pentapy Documentation

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CHAPTER 1

PENTAPY QUICKSTART

pentapy is a toolbox to deal with pentadiagonal matrices in Python and solve the corresponding linear equation systems.

1.1 Installation

The package can be installed via pip. On Windows you can install WinPython to get Python and pip running.

```
pip install pentapy
```

There are pre-built wheels for Linux, MacOS and Windows for most Python versions (2.7, 3.4-3.7).

If your system is not supported and you want to have the Cython routines of pentapy installed, you have to provide a c-compiler and run:

```
pip install numpy cython
pip install pentapy
```

To get the scipy solvers running, you have to install scipy or you can use the extra argument:

```
pip install pentapy[all]
```

Instead of "all" you can also typ "scipy" or "umfpack".

1.2 References

The solver is based on the algorithms `PTRANS-I` and `PTRANS-II` presented by Askar et al. 2015.

1.3 Examples

Solving a pentadiagonal linear equation system

This is an example of how to solve a LES with a pentadiagonal matrix.

```python
import numpy as np
import pentapy as pp

size = 1000
# create a flattened pentadiagonal matrix
M_flat = (np.random.random((5, size)) - 0.5) * 1e-5
V = np.random.random(size) * 1e5
# solve the LES with M_flat as row-wise flattened matrix
X = pp.solve(M_flat, V, is_flat=True)

# create the corresponding matrix for checking
M = pp.create_full(M_flat, col_wise=False)
# calculate the error
print(np.max(np.abs(np.dot(M, X) - V)))
```

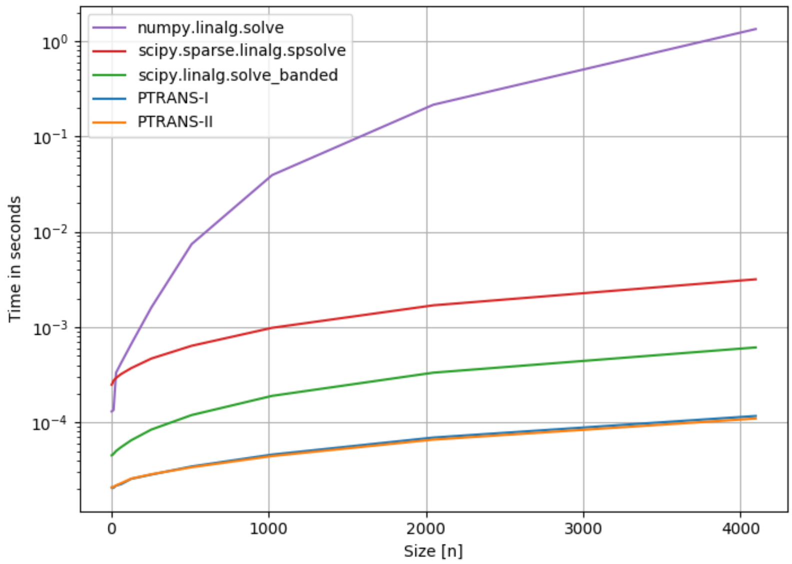
This should give something like:

```
4.257890395820141e-08
```

Performance

In the following, a couple of solvers for pentadiagonal systems are compared:

- Solver 1: Standard linear algebra solver of Numpy `np.linalg.solve` (link)
- Solver 2: `scipy.sparse.linalg.spsolve` (link)
- Solver 3: Scipy banded solver [`scipy.linalg.solve_banded`](scipy.github.io/devdocs/generated/scipy.linalg.solve_ba
- Solver 4: pentapy.solve with `solver=1`
- Solver 5: pentapy.solve with `solver=2`



The performance plot was created with `perfplot` (link).

1.4 Requirements

- Numpy >= 1.14.5

Optional

- SciPy
- scikit-umfpack

1.5 License

CHAPTER 2

PENTAPY TUTORIALS

In the following you will find Tutorials on how to use pentapy.

2.1 Tutorial 1: Solving a pentadiagonal system

Pentadiagonal systems arise in many areas of science and engineering, for example in solving differential equations with a finite difference sceme.

Theoretical Background

A pentadiagonal system is given by the equation: $M \cdot X = Y$, where M is a quadratic $n \times n$ matrix given by:

$$M = \begin{pmatrix} d_1 & d_1^{(1)} & d_1^{(2)} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ d_2^{(-1)} & d_2 & d_2^{(1)} & d_2^{(2)} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ d_3^{(-2)} & d_3^{(-1)} & d_3 & d_3^{(1)} & d_3^{(2)} & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & d_4^{(-2)} & d_4^{(-1)} & d_4 & d_4^{(1)} & d_4^{(2)} & 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & d_{n-2}^{(-2)} & d_{n-2}^{(-1)} & d_{n-2} & d_{n-2}^{(1)} & d_{n-2}^{(2)} \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & d_{n-1}^{(-2)} & d_{n-1}^{(-1)} & d_{n-1} & d_{n-1}^{(1)} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & d_n^{(-2)} & d_n^{(-1)} & d_n \end{pmatrix}$$

The aim is now, to solve this equation for X.

Memory efficient storage

To store a pentadiagonal matrix memory efficient, there are two options:

1. row-wise storage:

$$M_{\text{row}} = \begin{pmatrix} d_1^{(2)} & d_2^{(2)} & d_3^{(2)} & \cdots & d_{n-2}^{(2)} & 0 & 0 \\ d_1^{(1)} & d_2^{(1)} & d_3^{(1)} & \cdots & d_{n-2}^{(1)} & d_{n-1}^{(1)} & 0 \\ d_1 & d_2 & d_3 & \cdots & d_{n-2} & d_{n-1} & d_n \\ 0 & d_2^{(-1)} & d_3^{(-1)} & \cdots & d_{n-2}^{(-1)} & d_{n-1}^{(-1)} & d_n^{(-1)} \\ 0 & 0 & d_3^{(-2)} & \cdots & d_{n-2}^{(-2)} & d_{n-1}^{(-2)} & d_n^{(-2)} \end{pmatrix}$$

Here we see, that the numbering in the above given matrix was aiming at the row-wise storage. That means, the indices were taken from the row-indices of the entries.

2. column-wise storage:

$$M_{\mathrm{col}} = \begin{pmatrix} 0 & 0 & d_1^{(2)} & \cdots & d_{n-4}^{(2)} & d_{n-3}^{(2)} & d_{n-2}^{(2)} \\ 0 & d_1^{(1)} & d_2^{(1)} & \cdots & d_{n-3}^{(1)} & d_{n-2}^{(1)} & d_{n-1}^{(1)} \\ d_1 & d_2 & d_3 & \cdots & d_{n-2} & d_{n-1} & d_n \\ d_2^{(-1)} & d_3^{(-1)} & d_4^{(-1)} & \cdots & d_{n-1}^{(-1)} & d_n^{(-1)} & 0 \\ d_3^{(-2)} & d_4^{(-2)} & d_5^{(-2)} & \cdots & d_n^{(-2)} & 0 & 0 \end{pmatrix}$$

The numbering here is a bit confusing, but in the column-wise storage, all entries written in one column were in the same column in the original matrix.

Solving the system using pentapy

To solve the system you can either provide M as a full matrix or as a flattened matrix in row-wise resp. col-wise flattened form.

If M is a full matrix, you call the following:

```
import pentapy as pp

M = ...  # your matrix
Y = ...  # your right hand side

X = pp.solve(M, Y)
```

If M is flattend in row-wise order you have to set the keyword argument `is_flat=True`:

```
import pentapy as pp

M = ...  # your flattened matrix
Y = ...  # your right hand side

X = pp.solve(M, Y, is_flat=True)
```

If you got a col-wise flattend matrix you have to set `index_row_wise=False`:

```
X = pp.solve(M, Y, is_flat=True, index_row_wise=False)
```

Tools

pentapy provides some tools to convert a pentadiagonal matrix.

diag_indices(n[, offset])	Indices for the main or minor diagonals of a matrix.
shift_banded(mat[, up, low, col_to_row, copy])	Shift rows of a banded matrix.
create_banded(mat[, up, low, col_wise, dtype])	Create a banded matrix from a given quadratic Matrix.
create_full(mat[, up, low, col_wise])	Create a (n x n) Matrix from a given banded matrix.

Example

This is an example of how to solve a LES with a pentadiagonal matrix. The matrix is given as a row-wise flattened matrix, that is filled with random numbers. Afterwards the matrix is transformed to the full quadradratic matrix to check the result.

```python
import numpy as np
import pentapy as pp

size = 1000
# create a flattened pentadiagonal matrix
M_flat = (np.random.random((5, size)) - 0.5) * 1e-5
V = np.random.random(size) * 1e5
# solve the LES with M_flat as row-wise flattened matrix
X = pp.solve(M_flat, V, is_flat=True)

# create the corresponding matrix for checking
M = pp.create_full(M_flat, col_wise=False)
# calculate the error
print(np.max(np.abs(np.dot(M, X) - V)))
```

This should give something small like:

```
4.257890395820141e-08
```

CHAPTER 3

PENTAPY API

3.1 Purpose

pentapy is a toolbox to deal with pentadiagonal matrizes in Python.

Solver

Solver for a pentadiagonal equations system.

solve(mat, rhs[, is_flat, index_row_wise, . . .])	Solver for a pentadiagonal system.

Tools

The following tools are provided:

diag_indices(n[, offset])	Indices for the main or minor diagonals of a matrix.
shift_banded(mat[, up, low, col_to_row, copy])	Shift rows of a banded matrix.
create_banded(mat[, up, low, col_wise, dtype])	Create a banded matrix from a given quadratic Matrix.
create_full(mat[, up, low, col_wise])	Create a (n x n) Matrix from a given banded matrix.

3.2 pentapy.core

The core module of pentapy.

The following functions are provided

`solve`(mat, rhs[, is_flat, index_row_wise, . . .])	Solver for a pentadiagonal system.

`pentapy.core.`**`solve`**(*mat, rhs, is_flat=False, index_row_wise=True, solver=1*)

Solver for a pentadiagonal system.

The matrix can be given as a full n x n matrix or as a flattend one. The flattend matrix can be given in a row-wise flattend form:

```
[[Dup2[0]  Dup2[1]  Dup2[2]  ... Dup2[N-2]  0          0        ]
 [Dup1[0]  Dup1[1]  Dup1[2]  ... Dup1[N-2]  Dup1[N-1]  0        ]
 [Diag[0]  Diag[1]  Diag[2]  ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [0        Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] Dlow1[N]]
 [0        0        Dlow2[2] ... Dlow2[N-2] Dlow2[N-2] Dlow2[N]]]
```

Or a column-wise flattend form:

```
[[0        0        Dup2[2]  ... Dup2[N-2]  Dup2[N-1]  Dup2[N] ]
 [0        Dup1[1]  Dup1[2]  ... Dup1[N-2]  Dup1[N-1]  Dup1[N] ]
 [Diag[0]  Diag[1]  Diag[2]  ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [Dlow1[0] Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] 0       ]
 [Dlow2[0] Dlow2[1] Dlow2[2] ... Dlow2[N-2] 0          0       ]]
```

Dup1 and Dup2 are the first and second upper minor-diagonals and Dlow1 resp. Dlow2 are the lower ones. If you provide a column-wise flattend matrix, you have to set:

```
index_row_wise=False
```

Parameters

- **`mat`** (`numpy.ndarray`) – The Matrix or the flattened Version of the pentadiagonal matrix.
- **`rhs`** (`numpy.ndarray`) – The right hand side of the equation system.
- **`is_flat`** (`bool`, optional) – State if the matrix is already flattend. Default: `False`
- **`index_row_wise`** (`bool`, optional) – State if the flattend matrix is row-wise flattend. Default: `True`
- **`solver`** (`int` or `str`, optional) – Which solver should be used. The following are provided:
  - `[1, "1", "PTRANS-I"]` : The PTRANS-I algorithm
  - `[2, "2", "PTRANS-II"]` : The PTRANS-II algorithm
  - `[3, "3", "lapack", "solve_banded"]` : scipy.linalg.solve_banded
  - `[4, "4", "spsolve"]` : The scipy sparse solver without umf_pack
  - `[5, "5", "spsolve_umf", "umf", "umf_pack"]` : The scipy sparse solver with umf_pack

  Default: `1`

Returns **result** – Solution of the equation system

Return type `numpy.ndarray`

3.3 pentapy.tools

The tools module of pentapy.

The following functions are provided

diag_indices(n[, offset])	Indices for the main or minor diagonals of a matrix.
shift_banded(mat[, up, low, col_to_row, copy])	Shift rows of a banded matrix.
create_banded(mat[, up, low, col_wise, dtype])	Create a banded matrix from a given quadratic Matrix.
create_full(mat[, up, low, col_wise])	Create a (n x n) Matrix from a given banded matrix.

pentapy.tools.**create_banded**(*mat*, *up=2*, *low=2*, *col_wise=True*, *dtype=None*)

Create a banded matrix from a given quadratic Matrix.

The Matrix will to be returned as a flattend matrix. Either in a column-wise flattend form:

```
[[0         0         Dup2[2]   ... Dup2[N-2]  Dup2[N-1]  Dup2[N] ]
 [0         Dup1[1]   Dup1[2]   ... Dup1[N-2]  Dup1[N-1]  Dup1[N] ]
 [Diag[0]   Diag[1]   Diag[2]   ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [Dlow1[0]  Dlow1[1]  Dlow1[2]  ... Dlow1[N-2] Dlow1[N-1] 0       ]
 [Dlow2[0]  Dlow2[1]  Dlow2[2]  ... Dlow2[N-2] 0          0       ]]
```

Then use:

```
col_wise=True
```

Or in a row-wise flattend form:

```
[[Dup2[0]   Dup2[1]   Dup2[2]   ... Dup2[N-2]  0          0       ]
 [Dup1[0]   Dup1[1]   Dup1[2]   ... Dup1[N-2]  Dup1[N-1]  0       ]
 [Diag[0]   Diag[1]   Diag[2]   ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [0         Dlow1[1]  Dlow1[2]  ... Dlow1[N-2] Dlow1[N-1] Dlow1[N]]
 [0         0         Dlow2[2]  ... Dlow2[N-2] Dlow2[N-2] Dlow2[N]]]
```

Then use:

```
col_wise=False
```

Dup1 and Dup2 or the first and second upper minor-diagonals and Dlow1 resp. Dlow2 are the lower ones. The number of upper and lower minor-diagonals can be altered.

Parameters

- **mat** (numpy.ndarray) – The full (n x n) Matrix.
- **up** (int) – The number of upper minor-diagonals. Default: 2
- **low** (int) – The number of lower minor-diagonals. Default: 2
- **col_wise** (bool, optional) – Use column-wise storage. If False, use row-wise storage. Default: True

Returns Bandend matrix

Return type numpy.ndarray

pentapy.tools.**create_full**(*mat*, *up=2*, *low=2*, *col_wise=True*)

Create a (n x n) Matrix from a given banded matrix.

The given Matrix has to be a flattend matrix. Either in a column-wise flattend form:

```
[[0         0         Dup2[2]   ... Dup2[N-2]  Dup2[N-1]  Dup2[N] ]
 [0         Dup1[1]   Dup1[2]   ... Dup1[N-2]  Dup1[N-1]  Dup1[N] ]
 [Diag[0]   Diag[1]   Diag[2]   ... Diag[N-2]  Diag[N-1]  Diag[N] ]
```

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```
 [Dlow1[0] Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] 0        ]
 [Dlow2[0] Dlow2[1] Dlow2[2] ... Dlow2[N-2] 0          0        ]]
```

Then use:

```
col_wise=True
```

Or in a row-wise flattend form:

```
[[Dup2[0]  Dup2[1]  Dup2[2]  ... Dup2[N-2]  0          0        ]
 [Dup1[0]  Dup1[1]  Dup1[2]  ... Dup1[N-2]  Dup1[N-1]  0        ]
 [Diag[0]  Diag[1]  Diag[2]  ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [0        Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] Dlow1[N]]
 [0        0        Dlow2[2] ... Dlow2[N-2] Dlow2[N-2] Dlow2[N]]]
```

Then use:

```
col_wise=False
```

Dup1 and Dup2 or the first and second upper minor-diagonals and Dlow1 resp. Dlow2 are the lower ones. The number of upper and lower minor-diagonals can be altered.

Parameters

- **mat** (`numpy.ndarray`) – The flattened Matrix.
- **up** (`int`) – The number of upper minor-diagonals. Default: 2
- **low** (`int`) – The number of lower minor-diagonals. Default: 2
- **col_wise** (`bool`, optional) – Input is in column-wise storage. If False, use as row-wise storage. Default: `True`

Returns Full matrix.

Return type `numpy.ndarray`

`pentapy.tools.`**`diag_indices`**(*n*, *offset=0*)

Indices for the main or minor diagonals of a matrix.

This returns a tuple of indices that can be used to access the main diagonal of an array *a* with `a.ndim == 2` dimensions and shape (n, n).

Parameters

- **n** (*int*) – The size, along each dimension, of the arrays for which the returned indices can be used.
- **offset** (*int, optional*) – The diagonal offset.

Returns

- **idx** (`numpy.ndarray`) – row indices
- **idy** (`numpy.ndarray`) – col indices

`pentapy.tools.`**`shift_banded`**(*mat*, *up=2*, *low=2*, *col_to_row=True*, *copy=True*)

Shift rows of a banded matrix.

Either from column-wise to row-wise storage or vice versa.

The Matrix has to be given as a flattend matrix. Either in a column-wise flattend form:

```
[[0        0        Dup2[2]  ... Dup2[N-2]  Dup2[N-1]  Dup2[N] ]
 [0        Dup1[1]  Dup1[2]  ... Dup1[N-2]  Dup1[N-1]  Dup1[N] ]
 [Diag[0]  Diag[1]  Diag[2]  ... Diag[N-2]  Diag[N-1]  Diag[N] ]
```

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```
 [Dlow1[0] Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] 0        ]
 [Dlow2[0] Dlow2[1] Dlow2[2] ... Dlow2[N-2] 0          0        ]]
```

Then use:

```
col_to_row=True
```

Or in a row-wise flattend form:

```
[[Dup2[0]  Dup2[1]  Dup2[2]  ... Dup2[N-2]  0          0        ]
 [Dup1[0]  Dup1[1]  Dup1[2]  ... Dup1[N-2]  Dup1[N-1]  0        ]
 [Diag[0]  Diag[1]  Diag[2]  ... Diag[N-2]  Diag[N-1]  Diag[N] ]
 [0        Dlow1[1] Dlow1[2] ... Dlow1[N-2] Dlow1[N-1] Dlow1[N]]
 [0        0        Dlow2[2] ... Dlow2[N-2] Dlow2[N-2] Dlow2[N]]]
```

Then use:

```
col_to_row=False
```

Dup1 and Dup2 are the first and second upper minor-diagonals and Dlow1 resp. Dlow2 are the lower ones. The number of upper and lower minor-diagonals can be altered.

Parameters

- **mat** (`numpy.ndarray`) – The Matrix or the flattened Version of the pentadiagonal matrix.
- **up** (`int`) – The number of upper minor-diagonals. Default: 2
- **low** (`int`) – The number of lower minor-diagonals. Default: 2
- **col_to_row** (`bool`, optional) – Shift from column-wise to row-wise storage or vice versa. Default: `True`
- **copy** (`bool`, optional) – Copy the input matrix or overwrite it. Default: `True`

Returns Shifted bandend matrix

Return type `numpy.ndarray`

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