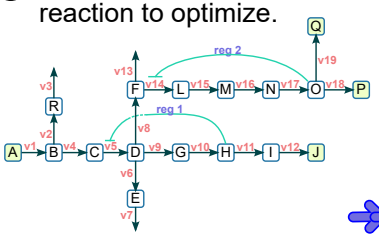
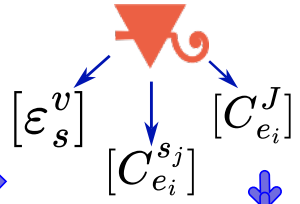
① **Choose a model** and the reaction to optimize.



② **Simulate ground truth values** using Tellurium.

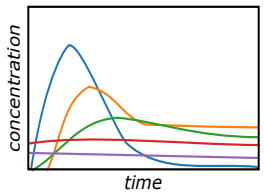


③ Creation of simulated datasets

(a) Select an enzyme and set it to the factor of the desired perturbation strength (e.g. 50%)

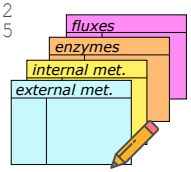
```
enzymei = enzymei * 50%
```

(b) Simulate the model to steady state.



c) Record the resulting data for all the data types

```
metabolite1 = 20.52
metabolite2 = 12.35
...
flux1 = 0.286
flux2 = 0.125
...
enzyme1 = 0.5
enzyme2 = 1
...
```



(d) Reset the model and the perturbed enzyme

(e) Repeat steps a-d until all enzymes have been perturbed and steady state responses have been recorded

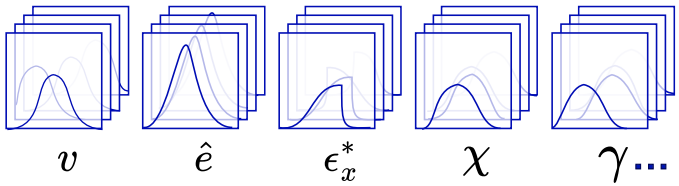
```
i += 1
enzymei = enzymei * 50%
```

④ BMCA

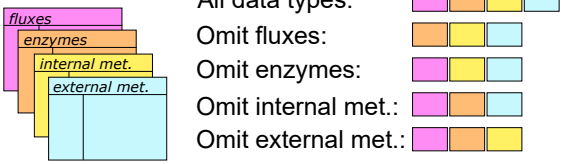
a) Write a system of linlog equations for all reactions in the network.

$$v = (v^* \hat{e})(1 + \epsilon_x^* \chi + \epsilon_y^* \gamma)$$

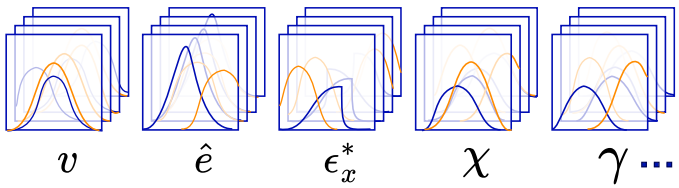
b) Establish priors for each variable in the linlog equation.



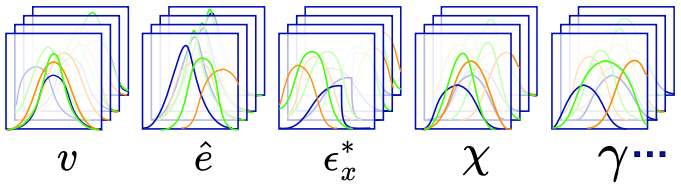
c) Choose which combination of simulated data from step 3 to use in BMCA.



d) Supply available data as observations.

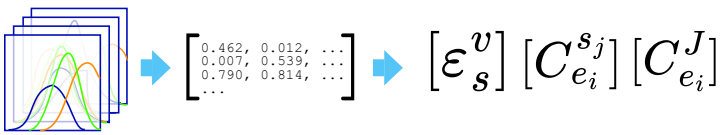


e) Approximate posterior distributions using ADVI.



⑤ Post-BMCA analysis

a) Calculate the predicted control coefficient values with the means of the highest density interval for each posterior distribution.



b) Compare predicted control coefficient values from step 5 with the ground truth values from step 2.