <math_expr> <relational_operator> <math_expr>
```

Supported Relational (Boolean) Operations

```
<: less than
>: greater than
<=: less than or equal to
>=: greater than or equal to
=: equal to
```

Supported Mathematical Operations

```
+, -, *, /: addition, subtraction, multiplication, division 

: exponentiation (to an integer power) 

sq, sqrt: square, square root 

sin, cos, tan: trigonometric functions 

asin, acos, atan: inverse trigonometric functions 

abs: absolute value 

ln, exp: natural logarithm, exponential
```

Solve Commands

```
pave: compute a paving for the feasible/infeasible set equilibrium: compute a paving for the equilibrium set bifurcation: compute a paving for the bifurcation set minmax: compute an enclosure for the minimum and maximum min: compute an enclosure for the minimum max: compute an enclosure for the maximum
```

Using the Library

The *Kodiak* library can be used in your own C++ programs. A good way to start is to take one of the existing .cpp files in the examples directory and adapt

to your purposes. You can either invoke the compiler directly with a link to the filib++ and Kodiak libraries, or else add a new entry to the makefile there.

The commands and keywords listed above have member function equivalents (see the source code), although some of the names vary slightly. For example, there is a difference between, e.g., sin and Sin; the former is the operator for floating-point numbers and intervals, the latter is the operator for real expressions. In some cases, care must be taken with the order in which commands are issued. All variables should be declared before any variable resolutions are set.

Copyright Notices

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PLY (Python Lex-Yacc) Version 3.4

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