
PyKrylov Documentation

Release 0.1

D. Orban

March 16, 2009

CONTENTS

1	Introduction to PyKrylov	3
1.1	Example	3
2	Generic Template for Krylov Methods	5
2.1	The <code>generic</code> Module	5
2.2	Writing a New Solver	5
3	The Conjugate Gradient Method	7
3.1	The <code>cg</code> Module	7
3.2	Example	7
4	The Conjugate Gradient Squared Method	9
4.1	The <code>cgs</code> Module	9
4.2	Example	9
5	The Bi-Conjugate Gradient Stabilized Method	11
5.1	The <code>bicgstab</code> Module	11
5.2	Example	11
6	The Transpose-Free Quasi-Minimum Residual Method	13
6.1	The <code>tfqmr</code> Module	13
6.2	Example	13
7	Benchmarking Solvers	15
7.1	Example with Preconditioning	16
8	Indices and tables	19
	Bibliography	21
	Module Index	23
	Index	25

Release 0.1

Date January 27, 2009

This is the general documentation for PyKrylov, a pure Python implementation of common Krylov methods for the solution of systems of linear equations. The aim of this document is to cover usage of the package and how it can serve to benchmark solvers or preconditioners. Because the framework is very general and does not concern any specific application, the style is light and examples keep things simple. This is intentional so users have as much freedom as possible in modifying the example scripts.

Some examples use the efficient [Pysparse](#) sparse matrix library to simulate functions that return matrix-vector products.

Comments on this document or the software package should be posted on the [Lighthouse PyKrylov](#) page.

Contents:

INTRODUCTION TO PYKRYLOV

PyKrylov aims to provide a flexible implementation of the most common Krylov method for solving systems of linear equations in pure Python. The sole requirement is Numpy for fast array operations.

PyKrylov is in the *very early* stages of development. If you give it a whirl, please let me know what you think at the [LightHouse PyKrylov page](#). Feel free to post bug reports, feature requests and praises.

1.1 Example

The following code snippet solves a linear system with a 1D Poisson coefficient matrix. Since this matrix is symmetric and positive definite, the conjugate gradient algorithm is used:

```
import numpy as np
from math import sqrt
from pykrylov.cg import CG

def Poisson1dMatvec(x):
    # Matrix-vector product with a 1D Poisson matrix
    y = 2*x
    y[:-1] -= x[1:]
    y[1:] -= x[:-1]
    return y

n = 100
e = np.ones(n)
rhs = Poisson1dMatvec(e)
cg = CG(Poisson1dMatvec, matvec_max=200)
cg.solve(rhs)

print 'Number of matrix-vector products: ', cg.nMatvec
print 'Residual: %8.2e' % cg.residNorm
print 'Error: %8.2e' % (np.linalg.norm(e - CG.bestSolution)/sqrt(n))
```

On my machine, the above script produces:

```
Number of matrix-vector products: 50
Residual: 7.39e-14
Error: 2.06e-15
```


GENERIC TEMPLATE FOR KRYLOV METHODS

2.1 The generic Module

class KrylovMethod (*matvec*, ***kwargs*)

A general template for implementing iterative Krylov methods. This module defines the *KrylovMethod* generic class. Other modules subclass *KrylovMethod* to implement specific algorithms.

For general references on Krylov methods, see [Demmel], [Greenbaum], [Kelley], [Saad] and [Templates].

References:

solve (*rhs*, ***kwargs*)

This is the `solve()` method of the abstract *KrylovMethod* class. The class must be specialized and this method overridden.

2.2 Writing a New Solver

Adding a new solver to *PyKrylov* should be done by subclassing *KrylovMethod* from the *generic* module and overriding the `solve()` method. A general template might look like the following:

```
import numpy as np
from pykrylov.generic import KrylovMethod

class NewSolver( KrylovMethod ):
    """
    Document your new class and give adequate references.
    """

    def __init__(self, matvec, **kwargs):
        KrylovMethod.__init__(self, matvec, **kwargs)

        self.name = 'New Krylov Solver'
        self.acronym = 'NKS'
        self.prefix = self.acronym + ': ' # Used when verbose=True

    def solve(self, rhs, **kwargs):
        """
        Solve a linear system with 'rhs' as right-hand side by the NKS
        method. The vector 'rhs' should be a Numpy array. An optional
```

```
argument 'guess' may be supplied, with an initial guess as a Numpy
array. By default, the initial guess is the vector of zeros.
"""
n = rhs.shape[0]
nMatvec = 0

# Initial guess is zero unless one is supplied
guess_supplied = 'guess' in kwargs.keys()
x = kwargs.get('guess', np.zeros(n))

r0 = rhs # Fixed vector throughout
if guess_supplied:
    r0 = rhs - self.matvec(x)

# Further initializations ...

# Compute initial residual norm. For example:
residNorm = np.linalg.norm(r0)
self.residNorm0 = residNorm

# Compute stopping threshold
threshold = max( self.abstol, self.reltol * self.residNorm0 )

if self.verbose:
    self._write('Initial residual = %8.2e\n' % self.residNorm0)
    self._write('Threshold = %8.2e\n' % threshold)

# Main loop
while residNorm > threshold and nMatvec < self.matvec_max:

    # Do something ...
    pass

# End of main loop

self.nMatvec = nMatvec
self.bestSolution = x
self.residNorm = residNorm
```

THE CONJUGATE GRADIENT METHOD

3.1 The `cg` Module

class `CG` (*matvec*, ****kwargs**)

Bases: `pykrylov.generic.generic.KrylovMethod`

A pure Python implementation of the conjugate gradient (CG) algorithm. The conjugate gradient algorithm may be used to solve symmetric positive definite systems of linear equations, i.e., systems of the form

$$A x = b$$

where the matrix A is square, symmetric and positive definite. This is equivalent to solving the unconstrained convex quadratic optimization problem

$$\text{minimize } -\langle b, x \rangle + 1/2 \langle x, Ax \rangle$$

in the variable x .

CG performs 1 matrix-vector product, 2 dot products and 3 daxpys per iteration.

If a preconditioner is supplied, it needs to solve one preconditioning system per iteration. Our implementation is standard and follows [\[Kelley\]](#) and [\[Templates\]](#).

solve (*rhs*, ****kwargs**)

Solve a linear system with *rhs* as right-hand side by the CG method. The vector *rhs* should be a Numpy array.

Keyword arguments and default values

<i>guess</i>	Initial guess (Numpy array)	0
<i>matvec_max</i>	Max. number of matrix-vector products	2n

3.2 Example

The following script runs through a list of symmetric positive definite matrices in [Matrix Market](#) format, builds the right-hand side so that the exact solution of the system is the vector of ones, and applies the conjugate gradient to each of them. The sparse matrices are handled by way of the [Pysparse](#) package.

```
from pykrylov.cg import CG
from pysparse import spmatrix
from pysparse.pysparseMatrix import PysparseMatrix as sp
import numpy as np
from math import sqrt

matrices = ['l138bus.mtx', 'bcsstk08.mtx', 'bcsstk09.mtx', 'bcsstk10.mtx']
```

```
matrices += ['bcsstk11.mtx', 'bcsstk18.mtx', 'bcsstk19.mtx' ]

hdr = '%15s %5s %5s %8s %8s %8s' % ('Name', 'Size', 'Mult',
                                     'Resid0', 'Resid', 'Error')

print hdr

for matName in matrices:
    A = sp( matrix=spmatrix.ll_mat_from_mtx(matName) )
    n = A.shape[0]
    e = np.ones(n)
    rhs = A * e
    cg = CG(lambd v: A*v, matvec_max=2*n)
    cg.solve(rhs)
    err = np.linalg.norm(cg.bestSolution - e)/sqrt(n)
    print '%15s %5d %5d %8.2e %8.2e %8.2e' % (matName, n, cg.nMatvec,
                                              cg.residNorm0,
                                              cg.residNorm, err)
```

The script above produces the following output:

Name	Size	Mult	Resid0	Resid	Error
1138bus.mtx	1138	1759	1.46e+03	1.44e-03	1.30e-05
bcsstk08.mtx	1074	1255	8.74e+10	7.41e+04	7.54e-02
bcsstk09.mtx	1083	180	3.17e+08	1.84e+02	8.59e-06
bcsstk10.mtx	1086	1753	8.10e+07	7.30e+01	1.04e-03
bcsstk11.mtx	1473	1689	5.43e+09	4.88e+03	5.68e-02
bcsstk18.mtx	11948	9729	2.79e+11	2.49e+05	2.85e-01
bcsstk19.mtx	817	468	1.34e+15	1.26e+09	8.09e-01

Note that the default relative stopping tolerance is $1.0e-6$ and is achieved in all cases.

THE CONJUGATE GRADIENT SQUARED METHOD

4.1 The `cgs` Module

class `CGS` (*matvec*, ***kwargs*)

Bases: `pykrylov.generic.generic.KrylovMethod`

A pure Python implementation of the conjugate gradient squared (CGS) algorithm. CGS may be used to solve unsymmetric systems of linear equations, i.e., systems of the form

$$A x = b$$

where the matrix A may be unsymmetric.

CGS requires 2 matrix-vector products with A , 3 dot products and 7 daxpys per iteration. It does not require products with the transpose of A .

If a preconditioner is supplied, CGS needs to solve two preconditioning systems per iteration. The original description appears in [Sonn89], which our implementation roughly follows.

Reference:

solve (*rhs*, ***kwargs*)

Solve a linear system with *rhs* as right-hand side by the CGS method. The vector *rhs* should be a Numpy array.

Keyword arguments and default values

<i>guess</i>	Initial guess (Numpy array)	0
<i>matvec_max</i>	Max. number of matrix-vector products	2n

4.2 Example

Here is an example using CGS on a linear system. The coefficient matrix is read from file in Matrix Market format:

```
import numpy as np
from pykrylov.cgs import CGS as KSolver
from pyparse import spmatrix
from pyparse.pyparseMatrix import PyparseMatrix as sp

A = sp(matrix=spmatrix.ll_mat_from_mtx('jpwh_991.mtx'))
n = A.shape[0]
e = np.ones(n)
```

```
rhs = A*e

ks = KSolver( lambda v: A*v,
              matvec_max=2*n,
              verbose=False,
              outputStream=sys.stderr,
              reltol = 1.0e-5 )
ks.solve(rhs, guess = 1+np.arange(n, dtype=np.float))

print 'Number of matvecs: ', ks.nMatvec
print 'Initial/final res: %8.2e/%8.2e' % (ks.residNorm0, ks.residNorm)
print 'Direct error: %8.2e' % (np.linalg.norm(ks.bestSolution-e)/sqrt(n))
```

Running this script produces the following output:

```
Number of matvecs: 64
Initial/final res: 8.64e+03/4.72e-03
Direct error: 1.47e-04
```

THE BI-CONJUGATE GRADIENT STABILIZED METHOD

5.1 The `bicgstab` Module

class `BiCGSTAB` (*matvec*, ***kwargs*)

Bases: `pykrylov.generic.generic.KrylovMethod`

A pure Python implementation of the bi-conjugate gradient stabilized (Bi-CGSTAB) algorithm. Bi-CGSTAB may be used to solve unsymmetric systems of linear equations, i.e., systems of the form

$$A x = b$$

where the matrix A is unsymmetric and nonsingular.

Bi-CGSTAB requires 2 matrix-vector products, 6 dot products and 6 daxpys per iteration.

In addition, if a preconditioner is supplied, it needs to solve 2 preconditioning systems per iteration.

The original description appears in [VdVorst92]. Our implementation is a preconditioned version of that given in [Kelley].

Reference:

solve (*rhs*, ***kwargs*)

Solve a linear system with *rhs* as right-hand side by the Bi-CGSTAB method. The vector *rhs* should be a Numpy array.

Keyword arguments and default values

<i>guess</i>	Initial guess (Numpy array)	0
<i>matvec_max</i>	Max. number of matrix-vector products	2n

5.2 Example

Here is an example using Bi-CGSTAB on a linear system. The coefficient matrix is read from file in Matrix Market format:

```
import numpy as np
from pykrylov.cgs import BiCGSTAB as KSolver
from pyparse import spmatrix
from pyparse.pysparseMatrix import PysparseMatrix as sp

A = sp(matrix=spmatrix.ll_mat_from_mtx('jpwh_991.mtx'))
n = A.shape[0]
```

```
e = np.ones(n)
rhs = A*e

ks = KSolver( lambda v: A*v,
              matvec_max=2*n,
              verbose=False,
              outputStream=sys.stderr,
              reltol = 1.0e-5 )
ks.solve(rhs, guess = 1+np.arange(n, dtype=np.float))

print 'Number of matvecs: ', ks.nMatvec
print 'Initial/final res: %8.2e/%8.2e' % (ks.residNorm0, ks.residNorm)
print 'Direct error: %8.2e' % (np.linalg.norm(ks.bestSolution-e)/sqrt(n))
```

Running this script produces the following output:

```
Number of matvecs:  57
Initial/final res: 8.64e+03/5.18e-02
Direct error: 3.35e-03
```


THE TRANSPOSE-FREE QUASI-MINIMUM RESIDUAL METHOD

6.1 The `tfqmr` Module

class `TFQMR` (*matvec*, ***kwargs*)

Bases: `pykrylov.generic.generic.KrylovMethod`

A pure Python implementation of the transpose-free quasi-minimum residual (TFQMR) algorithm. TFQMR may be used to solve unsymmetric systems of linear equations, i.e., systems of the form

$$A x = b$$

where the matrix A may be unsymmetric.

TFQMR requires 2 matrix-vector products with A , 4 dot products and 10 daxpys per iteration. It does not require products with the transpose of A .

If a preconditioner is supplied, TFQMR needs to solve 2 preconditioning systems per iteration. Our implementation is inspired by the original description in [\[Freund\]](#) and that of [\[Kelley\]](#).

References:

solve (*rhs*, ***kwargs*)

Solve a linear system with *rhs* as right-hand side by the TFQMR method. The vector *rhs* should be a Numpy array.

Keyword arguments and default values

<i>guess</i>	Initial guess (Numpy array)	0
<i>matvec_max</i>	Max. number of matrix-vector products	2n

6.2 Example

Here is an example using TFQMR on a linear system. The coefficient matrix is read from file in Matrix Market format:

```
import numpy as np
from pykrylov.tfqmr import TFQMR as KSolver
from pyparse import spmatrix
from pyparse.pyparseMatrix import PyparseMatrix as sp

A = sp(matrix=spmatrix.ll_mat_from_mtx('jpwh_991.mtx'))
n = A.shape[0]
e = np.ones(n)
```

```
rhs = A*e

ks = KSolver( lambda v: A*v,
              matvec_max=2*n,
              verbose=False,
              outputStream=sys.stderr,
              reltol = 1.0e-5 )
ks.solve(rhs, guess = 1+np.arange(n, dtype=np.float))

print 'Number of matvecs: ', ks.nMatvec
print 'Initial/final res: %8.2e/%8.2e' % (ks.residNorm0, ks.residNorm)
print 'Direct error: %8.2e' % (np.linalg.norm(ks.bestSolution-e)/sqrt(n))
```

Running this script produces the following output:

```
Number of matvecs: 70
Initial/final res: 8.64e+03/6.23e-04
Direct error: 2.77e-05
```

BENCHMARKING SOLVERS

You may have noticed that in the examples of sections *The Conjugate Gradient Method*, *The Conjugate Gradient Squared Method*, *The Bi-Conjugate Gradient Stabilized Method* and *The Transpose-Free Quasi-Minimum Residual Method*, the only line that differs in the example scripts has the form

```
from pykrylov.tfqmr import TFQMR as KSolver
```

The rest of the code fragment is exactly the same across all examples. This similarity could be used, for instance, to benchmark solvers on a set of test problems.

Consider the script:

```
import numpy as np
from pykrylov.cgs import CGS
from pykrylov.tfqmr import TFQMR
from pykrylov.bicgstab import BiCGSTAB
from pyparse import spmatrix
from pyparse.pyparseMatrix import PyparseMatrix as sp

from math import sqrt

hdr = '%10s %6s %8s %8s %8s' % ('Name', 'Matvec', 'Resid0', 'Resid', 'Error')
fmt = '%10s %6d %8.2e %8.2e %8.2e'
print hdr

A = sp(matrix=spmatrix.ll_mat_from_mtx('jpwh_991.mtx'))

n = A.shape[0]
e = np.ones(n)
rhs = A*e

# Loop through solvers using tighter stopping tolerance
for KSolver in [CGS, TFQMR, BiCGSTAB]:
    ks = KSolver(lambda v: A*v, reltol=1.0e-8)
    ks.solve(rhs, guess = 1*np.arange(n, dtype=np.float), matvec_max=2*n)

    err = np.linalg.norm(ks.bestSolution-e)/sqrt(n)
    print fmt % (ks.acronym, ks.nMatvec, ks.residNorm0, ks.residNorm, err)
```

Executing the script above produces the formatted output:

Name	Matvec	Resid0	Resid	Error
CGS	82	8.64e+03	3.25e-05	2.35e-06

TFQMR	84	8.64e+03	8.97e-06	1.22e-06
Bi-CGSTAB	84	8.64e+03	5.57e-05	4.04e-06

7.1 Example with Preconditioning

A preconditioner can be supplied to any Krylov solver via the *precon* keyword argument upon instantiation.

For example, we could supply a simple (and naive) diagonal preconditioner by modifying the benchmarking script as:

```
import numpy as np
from pykrylov.cgs import CGS
from pykrylov.tfqmr import TFQMR
from pykrylov.bicgstab import BiCGSTAB
from pyparse import spmatrix
from pyparse.pyparseMatrix import PyparseMatrix as sp

from math import sqrt

hdr = '%10s %6s %8s %8s %8s' % ('Name', 'Matvec', 'Resid0', 'Resid', 'Error')
fmt = '%10s %6d %8.2e %8.2e %8.2e'
print hdr

A = sp(matrix=spmatrix.ll_mat_from_mtx('jpwh_991.mtx'))

# Extract diagonal of A and make it sufficiently positive
diagA = np.maximum(np.abs(A.takeDiagonal()), 1.0)

n = A.shape[0]
e = np.ones(n)
rhs = A*e

# Loop through solvers using default stopping tolerance
for KSolver in [CGS, TFQMR, BiCGSTAB]:
    ks = KSolver(lambda v: A*v,
                  precon=lambda u: u/diagA,
                  reltol=1.0e-8)
    ks.solve(rhs, guess = 1+np.arange(n, dtype=np.float), matvec_max=2*n)

    err = np.linalg.norm(ks.bestSolution-e)/sqrt(n)
    print fmt % (ks.acronym, ks.nMatvec, ks.residNorm, err)
```

This time, the output is a bit better than before:

Name	Matvec	Resid0	Resid	Error
CGS	70	8.64e+03	7.84e-06	2.33e-07
TFQMR	70	8.64e+03	7.61e-06	2.47e-07
Bi-CGSTAB	64	8.64e+03	8.54e-05	4.93e-06

Much in the same way, a modification of the script above could be used to loop through preconditioners with a given solver.

Note that preconditioners need not be functions but can be more general objects. The only requirement is that they should be callable. For example, the same effect as above can be achieved by instead defining the preconditioner as:

```
class DiagonalPrec:

    def __init__(self, A, **kwargs):
        self.name = 'Diag'
        self.shape = A.shape
        self.diag = np.maximum( np.abs(A.takeDiagonal()), 1.0)

    def __call__(self, y, **kwargs):
        "Return the result of applying preconditioner to y"
        return y/self.diag
```

If *dp* is an instance of the *DiagonalPrec* class and *y* is a Numpy array of appropriate size, one solves preconditioning systems by simply calling $x=dp(y)$. A call to a Krylov solver might thus look like:

```
# Create diagonal preconditioner
dp = DiagonalPrec(A)

ks = KSolver(lambda v: A*v, precon=dp, reltol=1.0e-8)
```


INDICES AND TABLES

- *Index*
- *Module Index*
- *Search Page*

BIBLIOGRAPHY

- [Demmel] J. W. Demmel, *Applied Numerical Linear Algebra*, SIAM, Philadelphia, 1997.
- [Greenbaum] A. Greenbaum, *Iterative Methods for Solving Linear Systems*, number 17 in *Frontiers in Applied Mathematics*, SIAM, Philadelphia, 1997.
- [Kelley] C. T. Kelley, *Iterative Methods for Linear and Nonlinear Equations*, number 16 in *Frontiers in Applied Mathematics*, SIAM, Philadelphia, 1995.
- [Saad] Y. Saad, *Iterative Methods for Sparse Linear Systems*, 2nd ed., SIAM, Philadelphia, 2003.
- [Templates] R. Barrett, M. Berry, T. F. Chan, J. Demmel, J. M. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine and H. Van der Vorst, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, 1993.
- [Sonn89] P. Sonneveld, *CGS, A Fast Lanczos-Type Solver for Nonsymmetric Linear Systems*, SIAM Journal on Scientific and Statistical Computing **10** (1), pp. 36–52, 1989.
- [VdVorst92] H. Van der Vorst, *Bi-CGSTAB: A Fast and Smoothly Convergent Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems*, SIAM Journal on Scientific and Statistical Computing **13** (2), pp. 631–644, 1992.
- [Freund] R. W. Freund, *A Transpose-Free Quasi-Minimal Residual Method for Non-Hermitian Linear Systems*, SIAM Journal on Scientific Computing, **14** (2), pp. 470–482, 1993.

MODULE INDEX

B

bicgstab, 11

C

cg, 7

cgs, 9

G

generic, 5

P

pykrylov, 1

T

tfqmr, 13

INDEX

B

BiCGSTAB (class in bicgstab), 11
bicgstab (module), 11

C

CG (class in cg), 7
cg (module), 7
CGS (class in cgs), 9
cgs (module), 9

G

generic (module), 5

K

KrylovMethod (class in generic), 5

P

pykrylov (module), 1

S

solve() (bicgstab.BiCGSTAB method), 11
solve() (cg.CG method), 7
solve() (cgs.CGS method), 9
solve() (generic.KrylovMethod method), 5
solve() (tfqmr.TFQMR method), 13

T

TFQMR (class in tfqmr), 13
tfqmr (module), 13