
Catacycle Documentation

catacycle

Jan 24, 2022

CONTENTS:

1	About Catacycle	1
2	Installation	3
3	Getting Started	5
4	Tutorials	7
5	Developer Documentation	9
6	API Documentation	11
6.1	catacycle.catacycle	11
6.2	catacycle.drawing_helpers	12
7	Indices and tables	17
	Python Module Index	19
	Index	21

ABOUT CATACYCLE

This page explains the conception and anticipated use cases of catacycle, as well as an introduction to the web interface.

INSTALLATION

This page details how to install Catacycle on your machine.

GETTING STARTED

This page details how to get started with Catacycle.

TUTORIALS

This page contains examples of how to handle specific use cases with Catacycle.

DEVELOPER DOCUMENTATION

This page details how Catacycle is structured and how to begin adding new features.

API DOCUMENTATION

A python visualization package for generating data-rich catalytic cycle drawings

Modules

<code>catacycle.catacycle</code>	Cyclic reaction pathway figure generator - Rusty Shack- leford 2018
<code>catacycle.drawing_helpers</code>	

6.1 catacycle.catacycle

Cyclic reaction pathway figure generator - Rusty Shackelford 2018

Functions

<code>draw</code> ([data, startrange, stoprange, ...])	
<code>draw_straight</code> (data[, startrange, stoprange, ...])	
<code>scaler</code> (forward_rates, rev_rates[, ...])	Transforming rates to be within specified range defined by startrange and stoprange:
<code>try_fallback</code> (dictionary, key, fb)	

6.1.1 catacycle.catacycle.draw

`catacycle.catacycle.draw(data=None, startrange=0.15, stoprange=0.85, f_format='svg', figsize=(8, 8), return_image=False)`

6.1.2 catacycle.catacycle.draw_straight

`catacycle.catacycle.draw_straight(data, startrange=0.15, stoprange=0.85, f_format='svg', figsize=(8, 8), return_image=False)`

6.1.3 catacycle.catacycle.scaler

`catacycle.catacycle.scaler(forward_rates, rev_rates, startrange=0.1, stoprange=0.8, scale_type='Linear')`
Transforming rates to be within specified range defined by startrange and stoprange:

Can use linear or logarithmic scale, which is preserved when transforming the data. :param forward_rates: a list of forward rates as floats or ints :param rev_rates: a list of reverse rates as floats or ints :param startrange: float, first number of the range you want output to take :param stoprange: float, last number of range for output to take :param scale_type: 'Linear', 'Logarithmic', or 'Preserve Multiples'. :return: (forward_rates, rev_rates), a tuple of the original lists scaled properly

6.1.4 catacycle.catacycle.try_fallback

`catacycle.catacycle.try_fallback(dictionary, key, fb)`

6.2 catacycle.drawing_helpers

Functions

<code>cart2pol(x, y)</code>	
<code>concatenate_paths(paths[, connect])</code>	
<code>curved_arrow_double(theta1, theta2, radius, ...)</code>	Construct the paths a double-sided reversible curved arrow.
<code>curved_arrow_single(theta1, theta2, radius, ...)</code>	Construct the path for an irreversible curved arrow
<code>ensure_all_valid_gaps(delta, gaps[, precision])</code>	
<code>ensure_valid_gap(delta, gap[, precision])</code>	
<code>ensure_valid_gaps(delta, gap1, gap0[, precision])</code>	
<code>filled_circular_arc(theta1, theta2, radius, ...)</code>	Construct the path for a circular arc
<code>get_intersect_segment_circle(p1, p2, r[, p_cent])</code>	https://codereview.stackexchange.com/questions/86421/line-segment-to-circle-collision-algorithm
<code>get_isosceles_arrowhead(radius, theta1, ...)</code>	

continues on next page

Table 3 – continued from previous page

<code>get_isosceles_arrowhead_old</code> (radius, theta1, ...)	
<code>get_perp_arrowhead</code> (radius, theta_tip, ...)	
<code>join_points</code> (points)	
<code>path_arc_cw</code> (theta1, theta2)	used if theta1 >= theta2
<code>path_arc_smart</code> (theta1, theta2)	
<code>scale_arc</code> (arc_path, scale)	
<code>set_ax_lims</code> (ax, paths)	
<code>shift_path_by_vec</code> (path, vec)	
<code>straight_arrow_double</code> (length, width_top, ...)	Construct the path for an irreversible straight arrow
<code>straight_arrow_single</code> (length, width[, ...])	Construct the path for an irreversible straight arrow

6.2.1 catacycle.drawing_helpers.cart2pol

`catacycle.drawing_helpers.cart2pol`(x, y)

6.2.2 catacycle.drawing_helpers.concatenate_paths

`catacycle.drawing_helpers.concatenate_paths`(paths, connect=True)

6.2.3 catacycle.drawing_helpers.curved_arrow_double

`catacycle.drawing_helpers.curved_arrow_double`(theta1, theta2, radius, width_outer, width_inner, origin=(0, 0), rel_head_width=1.5, f_abs_head_len=None, r_abs_head_len=None, rel_head_len=0.1, reverse=False)

Construct the paths a double-sided reversible curved arrow.

Returns the paths for both the outer and inner arrows. Radius is the distance from the origin to the inside of the outer arrow

6.2.4 catacycle.drawing_helpers.curved_arrow_single

`catacycle.drawing_helpers.curved_arrow_single`(theta1, theta2, radius, width, origin=(0, 0), rel_head_width=1.5, rel_head_len=0.1, abs_head_len=None, reverse=False)

Construct the path for an irreversible curved arrow

6.2.5 `catacycle.drawing_helpers.ensure_all_valid_gaps`

`catacycle.drawing_helpers.ensure_all_valid_gaps(delta, gaps, precision=1)`

6.2.6 `catacycle.drawing_helpers.ensure_valid_gap`

`catacycle.drawing_helpers.ensure_valid_gap(delta, gap, precision=1)`

6.2.7 `catacycle.drawing_helpers.ensure_valid_gaps`

`catacycle.drawing_helpers.ensure_valid_gaps(delta, gap1, gap0, precision=1)`

6.2.8 `catacycle.drawing_helpers.filled_circular_arc`

`catacycle.drawing_helpers.filled_circular_arc(theta1, theta2, radius, width, origin=(0, 0))`
Construct the path for a circular arc

6.2.9 `catacycle.drawing_helpers.get_intersect_segment_circle`

`catacycle.drawing_helpers.get_intersect_segment_circle(p1, p2, r, p_cent=array([0, 0]))`
<https://codereview.stackexchange.com/questions/86421/line-segment-to-circle-collision-algorithm>

6.2.10 `catacycle.drawing_helpers.get_isosceles_arrowhead`

`catacycle.drawing_helpers.get_isosceles_arrowhead(radius, theta1, theta2, base_width)`

6.2.11 `catacycle.drawing_helpers.get_isosceles_arrowhead_old`

`catacycle.drawing_helpers.get_isosceles_arrowhead_old(radius, theta1, theta2, base_width)`

6.2.12 `catacycle.drawing_helpers.get_perp_arrowhead`

`catacycle.drawing_helpers.get_perp_arrowhead(radius, theta_tip, f_angle_offset, width, rel_head_width, reverse)`

6.2.13 `catacycle.drawing_helpers.join_points`

`catacycle.drawing_helpers.join_points(points)`

6.2.14 `catacycle.drawing_helpers.path_arc_cw`

`catacycle.drawing_helpers.path_arc_cw(theta1, theta2)`
used if $\theta_1 \geq \theta_2$

6.2.15 `catacycle.drawing_helpers.path_arc_smart`

`catacycle.drawing_helpers.path_arc_smart(theta1, theta2)`

6.2.16 `catacycle.drawing_helpers.scale_arc`

`catacycle.drawing_helpers.scale_arc(arc_path, scale)`

6.2.17 `catacycle.drawing_helpers.set_ax_lims`

`catacycle.drawing_helpers.set_ax_lims(ax, paths)`

6.2.18 `catacycle.drawing_helpers.shift_path_by_vec`

`catacycle.drawing_helpers.shift_path_by_vec(path, vec)`

6.2.19 `catacycle.drawing_helpers.straight_arrow_double`

`catacycle.drawing_helpers.straight_arrow_double(length, width_top, width_bottom, origin=(0, 0),
rel_head_width=0.5, f_abs_head_len=None,
r_abs_head_len=None, rel_head_len=0.2,
reverse=False)`

Construct the path for an irreversible straight arrow

6.2.20 `catacycle.drawing_helpers.straight_arrow_single`

`catacycle.drawing_helpers.straight_arrow_single(length, width, origin=(0, 0), rel_head_width=0.5,
abs_head_len=None, rel_head_len=0.2,
reverse=False)`

Construct the path for an irreversible straight arrow

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`

PYTHON MODULE INDEX

C

`catacycle`, [11](#)

`catacycle.catacycle`, [11](#)

`catacycle.drawing_helpers`, [12](#)

INDEX

C

`cart2pol()` (in module `catacycle.drawing_helpers`), 13
`catacycle`
 module, 11
`catacycle.catacycle`
 module, 11
`catacycle.drawing_helpers`
 module, 12
`concatenate_paths()` (in module `catacycle.drawing_helpers`), 13
`curved_arrow_double()` (in module `catacycle.drawing_helpers`), 13
`curved_arrow_single()` (in module `catacycle.drawing_helpers`), 13

D

`draw()` (in module `catacycle.catacycle`), 12
`draw_straight()` (in module `catacycle.catacycle`), 12

E

`ensure_all_valid_gaps()` (in module `catacycle.drawing_helpers`), 14
`ensure_valid_gap()` (in module `catacycle.drawing_helpers`), 14
`ensure_valid_gaps()` (in module `catacycle.drawing_helpers`), 14

F

`filled_circular_arc()` (in module `catacycle.drawing_helpers`), 14

G

`get_intersect_segment_circle()` (in module `catacycle.drawing_helpers`), 14
`get_isosceles_arrowhead()` (in module `catacycle.drawing_helpers`), 14
`get_isosceles_arrowhead_old()` (in module `catacycle.drawing_helpers`), 14
`get_perp_arrowhead()` (in module `catacycle.drawing_helpers`), 14

J

`join_points()` (in module `catacycle.drawing_helpers`), 14

M

module
 `catacycle`, 11
 `catacycle.catacycle`, 11
 `catacycle.drawing_helpers`, 12

P

`path_arc_cw()` (in module `catacycle.drawing_helpers`), 15
`path_arc_smart()` (in module `catacycle.drawing_helpers`), 15

S

`scale_arc()` (in module `catacycle.drawing_helpers`), 15
`scaler()` (in module `catacycle.catacycle`), 12
`set_ax_lims()` (in module `catacycle.drawing_helpers`), 15
`shift_path_by_vec()` (in module `catacycle.drawing_helpers`), 15
`straight_arrow_double()` (in module `catacycle.drawing_helpers`), 15
`straight_arrow_single()` (in module `catacycle.drawing_helpers`), 15

T

`try_fallback()` (in module `catacycle.catacycle`), 12