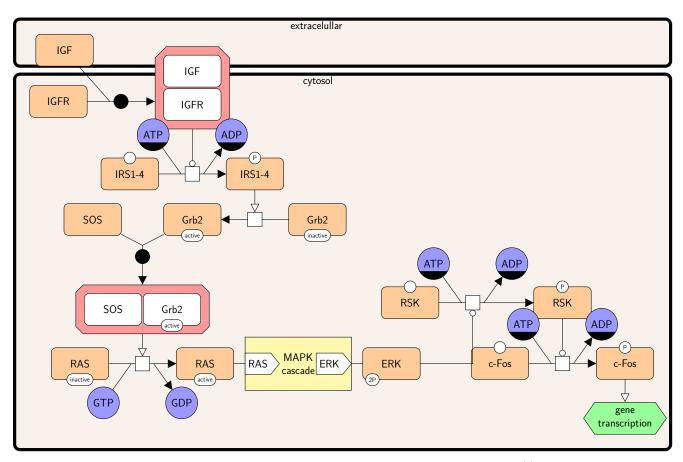
# sbgntikz

## manual for version 1.0.\*

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 ${\it Map\ adapted\ from\ SBGN\ PD\ language\ L1V1.3,\ Journal\ of\ Integrative\ Bioinformatics,\ 2015\ Sep\ 4;12(2):263}$ 

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#### 1 Introduction

#### 1.1 About

sbgntikz is a TikZ [1] library to draw SBGN PD, AF or ER maps [2] directly into LATEX documents. It basically encodes SBGN glyphs into TikZ shapes and arrowheads named by keywords, making them straightforwardly drawable within a TikZ picture. Drawing a specific glyph is then as simple as specifying its corresponding keyword in some TikZ command.

The present manual is intended for an audience that knows SBGN but not particularly TikZ. The rest of the present section is dedicated to the first steps in using sbgntikz: installing the library and drawing a first map (while introducing some basic TikZ syntax). Section 2 references all glyphs and their associated keywords, whereas section 3 gives some TikZ options and syntaxes that I find most useful to draw SBGN maps. I believe users already familiar with TikZ will mostly be interested in reading section 2, and might have different (and maybe better) solutions to the issues presented in section 3.

#### 1.2 Installation and usage

The directory tikz-sbgn/ should be copied to a directory where it can be found by the TFX engine:

- in the directory of your LATEX source file
- in your local texmf directory. This directory is usually /home/<user>/texmf/ under Linux, /Users/Library/texmf/ under MacOS, and C:/Users/<user>/texmf under Windows, but it can depend on your OS version and TFX distribution.

Your texmf directory can be found using the kpsewhich -var-value=TEXMFHOME command.

Usually, TikZ is installed within your TEX distribution, so TikZ and sbgntikz can be imported directly into your IETEX source file with no further installation adding the following two commands to your preamble:

```
\usepackage{tikz}
\usetikzlibrary{sbgn}
```

An SBGN map can then be drawn within a TikZ picture using the sbgn key:

```
\begin{tikzpicture}[sbgn]
% tikz code to draw an SBGN map
\end{tikzpicture}
```

#### 1.3 A first map

SBGN is all about drawing nodes with specific shapes and arcs with specific arrow heads. Fortunately, drawing TikZ pictures is not different, making it pretty straightforward to draw SBGN maps using sbgntikz: the  $\node$  command is used to draw nodes, while the  $\draw$  command is used to draw arcs. The code to draw an SBGN node (or an attribute) will usually look like the following:

```
\node[<sbgn node>, ...] (name) at (point) {LABEL};
```

where

- <sbgn node> is a keyword corresponding to the type of node to be drawn (e.g. simple chemical for a simple chemical);
- ... is a list of other options for the node (e.g. its relative positioning towards another node, color, line width ...);
- (name) specifies the name of the node (optional);
- at (point) specifies the point on the canvas where to draw the node (optional, by default (0,0) if no relative positioning is specified in the nodes' options);
- {LABEL} specifies the label of the node that will be displayed (mandatory but can be empty).

As for arcs, they can be drawn using the following piece of code:

```
\draw[<sbgn arc>, ...] (a) -- (b);
```

where

- <sbgn arc> is a keyword corresponding to the type of arc to be drawn (e.g. necessary stimulation for a necessary stimulation);
- ... is a list of other options for the arc (e.g. its color, line width ...);
- (a) is a point on the canvas or the name of a node from which the arc will depart;
- (b) is a point on the canvas or the name of a node on which the arc will arrive.

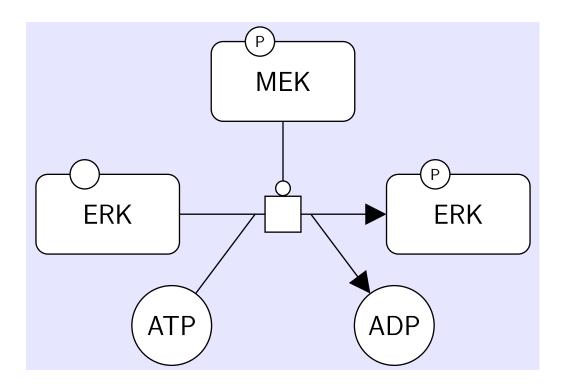
Knowing those two basic syntaxes, one can draw pretty much any desired SBGN map. Following is an example of code to draw a simple PD map. It relies on relative positioning provided by TikZ's positioning library, as positioning all nodes with absolute coordinates would be too cumbersome (see section 3 for few more details, or the PGF/TikZ manual for lot more details).

```
\documentclass{standalone}
\usepackage{tikz}
\usetikzlibrary{positioning, sbgn}
\begin{document}
\begin{tikzpicture}[sbgn]
\node[macromolecule] (erk) {ERK};
                                      % this node has no absolute nor relative positioning, so it
\hookrightarrow is placed at (0,0) by default
\node[sv] at (erk.120) {}; % the state variable is placed on the border of the node, at an angle
\hookrightarrow of 120 deg
\node[generic process, connectors = horizontal, right = of erk] (p) {}; % we add connectors, and

→ use relative positioning

\node[macromolecule, right = of p] (perk) {ERK};
\node[sv] at (perk.120) {P};
\node[simple chemical, below left = of p] (atp) {ATP};
\node[simple chemical, below right = of p] (adp) {ADP};
\node[macromolecule, above = 2cm of p] (pmek) {MEK};
\node[sv] at (pmek.120) {P};
\draw[consumption] (erk) -- (p.west); % p being the name of the process node, p.west is the tip
\hookrightarrow of its left connector
\draw[consumption] (atp) -- (p.west);
\draw[production] (p.east) -- (perk);
\draw[production] (p.east) -- (adp);
\draw[catalysis] (pmek) -- (p);
\end{tikzpicture}
\end{document}
```

Compiling the above code would produce the following figure:



# 2 Drawing glyphs

#### 2.1 Nodes

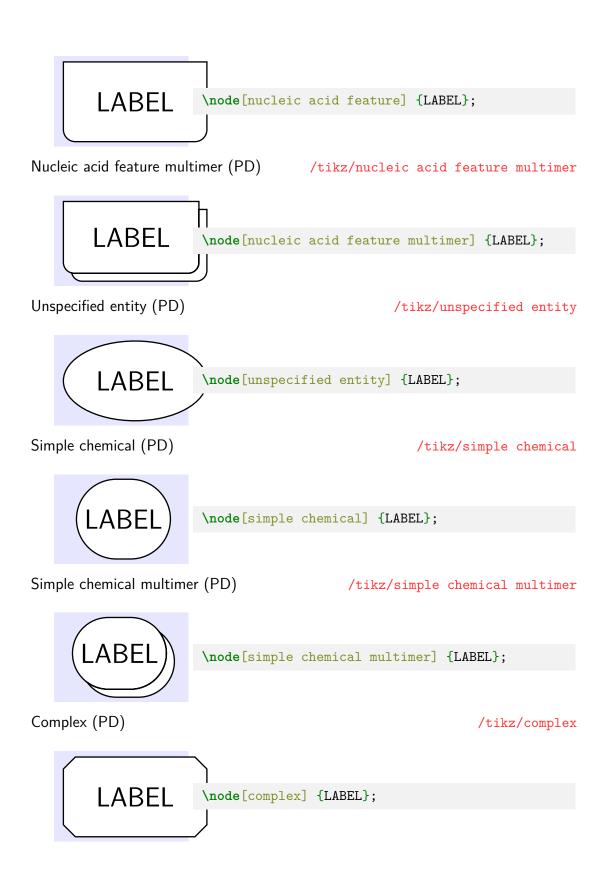
Macromolecule (PD)

LABEL \node[macromolecule] {LABEL};

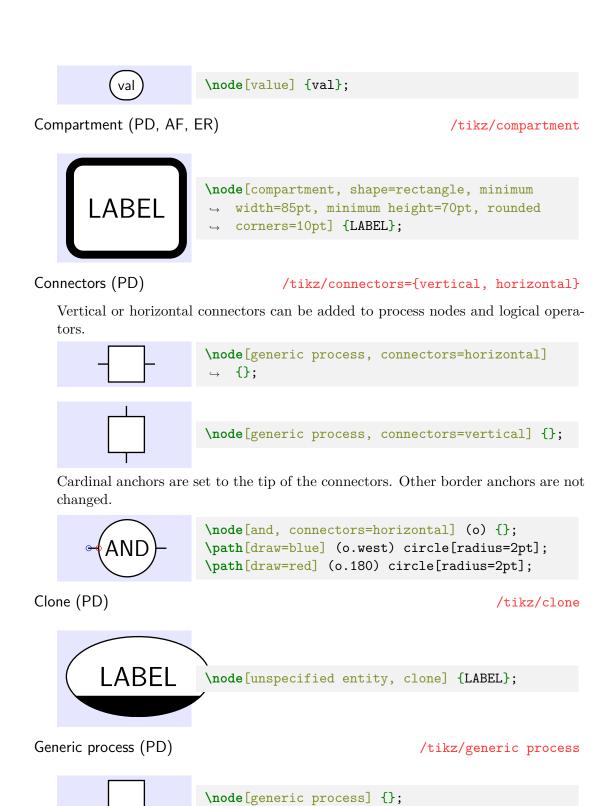
Macromolecule multimer (PD) /tikz/macromolecule multimer

LABEL \node[macromolecule multimer] {LABEL};

Nucleic acid feature (PD) /tikz/nucleic acid feature

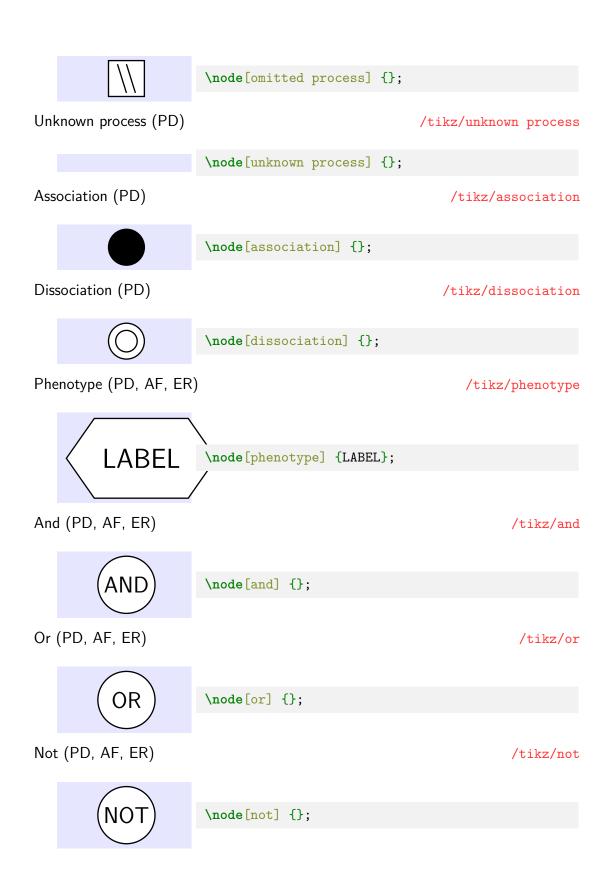


```
Complex multimer (PD)
                                                 /tikz/complex multimer
        LABEL
                      \node[complex multimer] {LABEL};
Perturbation (PD)
                                                     /tikz/perturbation
         LABEL
                      \node[perturbation] {LABEL};
Emptyset (PD)
                                                         /tikz/emptyset
                      \node[empty set] {};
Biological activity (AF)
                                              /tikz/biological activity
        LABEL
                      \node[biological activity] {LABEL};
Entity (ER)
                                                           /tikz/entity
        LABEL
                      \node[entity] {LABEL};
Outcome (ER)
                                                          /tikz/outcome
                      \node[outcome] {};
Value (ER)
                                                            /tikz/value
```



/tikz/omitted process

Omitted process (PD)



```
Delay (PD, AF, ER)
                                                              /tikz/delay
                       \node[delay] {};
Submap (PD)
                                                             /tikz/submap
                       \node[submap, minimum width=85pt, minimum
       LABEL
                        → height=70pt] {LABEL};
Tag (PD)
                                                                /tikz/tag
      LABEL
                       \node[tag] {LABEL};
2.2 Arcs
Logic arc (PD, AF, ER)
                                                          /tikz/logic arc
                       \draw[logic arc] (0,0) -- (2cm,0);
Equivalence arc (PD)
                                                    /tikz/equivalence arc
                       \draw[equivalence arc] (0,0) -- (2cm,0);
Consumption (PD)
                                                        /tikz/consumption
                       \draw[consumption] (0,0) -- (2cm,0);
Production (PD)
                                                         /tikz/production
                       \draw[production] (0,0) -- (2cm,0);
Reversible (PD)
                                                         /tikz/reversible
                       \draw[reversible] (0,0) -- (2cm,0);
```

```
Modulation (PD, AF, ER)
                                                              /tikz/modulation
                         \displaystyle \operatorname{Modulation} (0,0) -- (2cm,0);
Stimulation (PD, AF, ER)
                                                             /tikz/stimulation
                         \draw[stimulation] (0,0) -- (2cm,0);
Necessary stimulation (PD, AF, ER)
                                                 /tikz/necessary stimulation
                         \draw[necessary stimulation] (0,0) -- (2cm,0);
Absolute stimulation (ER)
                                                  /tikz/absolute stimulation
                         \draw[absolute stimulation] (0,0) -- (2cm,0);
Inhibition (PD, AF, ER)
                                                              /tikz/inhibition
                         \draw[inhibition] (0,0) -- (2cm,0);
Absolute inhibition (ER)
                                                   /tikz/absolute inhibition
                         \draw[absolute inhibition] (0,0) -- (2cm,0);
Assignment (ER)
                                                              /tikz/assignment
                         \displaystyle \operatorname{lassignment} (0,0) -- (2cm,0);
Interaction (ER)
                                                             /tikz/interaction
                         \draw[interaction] (0,0) -- (2cm,0);
   N-ary interactions can be drawn using the nary node:
                         \draw[interaction] (0,0) -- node[nary, pos=0.5]
                         \rightarrow (a) {} (2cm,0);
                         \node[outcome] at (a.100) {};
Anchor point (ER)
                                                           /tikz/anchor point
                         \draw[interaction] (0,0) -- coordinate[anchor
                         \rightarrow point, pos = 0.5] (a) (2,0);
                         \draw[stimulation] (1,1) -- (a);
```

#### 2.3 Nodes' and arcs' attributes

Unit of information (PD, ER)

State variable (PD, ER) /tikz/sv val@var \node[entity, draw=gray!60] (m) {}; \node[sv] at (m.north) {val@var}; Existence state variable (ER) /tikz/sv existence \node[entity, draw=gray!60] (m) {}; \node[sv existence] at (m.north) {}; Location state variable (ER) /tikz/sv location \node[entity, draw=gray!60] (m) {}; \node[sv location] at (m.north) {};

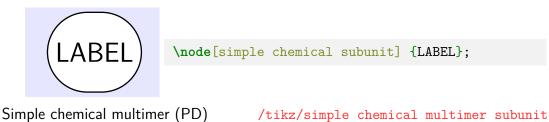
/tikz/ui

```
pre:label
                       \node[entity, draw=gray!60] (m) {};
                       \node[ui] at (m.north) {pre:label};
   In PD, stoichiometry can be drawn using a unit of information along an arc:
                       \draw[production] (0,0) -- node[ui, above,
                       \rightarrow pos=0.5] {\tiny N:5} (2cm,0);
Unit of information simple chemical (AF)
                                                 /tikz/ui simple chemical
           LABEL
                       \node[biological activity, draw=gray!60] (m) {};
                       \node[ui simple chemical] at (m.north) {LABEL};
Unit of information nucleic acid feature (AF) /tikz/ui nucleic acid feature
           LABEL
                       \node[biological activity, draw=gray!60] (m) {};
                       \node[ui nucleic acid feature] at (m.north)
                        Unit of information macromolecule (AF)
                                                  /tikz/ui macromolecule
           LABEL
                       \node[biological activity, draw=gray!60] (m) {};
                       \node[ui macromolecule] at (m.north) {LABEL};
Unit of information perturbation (AF)
                                                    /tikz/ui perturbation
          LABEL
                       \node[biological activity, draw=gray!60] (m) {};
                       \node[ui perturbation] at (m.north) {LABEL};
```

```
Unit of information complex (AF)
                                                      /tikz/ui complex
           LABEL
                      \node[biological activity, draw=gray!60] (m) {};
                      \node[ui complex] at (m.north) {LABEL};
Unspecidied entity subunit (PD)
                                     /tikz/unspecified entity subunit
        LABEL
                      \node[unspecified entity subunit] {LABEL};
Macromolecule subunit (PD)
                                           /tikz/macromolecule subunit
        LABEL
                      \node[macromolecule subunit] {LABEL};
Macromolecule multimer subunit (PD) /tikz/macromolecule multimer subunit
        LABEL
                      \node[macromolecule multimer subunit] {LABEL};
Nucleic acid feature subunit (PD)
                              /tikz/nucleic acid feature subunit
        LABEL
                      \node[nucleic acid feature subunit] {LABEL};
Nucleic acid feature multimer subunit (PD)
                                     /tikz/nucleic acid feature
multimer subunit
                      \node[nucleic acid feature multimer subunit]
        LABEL
```

```
Simple chemical subunit (PD)
```

/tikz/simple chemical subunit





\node[simple chemical multimer subunit] {LABEL};

Complex subunit (PD)

/tikz/complex subunit



Complex multimer subunit (PD)

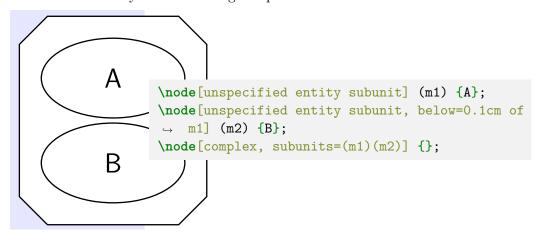
/tikz/complex multimer subunit



Subunits (PD)

/tikz/subunits

The subunits key allows drawing complexes around subunits:



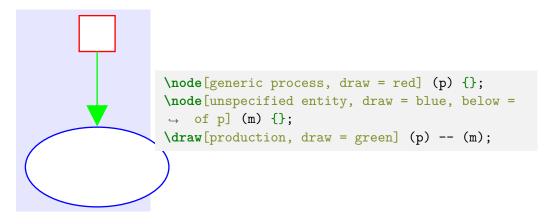
### 3 Customizing and drawing maps effectively

#### 3.1 Useful options for nodes and arcs

The style of nodes and arcs (and their attributes) can be customized at will using the numerous options offered by TikZ. Following are a few options that might be useful for customizing SBGN maps.

Foreground color (Nodes, Arcs)

/tikz/draw



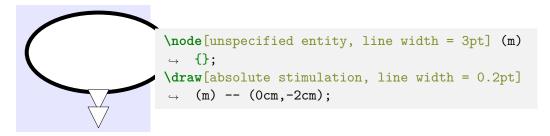
Background color (Nodes)

/tikz/fill



Line width (Nodes, Arcs)

/tikz/line width



Minimum width (Nodes)

/tikz/minimum width

```
\text{\node[complex, minimum width = 20pt] (m) {}; \node[simple chemical, minimum width = 70pt] at \to (0cm,-2cm) (m) {};

Minimum height (Nodes)

\text{\text{\text{\text{ninimum height}}} = 20pt] (m) {}; \node[complex, minimum height = 20pt] (m) {}; \node[simple chemical, minimum height = 70pt] at \to (0cm,-2cm) (m) {};
```

#### 3.2 Positioning of nodes, arcs, and their attributes

TikZ offers two ways of positioning nodes: with absolute coordinates and relatively to other nodes. We discourage using absolute coordinates as those cannot be changed easily through the drawing process. Drawing maps is far easier using relative positioning. For example, state variables can be placed using the border anchor of the entity pool node they decorate:

```
val@var

\node[macromolecule] at (0,0) (m) {};
\node[sv] at (m.140) {val@var};
```

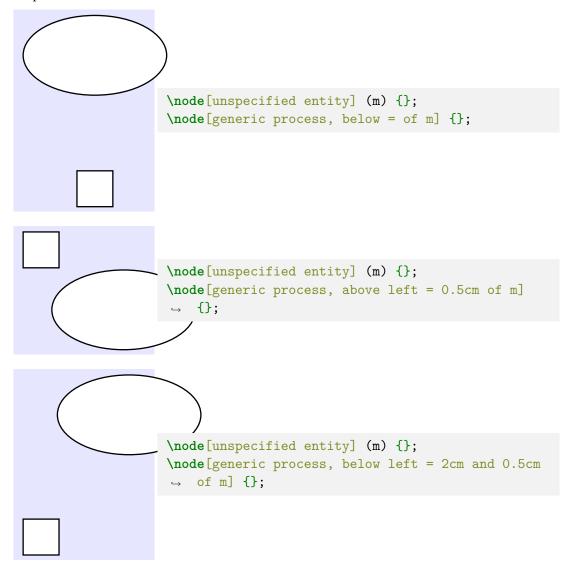
Here, we decided to place the state variable at an angle of 140° on the border of the entity pool node. Now, if we want to change the position of the entity pool node, we don't have to change the position of the state variable:

```
\node[macromolecule] at (0,2) (m) {};
\node[sv] at (m.140) {val@var};
```

Nodes can also be easily be placed relatively to other nodes using the positioning TikZ library, with the following syntax:

```
\node[<sbgn_node>, <direction> = <distance> of <node_name>] ...;
```

Here, <direction> defines in what direction the node should be place relatively to a previously defined node named <node\_name>. This direction can be unitary (left, right, above, below) or composed of two values (vertical direction first, e.g. above left). The node will be placed in that direction at the distance <distance> of the border of node <node\_name>. In case of a composed direction, one can define a distance for each sub-direction: <distance1> and <distance2>. If no distance is provided, the node will be placed at a distance of 1.5cm (default in sbgntikz). Following are some usage examples:



To make the node closer to the other one, a negative distance can be defined:

#### 3.3 Bended arcs, multi-part arcs

TikZ offers a simple way to bend arcs with the following syntax:

```
\draw (a) to [in=<in_angle>, out=<out_angle>] (b);
```

where <in\_angle> specifies the angle at which the arc leaves the source point or node and <out\_angle> the angle at which the arc arrives on the target point or node. Both angles are defined relatively to the picture's coordinate.

One can also use the following shortcut:

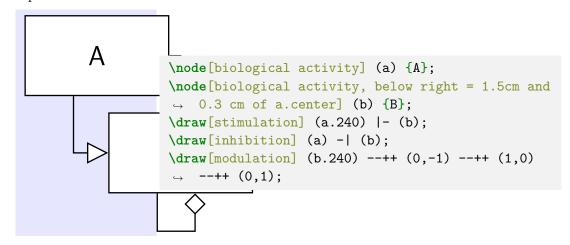
```
\draw (a) to [bend <direction>=<angle>] (b);
```

where <direction>={left, right} specifies the direction where to bend the arc and <angle> the angle at which the arc leaves the source point or node. The angle is this time defined relatively to the line passing through both points/nodes.

```
A
\[ \node[biological activity] (a) {A};
\[ \node[biological activity, below = of a] (b) {B};
\[ \draw[modulation] (a) to [out=-120, in=80] (b);
\] \[ \draw[stimulation] (a) to [bend left=40] (b);
\[ \draw[inhibition] (a) to [bend right=80] (b);
\]
\[ B
```

It is often necessary to break arcs into muliple parts for improved readability. TikZ offers very simple operations to break arcs into horizontal and vertical sub-parts, that replace the default -- operation. The |- operation will produce an horizontal sub-part followed by a vertical one, and the -| a vertical sub-part followed by a horizontal one.

It can also be convenient to use the --+ and --++ to draw arcs with more than two sub-parts.



#### 3.4 Nodes along paths for ER maps

In ER maps, outcomes should be drawn along interaction or assignment arcs. TikZ provides a handy syntax to do so:

```
\draw[interaction] (0,0) -- (2,0)
\( \to \text{ node[outcome, pos = 0.7] (o) } \};
```

Here, the outcome is added along the path using the node command (with no \), as if it was a normal node. The pos option allows defining the distance of the node from the source of the arc relatively to the length of the arc. Here, we placed the outcome at a distance of 70%. More than one outcome can be placed along an arc, by repeating the node syntax:

```
\draw[interaction] (0,0) -- (2,0)

→ node[outcome, pos = 0.3] (o1) {}

→ node[outcome, pos = 0.5] (o2) {}

→ node[outcome, pos = 0.7] (o3) {};
```

One other particularity of drawing ER maps is that one might have to draw arcs targeting other arcs. This is not straightforwardly possible in TikZ, as arcs must target points or nodes. One solution provided by sbgntikz is to draw anchor point coordinates along arcs, as in the following example:

```
\draw[interaction] (0,0) -- (2,0)

coordinate[anchor point, pos = 0.5] (a);
\draw[stimulation] (1,1) -- (a);
```

Here, the anchor point coordinate (which is a circle with no drawing, no label and a radius of 2pt) is placed halfway along the interaction arc.

Often in ER maps, one wants to draw horizontal or vertical modulation arcs departing from outcomes. These particular cases, on the other hand, can be easily achieved using TikZ's  $\mid$ - syntax:

```
\draw[interaction] (0,0) -- (2,0);
\draw[stimulation] (1,1) -- (1,1 |- 2,0);
```

Additional space between the tip of the modulation arc and the target arc can be added (here 2pt, that is the anchor point's default radius):

```
\\draw[interaction] (0,0) -- (2,0);
\\draw[inhibition] (1,1) -- ($(1,1 |-
\to 2,0)+(0,2pt)$);
```

Drawing vertical or horizontal modulation arcs can also be achieved using anchor points and TikZ's let syntax, which allows to place the anchor point at the X-coordinate (for a vertical arc) or Y-coordinate (for an horizontal arc) of the outcome. Following is an example:

```
\draw[interaction] (0,0) -- (2,0) node[outcome,

pos = 0.7] (o1) {};
\draw[interaction] let \p1=(o1) in (0,-2) --

(2,-2) coordinate[anchor point] (a) at

(\x1,-2) node[outcome, pos = 0.3] (o2) {};
\draw[stimulation] (o1) -- (a);
```

In the second interaction, we define the point \p1 as being the outcome of the second interaction, and we use its X-coordinate defined as \x1 to place the anchor point. More coordinates can be defined and accessed using the let command, always using the syntax \pi and \xi,\yi:

```
\draw[interaction] (0,0) -- (2,0) node[outcome,

→ pos = 0.7] (o1) {};

\draw[interaction] (-0.7,-0.5) -- (1.3,-0.5)

→ node[outcome, pos = 0.7] (o2) {};

\draw[interaction] let \p1=(o1), \p2=(o2) in

→ (0,-2) -- (2,-2) coordinate[anchor point] (a1)

→ at (\x1,-2) coordinate[anchor point] (a2) at

→ (\x2,-2);

\draw[stimulation] (o1) -- (a1);

\draw[absolute inhibition] (o2) -- (a2);
```

#### References

[1] Till Tantau. The TikZ and PGF Packages.

[2] Nicolas Le Novere, Michael Hucka, Huaiyu Mi, Stuart Moodie, Falk Schreiber, Anatoly Sorokin, Emek Demir, Katja Wegner, Mirit I Aladjem, Sarala M Wimalaratne, et al. The systems biology graphical notation. *Nature biotechnology*, 27(8):735, 2009.

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