pyknotid Documentation

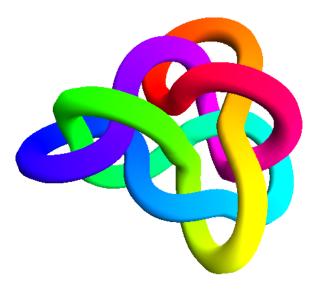
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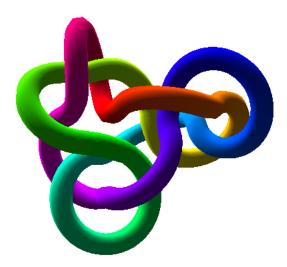
pyknotid is a Python module for identifying knot types and other topological quantities. It can take as input spacecurves (such as visualised above) or standard topological notations.

See the *overview* for an introduction to pyknotid's functionality, or find specific topics in the index below.

CHAPTER 1

Contents

1.1 Overview



pyknotid is a Python module for doing calculations on knots or links, whether specified as space-curves, or via standard topological notations.

Visit Knot ID for an online interface to some of these tools.

1.1.1 Installation

You can install pyknotid via pip:

\$ pip install pyknotid

By default pyknotid will try to compile some cython modules, but if this fails (normally because cython is not installed) it will only print a message and continue without errors. This won't impact your use of pyknotid except that the cython calculations would be, especially during space-curve analysis. If you want to use the improved speed of the cython implementations but did not initially install them, you should uninstall pyknotid, install cython, and reinstall pyknotid.

You can also install the pyknotid development version from github at https://github.com/SPOCKnots/pyknotid.

1.1.2 Space curve analysis

pyknotid can perform many calculations on space curves specified as a set of points, as well as plotting the curves in three dimensions or in projection. See the *space curve documentation* for more information.

Some topological calculations can only be performed for relatively short, simple curves, but in general pyknotid can work fine even for space-curves with many thousands of points.

Example:

```
from pyknotid.make import trefoil
from pyknotid.spacecurves import Knot
k = Knot(trefoil())
k.determinant() # 3
k.gauss_code() # 1+a,2-a,3+a,1-a,2+a,3-a
k.identify() # [<Knot 3_1>]
```

1.1.3 Topological representations

pyknotid can accept input using several standard topological notations including the Gauss code, planar diagram or Dowker-Thistlethwaite notation. You can then calculate topological invariants, or even reconstruct a 3D space curve. See the *representation documentation* for more information.

Example:

1.1.4 Knot catalogue

pyknotid can look up knot types in a prebuilt database containing various invariants for knots with up to 15 crossings. They can be looked up by the knot name (e.g. 3_1 for the trefoil knot, 4_1 for the figure-eight knot etc.), or the values of different knot invariants. See the *knot catalogue documentation* for more information.

Example:

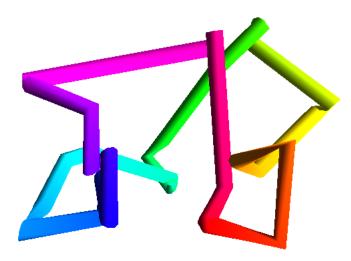
1.1.5 Example knots

pyknotid includes several functions for creating example knotted space curves. See the example knots documentation for more details.

Example:

```
from pyknotid.make import torus_knot
k = torus_knot(p=5, q=2)
k.identify() # [<Knot 5_1>]
from pyknotid.make import torus_link
l = torus_link(p=2, q=8) # a 2-component link
l.linking_number() # 8
from pyknotid.make import figure_eight
k = figure_eight()
k.determinant() # 5
```

1.2 Space curve analysis



This module contains classes and functions for working with knots and links as three-dimensional space curves, or calling functions elsewhere in pyknotid to perform topological analysis. Functionality includes manipulating knots/links via translation, rotation and scaling, plotting diagrams, finding crossings and identifying knots.

1.2.1 Different knot classes

pyknotid includes the following classes for topological calculation:

- *SpaceCurve*: Provides functions for calculations on a single curve, including plotting, some geometrical properties and finding crossings in projection.
- *Knot*: Provides functions for topological calculations on a single curve, such as the Alexander polynomial or Vassiliev invariants.
- *OpenKnot*: Provides functions for topological calculations on an open curve that does not form a closed loop. Open curves are topologically trivial from a mathematical perspective, but can be analysed in terms of the topology of different closures.
- Link: Provides the same interface to collections of multiple curves, and can calculate linking invariants.
- PeriodicCell: Provides some convenience functions for managing collections of curves in periodic boundaries.

1.2.2 Creating space curves

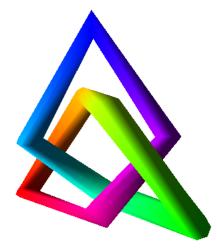
The space curve classes are specified via N by 3 arrays of points in three dimensions, representing a piecewise linear curve.

For instance, the following code produces and plots a *Knot* from a set of manually specified points:

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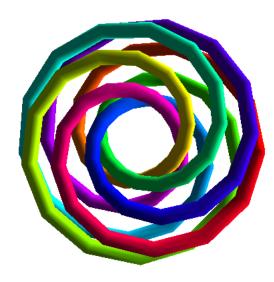
(continued from previous page)

```
[-4.5, -7.79, -7.35e-16],
[3.45, -2.89, 2.6],
[3.45, 2.89, -2.6],
[-4.5, 7.79, 0.0],
[-4.23, -1.54, 2.6],
[0.781, -4.43, -2.6]])
k = Knot(points)
k.plot()
```



The pyknotid.make module provides functions for creating many types of example knots, such as torus knots or some specific knot types:

```
import numpy as np
from pyknotid.make import torus_knot
    k = torus_knot(7, 4)
    k.plot()
```



1.2.3 SpaceCurve

The *SpaceCurve* class is the base for all space-curve analysis in pyknotid. It provides methods for geometrical manipulation (translation, rotation etc.), calculating geometrical characteristics such as the writhe, and obtaining topological representations of the curve by analysing its crossings in projection.

pyknotid provides other classes for topological analysis of the curves:

- Knot for calculating knot invariants of the space-curve.
- *Link* to handle multiple SpaceCurves and calculate linking invariants.
- Cell for handling multiple space-curves in a box with periodic boundaries.

API documentation

Bases: object

Class for holding the vertices of a single line, providing helper methods for convenient manipulation and analysis.

The methods of this class are largely geometrical (though this includes listing the crossings in projection and extracting a Gauss code etc.). For topological measurements, you should use a *Knot*.

This class deliberately combines methods to do many different kinds of measurements or manipulations. Some of these are externally available through other modules in pyknotid - if so, this is usually indicated in the method docstrings.

Parameters

- **points** (*array-like*) The 3d points (vertices) of a piecewise linear curve representation
- **verbose** (*bool*) Indicates whether the SpaceCurve should print information during processing
- **add_closure** (*bool*) If True, adds a final point to the knot near to the start point, so that it will appear visually to close when plotted.
- **zero_centroid** (*bool*) If True, shifts the coordinates of the points so that their centre of mass is at the origin.

arclength (include_closure=True)

Returns the arclength of the line, the sum of lengths of each piecewise linear segment.

Parameters include_closure (bool) – Whether to include the distance between the final and first points. Defaults to True.

average_crossing_number (samples=10, recalculate=False, **kwargs)

The (approximate) average crossing number of the space curve, obtained by averaging the planar writhe over the given number of directions.

- **samples** (*int*) The number of directions to average over.
- **recalculate** (*bool*) Whether to recalculate the ACN.
- ****kwargs** These are passed directly to *raw_crossings()*.

close()

Adds the starting point to the end of the curve, so that it ends exactly where it began.

classmethod closing_on_sphere(*line*, *com*=(0.0, 0.0, 0.0))

Adds new vertices to close the line at its maximum radius, returning a SpaceCurve representing the result.

Parameters

- line (ndarray) The points of the line.
- **com** (*iterable*) Optional additional centre of mass to shift by before closing

copy()

Returns another knot with the same points and verbosity as self. Other attributes (e.g. cached crossings) are not preserved.

cuaps (*include_closure=True*)

Returns a list of the 'cuaps', where the curve is parallel to the positive x-axis. See D Bar-Natan and R van der Veen, "A polynomial time knot polynomial", 2017.

curvatures (closed=True)

Returns curvatures at each vertex (or really line segment).

classmethod from_braid_word(word)

Returns a *SpaceCurve* instance formed from the given braid word.

The braid word should be of the form 'aAbBcC' (i.e. capitalisation denotes inverse).

Parameters word (*str*) – The braid word to interpret.

classmethod from_csv (filen, **kwargs)

Loads knot points from the given csv file, and returns a *SpaceCurve* with those points.

Arguments are passed straight to pyknot.io.from_csv().

classmethod from_gauss_code(code)

Creates a Knot from the given code, which must be provided as a string and may optionally include crossing orientations (these are actually ignored).

classmethod from_json(filen)

Loads knot points from the given filename, assuming json format, and returns a *SpaceCurve* with those points.

classmethod from_lattice_data(*line*)

Returns a *SpaceCurve* instance in which the line has been slightly translated and rotated, in order to (practically) ensure no self intersections in closure or coincident points in projection.

Parameters line (*array-like*) – The list of points in the line. May be any type that Space-Curve normally accepts.

Returns

Return type SpaceCurve

classmethod from_periodic_line(line, shape, perturb=True, **kwargs)

Returns a *SpaceCurve* instance in which the line has been unwrapped through the periodic boundaries.

- line (array-like) The Nx3 vector of points in the line
- shape (array-like) The x, y, z distances of the periodic boundary
- **perturb** (bool) If True, translates and rotates the knot to avoid any lattice problems.

gauss_code (recalculate=False, **kwargs)

Returns a *GaussCode* instance representing the crossings of the knot.

The GaussCode instance is cached internally. If you want to recalculate it (e.g. to get an unsimplified version if you have simplified it), you should pass *recalculate=True*.

This method passes kwargs directly to *raw_crossings()*, see the documentation of that function for all options.

gauss_diagram(simplify=False, **kwargs)

Returns a GaussDiagram instance representing the crossings of the knot.

This method passes kwargs directly to *raw_crossings()*, see the documentation of that function for all options.

interpolate (num_points, s=0, **kwargs)

Replaces self.points with points from a B-spline interpolation.

This method uses scipy.interpolate.splprep. kwargs are passed to this function.

octree_simplify (runs=1, plot=False, rotate=True, obey_knotting=True, **kwargs)
Simplifies the curve via the octree reduction of :module:'pyknotid.simplify.octree'.

Parameters

- **runs** (*int*) The number of times to run the octree simplification. Defaults to 1.
- plot (bool) Whether to plot the curve after each run. Defaults to False.
- **rotate** (*bool*) Whether to rotate the space curve before each run. Defaults to True as this can make things much faster.
- **obey_knotting** (*bool*) Whether to not let the line pass through itself. Defaults to True as this is always what you want for a closed curve.
- ****kwargs** Any remaining kwargs are passed to the pyknotid.simplify. octree.OctreeCell constructor.

planar_diagram(**kwargs)

Returns a *PlanarDiagram* instance representing the crossings of the knot.

This method passes kwargs directly to *raw_crossings()*, see the documentation of that function for all options.

planar_second_order_writhe(**kwargs)

The second order writhe (type 2, i1,i3,i2,i4) of the projection of the curve along the z axis.

planar_writhe(**kwargs)

Returns the current planar writhe of the knot; the signed sum of crossings of the current projection.

The 'true' writhe is the average of this quantity over all projection directions, and is available from the writhe() method.

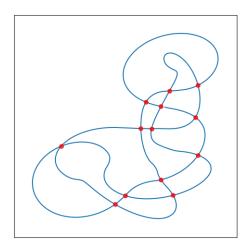
Parameters **kwargs – These are passed directly to *raw_crossings()*.

plot (mode='auto', clf=True, closed=False, **kwargs)

Plots the line. See *pyknotid*.visualise.plot_line() for full documentation.

Plots a 2D diagram of the knot projected along the current z-axis. The crossings, and start point of the curve, can optionally be marked.

The projection is drawn using matplotlib.



Parameters

- with_crossings (bool) If True, marks the location of each self-intersection in projection. Defaults to True.
- mark_start (bool) If True, marks the first point of the curve. Default to False.
- **fig_ax** (*tuple*) A 2-tuple of the matplotlib (fig, ax) to use, or None to create a new pair.
- show (bool) If True, opens a new window showing the drawing. Defaults to True.

Returns

Return type A 2-tuple of the matplotlib (fig, ax) used for the drawing.

points

The points of the spacecurve, as an Nx3 numpy array.

radius_of_gyration()

Returns the radius of gyration of the points of self, assuming each has equal weight and ignoring the connecting lines.

raw_crossings (mode='use_max_jump', include_closure=True, recalculate=False, try cython=True)

Returns the crossings in the diagram of the projection of the space curve into its z=0 plane.

The crossings will be calculated the first time this function is called, then cached until an operation that would change the list (e.g. rotation, or changing self.points).

Multiple modes are available (see parameters) - you should be aware of this because different modes may be vastly slower or faster depending on the type of line.

- mode (*str*, *optional*) One of 'count_every_jump' or 'use_max_jump' or 'naive'. In the first case, walking along the line uses information about the length of every step. In the second, it guesses that all steps have the same length as the maximum step length. In the last, no optimisation is made and every crossing is checked. The optimal choice depends on the data but is usually 'use_max_jump', which is the default.
- **include_closure** (*bool*, *optional*) Whether to include crossings with the line joining the start and end points. Defaults to True.
- **recalculate** (*bool*, *optional*) Whether to force a recalculation of the crossing positions. Defaults to False.

- **try_cython** (*bool*, *optional*) Whether to force the use of the python (as opposed to cython) implementation of find_crossings. This will make no difference if the cython could not be loaded, in which case python is already used automatically. Defaults to True.
- **Returns** The raw array of floats representing crossings, of the form [[line_index, other_index, +-1, +-1], ...], where the line_index and other_index are in arclength parameterised by integers for each vertex and linearly interpolated, and the +-1 represent over/under and clockwise/anticlockwise respectively.

Return type array-like

```
reparameterised (mode='arclength', num_points=None, interpolation='linear')
```

Returns a new *SpaceCurve* where new points have been selected by interpolating the current ones.

Warning: This doesn't do what you expect! The new segments will probably not all be separated by the right amount in terms of the new parameterisation.

Parameters

- **mode** (*str*) The function to reparameterise by. Defaults to 'arclength', which is currently the only option.
- **num_points** (*int*) The number of points in the new parameterisation. Defaults to None, which means the same as the current number.
- **interpolation** (*str*) The type of interpolation to use, passed directly to the kind option of scipy.interpolate.interpld. Defaults to 'linear', and other options have not been tested.

representation (*recalculate=False*, **kwargs)

Returns a *Representation* instance representing the crossings of the knot.

The Representation instance is cached internally. If you want to recalculate it (e.g. to get an unsimplified version if you have simplified it), you should pass *recalculate=True*.

This method passes kwargs directly to *raw_crossings()*, see the documentation of that function for all options.

rotate (angles=None)

Rotates all the points of self by the given angles in each axis.

```
Parameters angles (array-like) – The rotation angles about x, y and z. If None, random angles are used. Defaults to None.
```

scale (factor)

Scales all the points of self by the given factor.

You can accomplish the same thing, or other more subtle transformations, by modifying self.:py:attr:points.

```
segment_arclengths()
```

Returns an array of arclengths of every step in the line defined by self.points.

simplify_straight_segments(closed=False)

Replaces successive curve segments with identical tangents with a single longer segment.

smooth (repeats=1, periodic=True, window_len=10, window='hanning')

Smooths each of the x, y and z components of self.points by convolving with a window of the given type and size.

Warning: This is *not* topologically safe, it can change the knot type of the curve. For topologically safe reduction, see *octree_simplify()*.

Parameters

- **repeats** (*int*) Number of times to run the smoothing algorithm. Defaults to 1.
- **periodic** (*bool*) If True, the convolution window wraps around the curve. Defaults to True.
- window_len (*int*) Width of the convolution window. Defaults to 10. Passed to pyknotid.spacecurves.smooth.smooth().
- window (*string*) The type of convolution window. Defaults to 'hanning'. Passed to pyknotid.spacecurves.smooth.smooth().

to_json(filen)

Writes the knot points to the given filename, in a json format that can be read later by *SpaceCurve*. *from_json()*. Uses pyknotid.io.to_json_file() internally.

to_txt (filen)

Writes the knot points to the given filename, formatted with each x,y,z component of each point spaceseparated on its own line, i.e.:

```
...
1.2 6.1 98.5
6.19 8.5 1.9
...
```

torsions (signed=False, closed=True)

Returns torsions at each vertex.

translate(vector)

Translates all the points of self by the given vector.

```
Parameters vector (array-like) - The x, y, z translation distances
```

writhe (samples=10, recalculate=False, method='integral', include_acn=False, **kwargs)

The (approximate) writhe of the space curve, obtained by averaging the planar writhe over the given number of directions.

Parameters

- **samples** (*int*) The number of directions to average over. Defaults to 10.
- **recalculate** (*bool*) Whether to recalculate the writhe even if a cached result is available. Defaults to False.
- **method** (*str*) If 'projections', averages the planar writhe over many projections. If 'integral', calculates the writhing integral.
- ****kwargs** These are passed directly to *raw_crossings()*.

zero_centroid()

Translate such that the centroid (average position of vertices) is at (0, 0, 0).

1.2.4 Knot

Class for dealing with curves as knots. Knot provides many methods for topological manipulation and calculations.

API documentation

classpyknotid.spacecurves.knot.Knot(points, verbose=True, zero_centroid=False)add_closure=False, add_closure=False, zero_centroid=False)Bases:pyknotid.spacecurves.spacecurve.SpaceCurve

Class for holding the vertices of a single line, providing helper methods for convenient manipulation and analysis.

A Knot just represents a single space curve, it may be topologically trivial!

This class deliberately combines methods to do many different kinds of measurements or manipulations. Some of these are externally available through other modules in pyknotid - if so, this is usually indicated in the method docstrings.

Parameters

- **points** (*array-like*) The 3d points (vertices) of a piecewise linear curve representation
- verbose (bool) Indicates whether the Knot should print information during processing
- **add_closure** (*bool*) If True, adds a final point to the knot near to the start point, so that it will appear visually to close when plotted.

alexander_at_root (root, round=True, **kwargs)

Returns the Alexander polynomial at the given root of unity, i.e. evaluated at exp(2 pi I / root).

The result returned is the absolute value.

Parameters

- **root** (*int*) The root of unity to use, i.e. evaluating at exp(2 pi I / root). If this is iterable, this method returns a list of the results at every value of that iterable.
- **round** (*bool*) If True and n in (1, 2, 3, 4), the result will be rounded to the nearest integer for convenience, and returned as an integer type.
- ****kwargs** These are passed directly to alexander_polynomial().

alexander_polynomial (*variable=-1*, *quadrant='lr'*, *mode='python'*, ***kwargs*)

Returns the Alexander polynomial at the given point, as calculated by *pyknotid.invariants. alexander()*.

See *pyknotid.invariants.alexander()* for the meanings of the named arguments.

copy()

Returns another knot with the same points and verbosity as self. Other attributes (e.g. cached crossings) are not preserved.

determinant()

Returns the determinant of the knot. This is the Alexander polynomial evaluated at -1.

exterior_manifold()

The knot complement manifold of self as a SnapPy class giving access to all of SnapPy's tools.

This method requires that Spherogram, and possibly SnapPy, are installed.

hyperbolic_volume()

Returns the hyperbolic volume at the given point, via pyknotid.representations. PlanarDiagram.as_spherogram().

Returns

• **volume** (*float*) – A float representing the volume returned.

- **accuracy** (*int*) The number of digits of precision. This is significant digits, e.g. 0.00021 with 1 digit precision = 2E-4.
- **solution_type** (*str*) The solution type of the manifold. Normally one of: 'contains degenerate tetrahedra' => may not be a valid result 'all tetrahedra positively oriented' =>

really probably hyperbolic

identify (*determinant=True*, *alexander=False*, *roots=*(2, 3, 4), *min_crossings=True*)

Provides a simple interface to *pyknotid.catalogue.identify.from_invariants()*, by passing the given invariants. This does *not* support all invariants available, or more sophisticated identification methods, so don't be afraid to use the catalogue functions directly.

Parameters

- **determinant** (*bool*) If True, uses the knot determinant in the identification. Defaults to True.
- **alexander** (bool) If True-like, uses the full alexander polynomial in the identification. If the input is a dictionary of kwargs, these are passed straight to self.alexander_polynomial.
- roots (*iterable*) A list of roots of unity at which to evaluate. Defaults to (2, 3, 4), the first of which is redundant with the determinant. Note that higher roots can be calculated, but aren't available in the database.
- min_crossings (bool) If True, the output is restricted to knots with fewer crossings than the current projection of this one. Defaults to True. The only reason to turn this off is to see what other knots have the same invariants, it is never not useful for direct identification.

isolate_knot()

Return indices of self.points within which the knot (if any) appears to lie, according to a simple closure algorithm.

This method is experimental and may not provide very good results.

planar_writhe_quantities (num_angles=100, **kwargs)

Returns the second order writhes, and arnold 2St+J+ values, for a range of different projection directions.

plot (**kwargs)

Plots the line. See *pyknotid*.visualise.plot_line() for full documentation.

plot_isolated(**kwargs)

Plots the curve in red, except for the isolated local knot which is coloured blue. The local knot is found with self.isolate_knot, which may not be reliable or have good resolution.

Parameters **kwargs – kwargs are passed directly to *Knot.plot()*.

points

The points of the spacecurve, as an Nx3 numpy array.

slipknot_alexander(num_samples=0, **kwargs)

Parameters

- **num_samples** (*int*) The number of indices to cut at. Defaults to 0, which means to sample at all indices.
- ****kwargs** Keyword arguments, passed directly to :meth: 'pyknotid.spacecurves.openknot.OpenKnot.alexander_fractions.

```
vassiliev_degree_2 (simplify=True, **kwargs)
```

Returns the Vassiliev invariant of degree 2 for the Knot.

Parameters

- **simplify** (bool) If True, simplifies the Gauss code of self before calculating the invariant. Defaults to True, but will work fine if you set it to False (and might even be faster).
- ****kwargs** These are passed directly to gauss_code().

```
vassiliev_degree_3 (simplify=True, try_cython=True, **kwargs)
```

Returns the Vassiliev invariant of degree 3 for the Knot.

Parameters

- **simplify** (bool) If True, simplifies the Gauss code of self before calculating the invariant. Defaults to True, but will work fine if you set it to False (and might even be faster).
- **try_cython** (bool) Whether to try and use an optimised cython version of the routine (takes about 1/3 of the time for complex representations). Defaults to True, but the python fallback will be *slower* than setting it to False if the cython function is not available.
- ****kwargs** These are passed directly to gauss_code ().

whitney_index()

The degree of the Gauss map mapping a point on the curve to the direction of the positive tangent vector at this point.

1.2.5 OpenKnot

Class for working with open (linear) curves, that do not form closed loops. *OpenKnot* provides methods for visualising these curves and analysing their topology via different kinds of closures.

API documentation

```
class pyknotid.spacecurves.openknot.OpenKnot(*args, **kwargs)
    Bases: pyknotid.spacecurves.spacecurve.SpaceCurve
```

Class for holding the vertices of a single line that is assumed to be an open curve. This class inherits from *SpaceCurve*, replacing any default arguments that assume closed curves, and providing methods for statistical analysis of knot invariants on projection and closure.

All knot invariant methods return the results of a sampling over many projections of the knot, unless indicated otherwise.

```
alexander_fractions(number_of_samples=10, **kwargs)
```

Returns each of the Alexander polynomials from self.alexander_polynomials, with the fraction of that type.

```
alexander_polynomials (number_of_samples=10, radius=None, recalculate=False,
zero centroid=False, optimise closure=True)
```

Returns a list of Alexander polynomials for the knot, closing on a sphere of the given radius, with the given number of sample points approximately evenly distributed on the sphere.

The results are cached by number of samples and radius.

Parameters

• number_of_samples (*int*) - The number of points on the sphere to sample. Defaults to 10.

- **optimise_closure** (*bool*) If True, doesn't really close on a sphere but at infinity. This lets the calculation be optimised slightly, and so is the default.
- **radius** (*float*) The radius of the sphere on which to close the knot. Defaults to None, which picks 10 times the largest Cartesian deviation from 0. This is *only* used if optimise_closure=False.
- **zero_centroid** (*bool*) Whether to first move the average position of vertices to (0, 0, 0). Defaults to True.

Returns A number_of_samples by 3 array of angles and alexander polynomials.

Return type ndarray

alexander_polynomials_multiroots (number_of_samples=10,

radius=None,

zero_centroid=False) Returns a list of Alexander polynomials for the knot, closing on a sphere of the given radius, with the given number of sample points approximately evenly distributed on the sphere. The Alexander polynomials are found at three different roots (2, 3 and 4) and a the knot types corresponding to these roots are returned also.

The results are cached by number of samples and radius.

Parameters

- **number_of_samples** (*int*) The number of points on the sphere to sample. Defaults to 10.
- **radius** (*float*) The radius of the sphere on which to close the knot. Defaults to None, which picks 10 times the largest Cartesian deviation from 0.
- **zero_centroid** (*bool*) Whether to first move the average position of vertices to (0, 0, 0). Defaults to True.

Returns A number_of_samples by 3 array of angles and alexander polynomials.

Return type ndarray

${\tt arclength}\,(\,)$

Calls pyknotid.spacecurves.spacecurve.SpaceCurve.arclength(), automatically not including the closure.

closing_distance()

Returns the distance between the first and last points.

closure_alexander_polynomial(*theta=0*, *phi=0*)

Returns the Alexander polynomial of the knot, when projected in the z plane after rotating the given theta and phi to the North pole.

Parameters

- theta (float) The sphere angle theta
- **phi** (*float*) The sphere angle phi

generalised_alexander()

Returns the generalised Alexander polynomial for the default projection of the open knot

multiroots_fractions (number_of_samples=10, **kwargs)

Returns each of the knot types from self.alexander_polynomials_multiroots, with the fraction of that type.

plot_alexander_map (number_of_samples=10, scatter_points=False, mode='imshow', interpola-

tion=100, **kwargs)

Creates (and returns) a projective diagram showing each different Alexander polynomial in a different colour according to a closure on a far away point in this direction.

Parameters

- number_of_samples (*int*) The number of points on the sphere to close at.
- **scatter_points** (*bool*) If True, plots a dot at each point on the map projection where a closure was made.
- mode (str) 'imshow' to plot the pixels of an image, otherwise plots filled contours. Defaults to 'imshow'.
- **interpolation** (*int*) The (short) side length of the interpolation grid on which the map projection is made. Defaults to 100.

plot_alexander_shell (number_of_samples=100, mode='mesh', radius=None, **kwargs)

Plots the curve in 3d via self.plot(), along with a translucent sphere coloured by the type of knot obtained by closing on each point.

Parameters are all passed to *OpenKnot.alexander_polynomials()*, except opacity and kwargs which are given to mayavi.mesh, and sphere_radius_factor which gives the radius of the enclosing sphere in terms of the maximum Cartesian distance of any point in the line from the origin.

plot_projections (number_of_samples)

Plots the projection of the knot at each of the given number of samples squared, rotated such that the sample direction is vertical.

The output (and return) is a matplotlib plot with number_of_samples x number_of_samples axes.

Creates (and returns) a projective diagram showing each different self linking number in a different colour according to a projection in this direction.

plot_self_linking_shell (number_of_samples=100, **kwargs)

Plots the curve in 3d via self.plot(), along with a translucent sphere coloured by the self linking number obtained by projecting from this point.

Parameters are all passed to *OpenKnot.virtual_checks()*, except opacity and kwargs which are given to mayavi.mesh, and sphere_radius_factor which gives the radius of the enclosing sphere in terms of the maximum Cartesian distance of any point in the line from the origin.

plot_virtual_map (number_of_samples=10, scatter_points=False, mode='imshow', **kwargs)

Creates (and returns) a projective diagram showing each different virtual Boolean in a different colour according to a projection in this direction.

plot_virtual_shell (number_of_samples=10, zero_centroid=False, sphere_radius_factor=2.0,

opacity=0.3, **kwargs)

Plots the curve in 3d via self.plot(), along with a translucent sphere coloured according to whether or not the projection from this point corresponds to a virtual knot or not.

Parameters are all passed to *OpenKnot.virtual_checks()*, except opacity and kwargs which are given to mayavi.mesh, and sphere_radius_factor which gives the radius of the enclosing sphere in terms of the maximum Cartesian distance of any point in the line from the origin.

points

The points of the spacecurve, as an Nx3 numpy array.

projection_invariant(**kwargs)

First checks if the projection of an open curve is virtual or classical. If virtual, a virtual knot invariant is calculated. Otherwise a classical invariant is calculated.

raw_crossings (mode='use_max_jump', virtual_closure=False, recalculate=False, try cython=False)

Calls pyknotid.spacecurves.spacecurve.SpaceCurve.raw_crossings(), but without

including the closing line between the last and first points (i.e. setting include_closure=False).

self_linking(theta=0, phi=0)

Takes an open curve, finds its Gauss code (for the default projection) and calculates its self linking number, J(K). See Kauffman 2004 for more information.

Returns The self linking number of the open curve

Return type self_link_counter : int

```
self_linking_fractions (number_of_samples=10, **kwargs)
```

Returns each of the self linking numbers from self.virtual.self_link.projections, with the fraction of each type.

self_linkings(number_of_samples=10, zero_centroid=False, **kwargs)

Returns a list of self linking numbers for the curve with a given number of projections taken from directions approximately evenly distributed.

Parameters

- number_of_samples (*int*) The number of points on the sphere to project from. Defaults to 10.
- **zero_centroid** (*bool*) Whether to first move the average position of vertices to (0, 0, 0). Defaults to False.

Returns A number_of_samples by 3 array of angles and self linking number

Return type ndarray

smooth (repeats=1, window_len=10, window='hanning')

Calls *pyknotid*.*spacecurve*.*spaceCurve*.*smooth()*, with the periodic argument automatically set to False.

vassiliev_degree_2_average (*samples=10*, *recalculate=False*, ***kwargs*)

Returns the average Vassliev degree 2 invariant calculated by averaging its combinatorial value over many different projection directions.

Parameters

- **samples** (*int*) The number of directions to average over. Defaults to 10.
- **recalculate** (*bool*) Whether to recalculate the writhe even if a cached result is available. Defaults to False.
- ****kwargs** These are passed directly to raw_crossings().

virtual_check()

Takes an open curve and checks (for the default projection) if its Gauss code corresponds to a virtual knot or not. Returns a Boolean of this information.

Warning: This only checks the distance by which entries in the Gauss code are separated, it is *not* guaranteed to detect virtual knots.

Returns virtual – True if the Gauss code corresponds to a virtual knot. False otherwise.

Return type bool

virtual_checks (number_of_samples=10, zero_centroid=False)

Returns a list of virtual Booleans for the curve with a given number if projections taken from directions

approximately evenly distributed. A value of True corresponds to the projection giving a virtual knot, with False returned otherwise.

Parameters

- number_of_samples (*int*) The number of points on the sphere to project from. Defaults to 10.
- **zero_centroid** (*bool*) Whether to first move the average position of vertices to (0, 0, 0). Defaults to False.

Returns A number_of_samples by 3 array of angles and virtual Booleans (True if virtual, False otherwise)

Return type ndarray

```
virtual_fractions (number_of_samples=10, **kwargs)
```

Returns each of the virtual booleans from self.virtual.check.projections, with the fraction of each type.

pyknotid.spacecurves.openknot.gall_peters(theta, phi)

Converts spherical coordinates to the Gall-Peters projection of the sphere, an area-preserving projection in the shape of a Rectangle.

Parameters

- theta (float) The latitude, in radians.
- **phi** (*float*) The longitude, in radians.

pyknotid.spacecurves.openknot.knot_db_to_string(database_object)

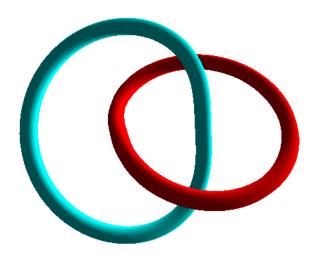
Takes output from from_invariants() and returns knot type as decimal. For example: <Knot 3_1> becomes 3.1 and <Knot K13n1496> becomes 13.1496

pyknotid.spacecurves.openknot.mollweide(phi, lambda_)

Converts spherical coordinates to the Mollweide projection of the sphere, an area-preserving projection in the shape of an ellipse.

- **phi** (*float*) The latitude, in radians.
- **lambda** (*float*) The longitude, in radians.

1.2.6 Link



Class for dealing with multiple curves as a link. *Link* provides methods for topological manipulation and calculations on multiple curves.

API documentation

```
class pyknotid.spacecurves.link.Link(lines, verbose=True)
```

Bases: object

Class for holding the vertices of multiple lines, providing helper methods for convenient manipulation and analysis.

The data is stored internally as multiple :class: 'Knot's.

Parameters

- lines (list of nx3 array-like or Knots) List with the points of each line.
- **verbose** (*bool*) Whether to print information during processing. Defaults to True.

arclength (include_closures=True)

Returns the sum of arclengths of the lines.

Parameters include_closures (*bool*) – Whether to include the distance between the final and first points of each line. Defaults to True.

classmethod from_periodic_lines (lines, shape, perturb=True)

Returns a *Link* instance in which the lines have been unwrapped through the periodic boundaries.

Parameters

- line (list) A list of the Nx3 vectors of points in the lines
- shape (array-like) The x, y, z distances of the periodic boundary
- perturb (bool) If True, translates and rotates the knot to avoid any lattice problems.

gauss_code (**kwargs)

Returns a *GaussCode* instance representing the crossings of the knot.

The GaussCode instance is cached internally. If you want to recalculate it (e.g. to get an unsimplified version if you have simplified it), you should pass *recalculate=True*.

This method passes kwargs directly to *raw_crossings()*, see the documentation of that function for all options.

linking_number(**kwargs)

Returns the linking number of the lines in the Link, the sum of signed crossings between them, ignoring crossings of a line with itself.

octree_simplify (runs=1, plot=False, rotate=True, obey_knotting=False, **kwargs)
Simplifies the curves via the octree reduction of :module:'pyknotid.simplify.octree'.

Parameters

- **runs** (*int*) The number of times to run the octree simplification. Defaults to 1.
- plot (bool) Whether to plot the curve after each run. Defaults to False.
- **rotate** (*bool*) Whether to rotate the space curve before each run. Defaults to True as this can make things much faster.
- **obey_knotting** (*bool*) Whether to not let the line pass through itself. Defaults to False knotting of individual components will be ignored! This is *much* faster than the alternative.

:param kwargs are passed to the pyknotid.simplify.octree.OctreeCell: :param constructor.:

plot (mode='vispy', clf=True, colours=None, **kwargs)

Plots all the lines. See *pyknotid*.visualise.plot_line() for full documentation.

raw_crossings (mode='use_max_jump', only_with_other_lines=True, include_closures=True, recalculate=False, try_cython=True)

Returns the crossings in the diagram of the projection of the space curve into its z=0 plane.

The crossings will be calculated the first time this function is called, then cached until an operation that would change the list (e.g. rotation, or changing self.points).

Multiple modes are available (see parameters) - you should be aware of this because different modes may be vastly slower or faster depending on the type of line.

- mode (*str*, *optional*) One of 'count_every_jump' and 'use_max_jump'. In the former case, walking along the line uses information about the length of every step. In the latter, it guesses that all steps have the same length as the maximum step length. The optimal choice depends on the data, but is usually 'use_max_jump', which is the default.
- **only_with_other_lines** (*bool*) If True, ignores self-crossings (i.e. the knot type of the loops) and returns only a list of crossings between the loops. Defaults to True
- **include_closures** (*bool*, *optional*) Whether to include crossings with the lines joining their start and end points. Defaults to True.
- **recalculate** (*bool*, *optional*) Whether to force a recalculation of the crossing positions. Defaults to False.
- **try_cython** (*bool*, *optional*) Whether to try to use a cython implementation of crossing finding. This will make no difference if the cython could not be loaded, in which case python is already used automatically. Defaults to True.
- **Returns** The raw array of floats representing crossings, of the form [[line_index, other_index, +-1, +-1], ...], where the line_index and other_index are in arclength parameterised by integers for each vertex and linearly interpolated, and the +-1 represent over/under and clockwise/anticlockwise respectively.

Return type array-like

rotate(angles=None)

Rotates all the points of each line of self by the given angle in each axis.

Parameters angles (*array-like*) – Rotation angles about x, y and z axes. If None, random angles are used. Defaults to None.

smooth(*args, **kwargs)

Smooths each of the x, y and z components of each of self.lines by convolving with a window of the given type and size.

kwargs are passed straight to pyknotid.spacecurves.spacecurve.SpaceCurve. smooth().

```
translate (vector, lines=None)
```

Translate all points in some or all lines of self.

Parameters

- vector (array-like) The x, y, z translation distances
- **lines** (*list or int*) The list of line indices to which the translation should be applied. Defaults to None, which applies the translation to all the lines of self. If an integer is supplied, only the line with this index is translated.

1.2.7 PeriodicCell

Tools for working with a periodic cell of spacecurves.

API documentation

Bases: object

Class for holding the vertices of some number of lines with periodic boundary conditions.

Parameters

- lines (list) Must be a list of Knots or ndarrays of vertices.
- **shape** (*tuble or int*) The shape of the cell, in whatever units the lines use.
- **periodic** (bool) Whether the cell is periodic. If True, lines are marked as 'nth' or 'loop' in self.line_types. Defaults to True.

```
classmethod from_qwer(qwer, shape, **kwargs)
```

Returns an instance of Cell from a quartet of differently classified lines in periodic boundaries.

Parameters

- **qwer** (*tuple*) Should be a 4-tuple of lists q, w, e, r. q is closed loops, w is lines with non-trivial homology, e is lines that terminate on the boundaries of the cell, r is any remaining (unclassified) lines.
- **shape** (*int* or *tuple*) The size of the cell along each axis. If a single number is passed, all axes are assumed to be the same length.

linking_matrix()

Get the linking numbers of each line in the cell with every other.

smooth (repeats=1, window_len=10)
Smooth each line in the curve, equivalent to smooth().

1.3 Invariants

Functions for retrieving invariants of knots and links.

Many of these functions can be called in a more convenient way via methods of the *space curve classes* (e.g. *Knot*) or the *Representation* class.

1.3.1 Mathematica

Functions whose name ends with _mathematica try to create an external Mathematica process to calculate the answer. They may hang or have other problems if Mathematica isn't available in your \$PATH, so be careful using them.

Warning: This module may be broken into multiple components at some point.

1.3.2 API documentation

pyknotid.invariants.alexander(representation, variable=-1, quadrant='lr', simplify=True,

mode='python')

Calculates the Alexander polynomial of the given knot. The representation *must* have just one knot component, or the calculation will fail or potentially give bad results.

The result is returned with whatever numerical precision the algorithm produces, it is not rounded.

The given representation *must* be simplified (RM1 performed if possible) for this to work, otherwise the matrix has overlapping elements. This is so important that this function automatically calls *pyknotid*. *representations.gausscode.GaussCode.simplify()*, you must disable this manually if you don't want to do it.

Note: If 'maxima' or 'mathematica' is chosen as the mode, the variable will automatically be set to t.

Note: If the mode is 'cypari', the quadrant argument will be ignored and the upper-left quadrant always used.

- **representation** (Anything convertible to a) GaussCode A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).
- **variable** (float or complex or sympy variable) The value to caltulate the Alexander polynomial at. Defaults to -1, but may be switched to the sympy variable t in the future. Supports int/float/complex types (fast, works for thousands of crossings) or sympy expressions (much slower, works mostly only for <100 crossings).

- **quadrant** (*str*) Determines what principal minor of the Alexander matrix should be used in the calculation; all choices *should* give the same answer. Must be 'lr', 'ur', 'ul' or 'll' for lower-right, upper-left or lower-left respectively.
- **simplify** (bool) Whether to call the GaussCode simplify method, defaults to True.
- **mode** (*string*) One of 'python', 'maxima', 'cypari' or 'mathematica'. denotes what tools to use; if python, the calculation is performed with numpy or sympy as appropriate. If maxima or mathematica, that program is called by the function this will only work if the external tool is installed and available. Defaults to python.

```
pyknotid.invariants.alexander_cypari(representation, quadrant='ul', verbose=False, sim-
plify=True)
```

Returns the Alexander polynomial of the given representation, by calculating the matrix determinant via cypari, a python interface to Pari-GP.

The function only supports evaluating at the variable t.

The returned object is a cypari query type.

Parameters

- **representation** (*Anything convertible to a*) *GaussCode* A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).
- **quadrant** (*str*) Determines what principal minor of the Alexander matrix should be used in the calculation; all choices *should* give the same answer. Must be 'lr', 'ur', 'ul' or 'll' for lower-right, upper-right,
- **verbose** (*bool*) Whether to print information about the procedure. Defaults to False.
- **simplify** (*bool*) If True, tries to simplify the representation before calculating the polynomial. Defaults to True.

Returns the Alexander polynomial of the given representation, by creating a Mathematica process and running its knot routines. The Mathematica installation must include the KnotTheory package.

The function only supports evaluating at the variable t.

- **representation** (*Anything convertible to a*) *GaussCode* A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).
- **quadrant** (*str*) Determines what principal minor of the Alexander matrix should be used in the calculation; all choices *should* give the same answer. Must be 'lr', 'ur', 'ul' or 'll' for lower-right, upper-right,
- **verbose** (bool) Whether to print information about the procedure. Defaults to False.
- via_file (bool) If True, calls Mathematica via a written file mathematicascript.m, otherwise calls Mathematica directly with runMath. The latter had a nasty bug in at least one recent Mathematica version, so the default is to True.
- **simplify** (*bool*) If True, tries to simplify the representation before calculating the polynomial. Defaults to True.

pyknotid.invariants.alexander_maxima(representation, quadrant='ul', verbose=False, sim-

```
plify=True)
```

Returns the Alexander polynomial of the given representation, by calculating the matrix determinant in maxima.

The function only supports evaluating at the variable t.

Parameters

- **representation** (*Anything convertible to a*) *GaussCode* A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).
- **quadrant** (*str*) Determines what principal minor of the Alexander matrix should be used in the calculation; all choices *should* give the same answer. Must be 'lr', 'ur', 'ul' or 'll' for lower-right, upper-right,
- **verbose** (*bool*) Whether to print information about the procedure. Defaults to False.
- **simplify** (*bool*) If True, tries to simplify the representation before calculating the polynomial. Defaults to True.

pyknotid.invariants.arnold_2St_2Jminus(representation)

Returns J- + 2 * St where J+ and St are Arnold's invariants of plane curves.

See 'Invariants of curves and fronts via Gauss diagrams', M Polyak, Topology 37, 1998.

pyknotid.invariants.arnold_2St_2Jplus(representation)

Returns J + + 2 * St where J + and St are Arnold's invariants of plane curves.

The calculation is performed by transforming the representation into a representation of an unknot by flipping crossings, then calculating the second order writhe.

See 'Invariants of curves and fronts via Gauss diagrams', M Polyak, Topology 37, 1998.

pyknotid.invariants.contract_points(planar_diagram)

For appropriately contracting :class: *Points* in a :class: *PlanarDiagram* According to the following rules:

P_a,b P_b,c -> P_a,c P_a,b P_a,b -> P_a,a

pyknotid.invariants.hyperbolic_volume(representation)

The hyperbolic volume, calculated by the SnapPy library for studying the topology and geometry of 3-manifolds. This function depends on the Spherogram module, distributed with SnapPy or available separately.

Parameters representation (A PlanarDiagram, or anything convertible to a) - GaussCode A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)), or a PlanarDiagram.

pyknotid.invariants.jones_mathematica(representation)

Returns the Jones polynomial of the given representation, by creating a Mathematica process and running its knot routines. The Mathematica installation must include the KnotTheory package.

The function only supports evaluating at the variable q.

Parameters representation (A PlanarDiagram, or anything convertible to a) - GaussCode A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)), or a PlanarDiagram.

pyknotid.invariants.second_order_writhe(representation)

Returns the second order writhe (i1,i3,i2,i4) of the representation, as defined in Lin and Wang.

pyknotid.invariants.self_linking(representation)

Returns the self linking number J(K) of the Gauss code, an invariant of virtual knots. See Kauffman 2004 for more information.

Currently only works for knots.

pyknotid.invariants.vassiliev_degree_2 (representation)

Calculates the Vassiliev invariant of degree 2 of the given knot. The representation must have just one knot component, this doesn't work for links.

Parameters representation (Anything convertible to a) - GaussCode A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).

pyknotid.invariants.vassiliev_degree_3 (representation, try_cython=True)

Calculates the Vassiliev invariant of degree 3 of the given knot. The representation must have just one knot component, this doesn't work for links.

Parameters

- **representation** (*Anything convertible to a*) *GaussCode* A pyknotid representation class for the knot, or anything that can automatically be converted into a GaussCode (i.e. by writing GaussCode (your_object)).
- **try_cython** (*bool*) Whether to try and use an optimised cython version of the routine (takes about 1/3 of the time for complex representations). Defaults to True, but the python fallback will be *slower* than setting it to False if the cython function is not available.

pyknotid.invariants.virtual_vassiliev_degree_3(representation)

Calculates the virtual Vassiliev invariant of degree 3 (for non-long-knots) of the given representation, as described in 'Finite type invariants of classical and virtual knots' by Goussarov, Polyak and Viro.

Parameters representation (*Representation*) – A representation class, or anything convertible to one (in principle).

1.4 Topological representations

Knots and links can be encoded in many different ways, generally by enumerating their self-intersections in projection along some axis. We provide here

This module contains classes and functions for representing knots in knot diagrams, mainly the *pyknotid*. *representations.gausscode.GaussCode* and *pyknotid.representations.planardiagram*. *PlanarDiagram*.

These provide convenient methods to convert between different representations, and to simplify via Reidemeister moves.

1.4.1 Creating representations

Knot representations can be calculated from space curves, or created directly by inputting standard notations.

From space curves

pyknotid's space curve classes can all return topological representations. For instance:

```
from pyknotid.spacecurves import Knot
from pyknotid.make import trefoil
k = Knot(trefoil())
```

You can extract a *GaussCode* object:

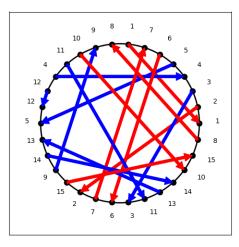
k.gauss_code() # 1+a,2-a,3+a,1-a,2+a,3-a

or a PlanarDiagram:

k.planar_diagram() # PD with 3: X_{2,5,3,6} X_{4,1,5,2} X_{6,3,1,4}

or a Gauss diagram:

k.gauss_diagram() # plots the diagram in a new window using matplotlib



or a generic Representation:

```
k.representation() # 1+a,2-a,3+a,1-a,2+a,3-a (but provides more methods than a_

→GaussCode)
```

By direct input

Gauss codes

A Gauss code is a list of crossings in a projection of a curve, labelled by numbers, and in each case indicating whether the curve passes over (+) or under (-) itself. Each crossing also has a local orientation, represented here by 'c' for clockwise, or 'a' for anticlockwise.

With these rules, you can enter Gauss codes as comma-separated lists:

```
from pyknotid.representations import GaussCode
gc = GaussCode('1+c,2-c,3+c,1-c,2+c,3-c')
```

If you do not know the crossing orientations (c/a), pyknotid can calculate them automatically:

gc = GaussCode.calculating_orientations('1+, 2-, 3+, 1-, 2+, 3-')

If you do this with a chiral not, the chirality is selected arbitrarily.

1.4.2 Calculating invariants

You can calculate many invariants using the functions of Invariants.

pyknotid also provides a more convenient interface using the *Representation* class. Internally this wraps a Gauss code:

```
from pyknotid.representations import Representation
rep = Representation('1-c,2+c,3-a,4+a,2-c,1+c,4-a,3+a')
```

You can then calculate many quantities via methods of this object:

```
rep.vassiliev_degree_2() # 1
rep.vassiliev_degree_3() # -1
rep.identify() # [<Knot 4_1>]
```

For a full list of available functions, see Representation.

1.4.3 GaussCode

Classes for working with Gauss codes representing planar projections of curves.

See class documentation for more details.

API documentation

class pyknotid.representations.gausscode.GaussCode(crossings=", verbose=True)
Bases: object

Class for containing and manipulating Gauss codes.

By default you must pass an extended Gauss code that includes the sign of each crossing ('c' for clockwise or 'a' for anticlockwise), e.g. 1+c, 2-c, 3+c, 1-c, 2+c, 3-c for the trefoil knot. If you do not know the crossing signs you can instead call *GaussCode.calculating_orientations()*, e.g. gc = GaussCode. calculating_orientations(), e.g. gc = GaussCode.

The length of a Gauss code (e.g. len (GaussCode ())) is the number of crossings in it.

Parameters

- crossings (array-like or string or PlanarDiagram or GaussCode)
 A raw_crossings array from a Knot or Link, or a string representation of the form (e.g.) 1+c, 2-c, 3+c, 1-c, 2+c, 3-c, with commas between entries, and with multiple link components separated by spaces and/or newlines. If a PlanarDiagram or GaussCode is passed, the code is duplicated.
- **verbose** (*bool*) Whether to print information during calculations. Defaults to True.

classmethod calculating_orientations (code)

Takes a Gauss code without crossing orientations and returns an equivalent Gauss code (though not necessarily of the same length).

This works by generating a space curve and finding its self-intersections on projection. This is overkill for the problem, but works.

flipped()

Returns a copy of self with crossing over/under switched.

mirrored()

Returns a copy of self with crossing orientations reversed.

reindex_crossings()

Replaces the indices of the crossings in the Gauss code with the integers from 1 to its length.

Note that this modifies the Gauss code in place, the previous indices are not recorded.

```
simplify (one=True, two=True, one_extended=True)
```

Simplifies the GaussCode, performing the given Reidemeister moves everywhere possible, as many times as possible, until the GaussCode is no longer changing.

This modifies the GaussCode - (non-topological) information may be lost!

Parameters

- one (bool) Whether to use Reidemeister 1, defaults to True.
- two (bool) Whether to use Reidemeister 2, defaults to True.
- **one_extended** (bool) Whether to use extended Reidemeister 1, which removes crossings connected by arcs which include only over or only under crossings (and which must thus be topologically irrelevant). Defaults to True.

without_virtual()

Returns a version of the Gauss code without explicit virtual crossings.

1.4.4 PlanarDiagram

Classes for working with planar diagram notation of knot diagrams.

See individual class documentation for more details.

API documentation

Bases: list

A single crossing in a planar diagram. Each *PlanarDiagram* is a list of these.

Parameters

- a (int or None) The first entry in the list of lines meeting at this Crossing.
- b (int or None) The second entry in the list of lines meeting at this Crossing.
- c (int or None) The third entry in the list of lines meeting at this Crossing.
- d (int or None) The fourth entry in the list of lines meeting at this Crossing.

as_mathematica()

Get a string of mathematica code that can represent the Crossing in mathematica's knot library.

The mathematica code won't be valid if any lines of self are None.

Return type str

components()

Returns a de-duplicated list of lines intersecting at this Crossing.

Return type list

update_line_number(old, new)

Replaces all instances of the given line number in self.

Parameters

- **old** (*int*) The old line number
- **new** (*int*) The number to replace it with

valid()

True if all intersecting lines are not None.

```
class pyknotid.representations.planardiagram.PlanarDiagram(crossings=")
```

Bases: list

A class for containing and manipulating planar diagrams.

Just provides convenient display and conversion methods for now. In the future, will support simplification.

Shorthand input may be of the form X_1, 4, 2, 5 X_3, 6, 4, 1 X_5, 2, 6, 3. This is (should be?) the same as returned by repr.

Parameters crossings (*array-like or string or* GaussCode) – The list of crossings in the diagram, which will be converted to an internal planar diagram representation. Currently these are mostly converted via a GaussCode instance, so in addition to the shorthand any array-like supported by *GaussCode* may be used.

as_mathematica()

Returns a mathematica code representation of self, usable in the mathematica knot tools.

as_networkx()

Get a networkx graph representing the planar diagram, where each node is a crossing and each edge is an arc. This is a non-directed non-multi graph; where two arcs join the same crossing, they are represented as a single edge, but information about duplicates is returned alongside the graph.

Returns

- **g** (*Graph*) The networkx graph
- duplicates (list) A list of tuples representing nodes joined by multiple edges.
- heights (*dict*) A dictionary of (start, end, arc_number) graph edges, containing the start and end height of each edge.
- first_edge (tuple) The first edge in the graph, including (start, end, arc_number).

as_networkx_extended()

(internal use only) Returns a networkx Graph along with extra information about the crossings.

as_spherogram()

Get a planar diagram class from the Spherogram module, which can be used to access SnapPy's manifold tools.

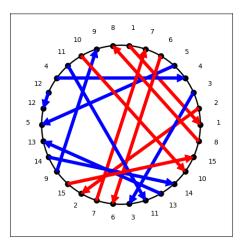
This method requires that spherogram and SnapPy are installed.

pyknotid.representations.planardiagram.index_height (index)

Returns the height based on the index of the crossing in an entry of a planar diagram; the 0th and 2nd indices are under crossings, and the 1st and 3rd are over crossings.

pyknotid.representations.planardiagram.**shorthand_to_crossings**(*s*) Takes a planar diagram shorthand string, and returns a list of :class: 'Crossing's.

1.4.5 GaussDiagram



Class for creating and viewing Gauss diagrams.

API documentation

```
class pyknotid.representations.gaussdiagram.GaussDiagram(representation)
    Bases: object
```

Class for containing and manipulating Gauss diagrams.

Parameters representation (Another representation of a knot.) -

plot (fig_ax=None)

Plots the Gauss diagram using matplotlib. This is called automatically on __init__.

Returns a tuple of the matplotlib figure and axis.

1.4.6 DTNotation

Classes for working with DT notation representing planar projections of curves.

API documentation

```
class pyknotid.representations.dtnotation.DTNotation(code)
    Bases: object
```

Class for containing and manipulation DT notation.

Parameters code (*str or array-like*) – The DT code. Must be either a string of entries separated by spaces, or an array.

gauss_code_string()

Returns a string containing a Gauss code, in the format accepted by GaussCode.

To get a GaussCode object, you can pass this string when initialising it, or use DTNotation. representation().

representation (**kwargs)

Returns a *Representation* representing the same DT code. The crossing orientations (and therefore resulting chirality) are chosen arbitrarily.

1.4.7 Representation

An abstract representation of a Knot, providing methods for the calculation of topological invariants.

API documentation

```
class pyknotid.representations.representation.CrossingGraph
    Bases: collections.defaultdict
```

align_nodes()

Orders the lines of each node to be in order, clockwise, depending on their incoming angle.

```
class pyknotid.representations.representation.Representation(crossings=",
```

verbose=True)

Bases: pyknotid.representations.gausscode.GaussCode

An abstract representation of a knot or link. Internally this is just a Gauss code, but it exposes extra topological methods and may in future be refactored to work differently.

alexander_at_root (root, round=True, **kwargs)

Returns the Alexander polynomial at the given root of unity, i.e. evaluated at exp(2 pi I / root).

The result returned is the absolute value.

Parameters

- **root** (*int*) The root of unity to use, i.e. evaluating at exp(2 pi I / root). If this is iterable, this method returns a list of the results at every value of that iterable.
- **round** (*bool*) If True and n in (1, 2, 3, 4), the result will be rounded to the nearest integer for convenience, and returned as an integer type.
- ****kwargs** These are passed directly to alexander_polynomial().
- **alexander_polynomial** (variable=-1, quadrant='lr', mode='python', force_no_simplify=False)

Returns the Alexander polynomial at the given point, as calculated by *pyknotid.invariants. alexander()*.

See *pyknotid.invariants.alexander()* for the meanings of the named arguments.

classmethod calculating_orientations (code, **kwargs)

Takes a Gauss code without crossing orientations and returns an equivalent Gauss code (though not necessarily of the same length).

This works by generating a space curve and finding its self-intersections on projection. This is overkill for the problem, but works.

exterior_manifold()

The knot complement manifold of self as a SnapPy class giving access to all of SnapPy's tools.

This method requires that Spherogram, and possibly SnapPy, are installed.

hyperbolic_volume()

Returns the hyperbolic volume at the given point, via pyknotid.representations. PlanarDiagram.as_spherogram().

Provides a simple interface to *pyknotid.catalogue.identify.from_invariants()*, by passing the given invariants. This does *not* support all invariants available, or more sophisticated identification methods, so don't be afraid to use the catalogue functions directly.

Parameters

- **determinant** (*bool*) If True, uses the knot determinant in the identification. Defaults to True.
- **alexander** (bool) If True-like, uses the full alexander polynomial in the identification. If the input is a dictionary of kwargs, these are passed straight to self.alexander_polynomial.
- roots (*iterable*) A list of roots of unity at which to evaluate. Defaults to (2, 3, 4), the first of which is redundant with the determinant. Note that higher roots can be calculated, but aren't available in the database.
- min_crossings (bool) If True, the output is restricted to knots with fewer crossings than the current projection of this one. Defaults to True. The only reason to turn this off is to see what other knots have the same invariants, it is never not useful for direct identification.
- **vassiliev_2** (*bool*) If True, uses the Vassiliev invariant of order 2. Defaults to True.
- **vassiliev_3** (bool) If True, uses the Vassiliev invariant of order 3. Defaults to None, which means the invariant is used only if the representation has less than 30 crossings.

is_virtual()

Takes an open curve and checks (for the default projection) if its Gauss code corresponds to a virtual knot or not. Returns a Boolean of this information.

Returns virtual – True if the Gauss code corresponds to a virtual knot. False otherwise.

Return type bool

self_linking()

Returns the self linking number J(K) of the Gauss code, an invariant of virtual knots. See Kauffman 2004 for more information.

Returns slink_counter – The self linking number of the open curve

Return type int

vassiliev_degree_2 (simplify=True)

Returns the Vassiliev invariant of degree 2 for the Knot.

Parameters

- **simplify** (bool) If True, simplifies the Gauss code of self before calculating the invariant. Defaults to True, but will work fine if you set it to False (and might even be faster).
- ****kwargs** These are passed directly to gauss_code().

vassiliev_degree_3 (simplify=True, try_cython=True)

Returns the Vassiliev invariant of degree 3 for the Knot.

Parameters

- **simplify** (bool) If True, simplifies the Gauss code of self before calculating the invariant. Defaults to True, but will work fine if you set it to False (and might even be faster).
- **try_cython** (bool) Whether to try and use an optimised cython version of the routine (takes about 1/3 of the time for complex representations). Defaults to True, but the python fallback will be *slower* than setting it to False if the cython function is not available.
- ****kwargs** These are passed directly to gauss_code ().

virtual_vassiliev_degree_3()

Returns the virtual Vassiliev invariant of degree 3 for the representation.

1.5 Knot catalogue

pyknotid provides knot lookup by name or invariant values, using a prebuilt database.

The knot database includes information about all knots with up to 15 crossings, with topological invariants following those indexed by the Knot Atlas and the KnotInfo Table of Knot Invariants, or calculated by pyknotid using the Dowker-Thistlethwaite codes of the knots.

1.5.1 Downloading the database

The database must normally be downloaded separately, and is currently approximately 230MB in size.

If you do not download the database, most of pyknotid will work fine. Only the explicit knot identification by database lookup, or direct database queries, are not available.

To download the knot database:

```
from pyknotid.catalogue.getdb import download_database
download_database()
```

After this has completed (it may take a few seconds), the database functions should all work immediately.

For other database management functions, see Database download module.

1.5.2 Lookup by name

Use pyknotid.catalogue.identify.get_knot():

```
from pyknotid.catalogue.identify import get_knot
trefoil = get_knot('3_1')
figure_eight = get_knot('4_1')
```

1.5.3 Lookup by invariants

Use pyknotid.catalogue.identify.from_invariants():

```
from pyknotid.catalogue.identify import from_invariants
```

```
from_invariants(determinant=5, max_crossings=9)
# returns [<Knot 4_1>, <Knot 5_1>]
```

(continues on next page)

(continued from previous page)

```
import sympy as sym
t = sym.var('t')
from_invariants(alexander=1-t+t**2, max_crossings=9)
# returns [<Knot 3_1>]
```

For a full list of lookup parameters, see from_invariants().

1.5.4 Exploring properties of knots

You can view more properties of any knot returned by the database:

```
from pyknotid.catalogue import get_knot, from_invariants
k = get_knot('5_2')
k.pretty_print() # prints some information from the database:
                  # Identifier: 5_2
                  # Min crossings: 5
                  # Fibered: False
                  # Gauss code: -1, 5, -2, 1, -3, 4, -5, 2, -4, 3
                    Planar diagram: X_1425 X_3849 X_5,10,6,1 X_9,6,10,7 X_7283
                  #
                    DT code: 4 8 10 2 6
                  #
                    Determinant: 7
                  #
                  # Signature: -2
                  # Alexander: 2*t**2 - 3*t + 2
                  # Jones: 1/q - 1/q**2 + 2/q**3 - 1/q**4 + q**(-5) - 1/q**6
                  # HOMFLY: -a**6 + a**4*z**2 + a**4 + a**2*z**2 + a**2
                  # Hyperbolic volume: 2.82812
                  # Vassiliev order 2: 2
                  # Vassiliev order 3: -3
                  # Symmetry: reversible
```

Properties of the knot can also be accessed directly:

k.determinant # 7

For a full list of attributes available, see *pyknotid.catalogue.database.Knot*.

1.5.5 Database download module

To download the database, call download_database().

The other functions in this module provide basic functionality for checking where the database is stored, and deleting old versions if necessary.

API documentation

```
pyknotid.catalogue.getdb.clean_all_databases()
    Deletes all database files.
```

```
pyknotid.catalogue.getdb.clean_old_databases()
    Deletes old database files (all but the most recent version).
```

```
pyknotid.catalogue.getdb.download_database()
    Downloads the knots database to download target dir().
```

find_db looks in the following locations, in order of precedence:

- 1. The local folder (containing getdb.py). This is convenient if you have built your own database.
- 2. The directory returned by appdirs.user_data_dir (depends on the OS).

If the database cannot be found, an exception is raised.

You can download a prebuilt database using *download_database()*.

Parameters db_version (*int*) – The database version to find. Defaults to None, in which case the current db_version from *pyknotid.catalogue.database* is used.

```
pyknotid.catalogue.getdb.require_database(func)
```

Decorator that causes a function to query find_database before returning.

1.5.6 Identify module

Functions for identifying knots based on their name or invariants.

API documentation

```
pyknotid.catalogue.identify.first_from_invariants (*args, **kwargs)
Returns the first Knot by crossing number (and arbitrary ordering within that) with the given invariant conditions.
```

Parameters **kwargs – Any set of invariant conditions. The accepted arguments are the same as for *from_invariants()*.

pyknotid.catalogue.identify.from_invariants(*args, **kwargs)

Takes invariants as kwargs, and does the appropriate conversion to return a list of database objects matching all the given criteria.

Note: This only searches within the indexed database available. Some invariant options return only results where the invariant both matches *and* is known, others return those that match *or* are not known. Check the source if depending on accurate results.

Does not support all available invariants. Currently, searching is supported by:

Parameters

- or name or id (*identifier*) The name of the knot following knot atlas conventions, e.g. '3_1'
- **min_crossings** (*int*) The minimal crossing number of the knot.
- **max_crossings** (*int*) The maximal known crossing number of the knot. This may be higher than its actual crossing number, it serves only to prune the results list.
- **signature** (*int*) The signature invariant.
- unknotting_number (*int*) The unknotting number of the knot.

- or alex (*alexander*) The Alexander polynomial, provided as a sympy expression in a single variable (ideally 't').
- or alexander_imag_2 (determinant) The Alexander polynomial at -1 (== exp(Pi I))
- alexander_imag_3 (*int*) The abs of the Alexander polynomial at exp(2 Pi I / 3)
- alexander_imag_4 (int) The abs of the Alexander polynomial at exp(Pi I / 2)
- **roots** (*iterable*) The abs of the Alexander polnomial at the given roots, assumed to start at 2, e.g. passing (3, 2, 1) is the same as identifying at determinant=3, alexander_imag_3=2, alexander_imag_4=1. An entry of None means the value is ignored in the lookup.
- jones (sympy) The Jones polynomial, provided as a sympy expression in a single variable (ideally 'q').
- homfly (sympy) The HOMFLY-PT polynomial, provided as a sympy expression in two variables.
- or hyp_vol or hypvol (hyperbolic_volume) The hyperbolic volume of the knot complement. The lookup is a string comparison based on the given number of significant digits.
- or vassiliev_2 or v_2 or v2 (vassiliev_order_2) The Vassiliev invariant of order 2. This will not prune knots where this invariant is not known (specifically, those with 12 or more crossings).
- or vassiliev_3 or v_3 or v3 (vassiliev_order_3) The Vassiliev invariant of order 3. This will not prune knots where this invariant is not known (specifically, those with 12 or more crossings).
- **symmetry** (*string*) The symmetry of the knot, one of 'reversible', 'positive amplicheiral', 'negative amplicheiral', 'chiral'.
- or planar_writhe (writhe) The writhe of the knot's minimal diagram as recorded by its dt code. This is not necessarily unique, only the value of the dt code stored is given.
- **composite** (*bool*) If True, will return only composite knots. If False, will return only prime knots. Defaults to None, meaning it will return any knot type.
- **prime** (bool) If True, will return only prime knots. If False, will return only composite knots. Defaults to None, meaning it will return any knot type.
- **other** (*iterable*) A list of other peewee terms that can be chained in where () calls, e.g. database.Knot.min_crossings < 5. This provides more flexibility than the other options.
- **return_query** (bool) If True, returns the database iterator for the objects, otherwise returns a list. Defaults to False (i.e. the list). This will be much slower if the list is very large, but is convenient for most searches.

```
For instance, trefoil = get_knot('3_1').
```

1.5.7 Database module

pyknotid looks up knot information via a prebuilt sqlite database, accessed using the peewee ORM. Other ORMs are not currently supported.

The model class is *pyknotid.catalogue.database.Knot*, documented below. For generic documentation about using the database, see *Knot catalogue*.

pyknotid also includes functions for creating a database from scratch (using knot information from the Knot Atlas), and improving an existing database by calculating new invariants or pulling information from other sources such as the KnotInfo database. These functions can be found in pyknotid.catalogue.build and pyknotid.catalogue.build and pyknotid.catalogue.improve, which are not included in the indexed documentation here.

API documentation

```
class pyknotid.catalogue.database.Knot (*args, **kwargs)
     Bases: pyknotid.catalogue.database.BaseModel
     Peewee model for storing a knot in a database.
     DoesNotExist
         alias of KnotDoesNotExist
     alexander = <TextField: Knot.alexander>
         Alexander polynomial, stored as a json list of coefficients from lowest to highest index, including zeros if
         there are any jumps in index.
     alexander_imag_3 = <IntegerField: Knot.alexander_imag_3>
         The absolute value of the Alexander polynomial at exp(2 \text{ pi } I / 3). This will always be an integer.
     alexander_imag_4 = <IntegerField: Knot.alexander_imag_4>
         The absolute value of the Alexander polynomial at exp(2 \text{ pi } I/4) == I. This will always be an integer.
     components
         A list tuples (identifier, index), where the knot with the given identifier occurs index times.
     composite = <BooleanField: Knot.composite>
         Whether the knot is composite or not.
     conway_notation = <CharField: Knot.conway_notation>
         Conway notation, as a string.
     determinant = <IntegerField: Knot.determinant>
         The knot determinant (Alexander polynomial at -1)
     dt_code = <CharField: Knot.dt_code>
         Dowker-Thistlethwaite code, as a string.
     fibered = <BooleanField: Knot.fibered>
         Whether the knot is fibered or not.
     qauss code = <CharField: Knot.gauss code>
         Gauss code, as a string.
     homfly = <TextField: Knot.homfly>
         HOMFLY-PT polynomial, stored as a json list.
     hyperbolic_volume = <CharField: Knot.hyperbolic_volume>
         Hyperbolic volume, stored as a string to avoid precision problems.
     identifier = <CharField: Knot.identifier>
         The standard knot notation, e.g. 3_1 for trefoil
     jones = <TextField: Knot.jones>
```

Jones polynomial, stored as a json list of coefficients and indices for each monomial.

```
min_crossings = <IntegerField: Knot.min_crossings>
    Minimal crossing number for the knot, e.g. 3 for trefoil
name = <CharField: Knot.name>
    The actual name (if any), e.g. trefoil
planar_diagram = <CharField: Knot.planar_diagram>
    Planar diagram representation, as a string.
planar_writhe = <IntegerField: Knot.planar_writhe>
    The writhe of the minimal diagram described by the DT_code. This is not necessarily unique (see Perko
    pair, I think?).
pretty_print()
    Pretty print all information contained about self.
signature = <IntegerField: Knot.signature>
    The knot signature
space_curve (verbose=True, **kwargs)
    Returns a Knot object representing this knot.
symmetry = <CharField: Knot.symmetry>
    The symmetry type of the knot; reversible, positive amphichiral, negative amphichiral fully amphichiral or
    chiral.
two_bridge = <CharField: Knot.two_bridge>
    Two-bridge notation, as a string.
unknotting number = <IntegerField: Knot.unknotting number>
    Unknotting number, stored as an integer.
url()
    The guessed url of this knot in the Knot Atlas. This page may not actually exist or be populated.
vassiliev_2 = <IntegerField:</pre>
                                     Knot.vassiliev_2>
    The Vassiliev invariant of order 2.
vassiliev_3 = <IntegerField:</pre>
                                      Knot.vassiliev_3>
    The Vassiliev invariant of order 3.
```

1.6 Visualise

Functions for plotting knots, supporting different toolkits and types of plot.

pyknotid primarily supports Vispy as the plotting mechanism. Mayavi is semi-supported but may not always work. Many of these functions can be called in a more convenient way via methods of the *space curve classes* (e.g. *Knot*).

1.6.1 API documentation

```
pyknotid.visualise.plot_line (points, mode='auto', clf=True, **kwargs)
Plots the given line, using the toolkit given by mode.
```

kwargs are passed to the toolkit specific function, except for:

Parameters

• **points** (*ndarray*) – The nx3 array to plot.

- **mode** (*str*) The toolkit to draw with. Defaults to 'auto', which will automatically pick the first available toolkit from ['mayavi', 'matplotlib', 'vispy'], or raise an exception if none can be imported.
- **clf** (bool) Whether the existing figure should be cleared before drawing the new one.

Plot the 2d projection of the given points, with optional markers for where the crossings are.

Parameters

- **points** (*array-like*) The nxm array of points in the line, with m >= 2.
- **crossings** (*array-like or None*) The nx2 array of crossing positions. If None, crossings are not plotted. Defaults to None.

```
pyknotid.visualise.plot_shell_vispy (func, points, number_of_samples=10, radius=None,
                                               zero_centroid=False, sphere_radius_factor=2.0, opac-
                                               ity=0.5, cmap='hsy', **kwargs)
     func must be a function returning values at angles and points, like OpenKnot._alexander_map_values.
pyknotid.visualise.plot_sphere_lambert_sharp_vispy (func,
                                                                                 circle_points=50,
                                                                                 output_size=500,
                                                                  depth=2,
                                                                  edge_color=None, cmap='brg',
                                                                                  mesh='circles',
                                                                  smooth=0,
                                                                  **kwargs)
     func must be a function of sphere angles theta, phi
pyknotid.visualise.plot_sphere_lambert_vispy (func,
                                                                    circle_points=50,
                                                                                        depth=2,
                                                          edge_color=None, cmap='hsv', smooth=0,
                                                          mesh='circles', **kwargs)
     func must be a function of sphere angles theta, phi
pyknotid.visualise.plot_sphere_mollweide_vispy (func,
                                                                     circle_points=50,
                                                                                        depth=2,
                                                                                     cmap='hsv',
                                                             edge_color=None,
                                                             smooth=0, mesh='circles', **kwargs)
     func must be a function of sphere angles theta, phi
pyknotid.visualise.plot sphere shell vispy (func, rows=100, cols=100, radius=1.0,
                                                        opacity=1.0, translation=(0.0, 0.0, 0.0),
                                                                                edge_color=None,
                                                        method='latitude',
                                                        cmap='hsv', smooth=0, cutoff=0.4, cut-
                                                        off_max=0.8,
                                                                            transparent_side=True,
                                                        **kwargs)
     func must be a function of sphere angles theta, phi
```

1.7 About pyknotid

pyknotid has been developed as part of Leverhulme Trust Programme Grant RP2013-K-009: Scientific Properties of Complex Knots, a collaboration between the University of Bristol and Durham University in the UK. For more information, see the SPOCK homepage.

A graphical interface to some of these tools is available online at Knot ID.

1.7.1 Contacts

Questions or comments are welcome, please email alexander.taylor@bristol.ac.uk.

1.7.2 Cite us

If you use pyknotid in your research, please cite us as follows:

A J Taylor and other SPOCK contributors. pyknotid knot identification toolkit. https://github.com/ SPOCKnots/pyknotid, 2017. Accessed YYYY-MM-DD.

In bibtex format:

```
@Misc{pyknotid,
  author = {Alexander J Taylor and other SPOCK contributors},
  title = {pyknotid knot identification toolkit},
  howpublished = {\url{https://github.com/SPOCKnots/pyknotid}},
  note = {Accessed YYYY-MM-DD},
  year = 2017,
}
```

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