From Quantitative SBML to Boolean Networks

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Modeling of Biological Systems

Example of a simple enzymatic reaction

$$S + E \underset{k_{off}}{\overset{k_{on}}{\rightleftharpoons}} ES \xrightarrow{k_{cat}} E + 2 \cdot P$$

Boolean Networks (BNs)

$\neg$: “not”; $\vee$: “or”; $\wedge$: “and”

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a Boolean network

$$\mathscr{B} = \begin{cases} f_{\mathrm{ES}} := \mathrm{S} \\ f_{\mathrm{P}} := \mathrm{ES} \\ f_{\mathrm{S}} := \mathrm{ES} \\ f_{\mathrm{E}} := \neg\mathrm{S} \end{cases}$$

Boolean Networks (BNs)

$\neg$: "not"; $\vee$: "or"; $\wedge$: "and"

a Boolean network, its interaction graph and gen. asyn. state transition graph

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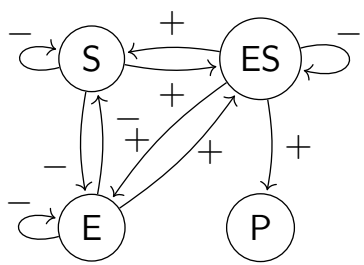

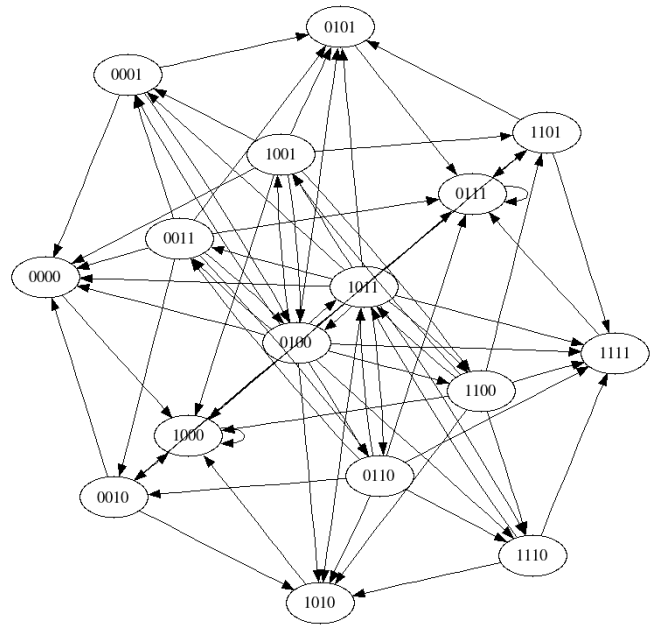

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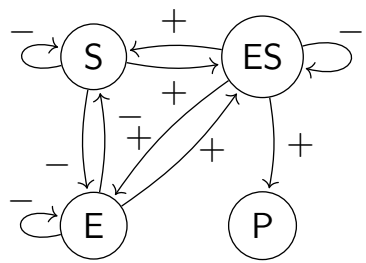
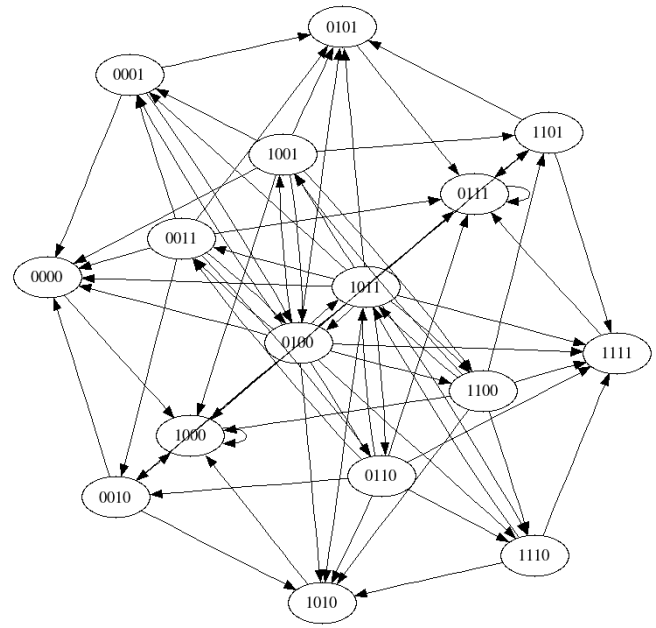




Synthetis of Boolean networks *compatible* with structural constraints (Prior Knowledge Network) and dynamical constraints (Time Series).

`REVEAL`, `Best-Fit`, `caspo-TS`, `ASKeD-BN`...

Our goal

Synthesise Boolean networks starting from SBML models

= Systems Biology Markup Language

chemical reactions network = set of reactions

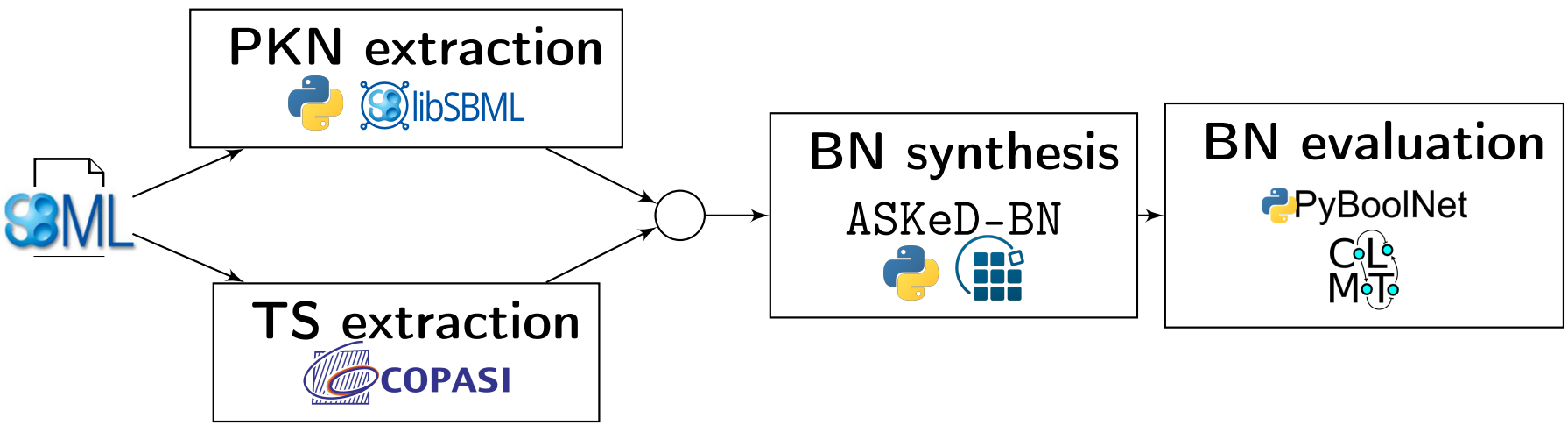
$$S + E \underset{k_{off}}{\overset{k_{on}}{\rightleftharpoons}} ES$$

$$ES \xrightarrow{k_{cat}} E + 2 \cdot P$$

some have all the necessary for us to extract a Time Series and a Prior Knowledge Network $\rightarrow$ *complete* quantitative SBML models

The SBML2BN Pipeline

input: a *complete* quantitative SBML model
output: a *set* of *compatible* Boolean networks



Pipeline Evaluation and Results

Pipeline ran on $>$ 200 SBML models from Biomodels

$\rightarrow$ Overall, our pipeline is good!
(runtime & quality of Boolean networks synthesised)

Reasons for coming...

- *complete* quantitative SBML models
- Boolean Networks *compatible* with an SBML model
- steps of the SBML2BN pipeline
- the actual results
- ...

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- your suggestions are welcomed
- I brought "Bergamotes de Nancy" (= candies)

Thanks for your attention.

Hope to {see, read} you.

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Enjoy the conference!