REACTION RATE EQUATIONS

$|M \to M + P|$, $\underbrace{kt}_{}$ X_M

STARTING POINT $\to$ POPULATION MODEL $\vec{X}_i$, $(\vec{v}_j, r_j(\vec{X}))$ $\quad \cancel{-1 \cdot \vec{e}_M} + \cancel{1 \cdot \vec{e}_M} + 1 \cdot \vec{e}_P$

$V = \vec{e}_P$

1) RRE, FLUID EQUATIONS

$$\frac{d\vec{X}}{dt} = \sum_j \vec{v}_j \cdot r_j(\vec{X}) \qquad \begin{cases} d\vec{x} = \sum_j \vec{v}_j \cdot \underbrace{r_j(\vec{x})\,dt} \end{cases} \leftarrow \text{AVERAGE "VARIATION" OF } \vec{X}.$$

$\approx$ prob of reaction j in state $\vec{X}$.

variation due to reaction j

DRIFT

2) CONCENTRATION AND SCALING.

$$\text{Volume} \cdot \underset{\text{AVOGADRO \#}}{N_A} = \gamma \qquad \vec{x} = \vec{X}/\gamma \quad \text{concentration (moles}/\ell)$$

X numerosità $\quad x$ concentration

$$\frac{dx}{dt} = \frac{1}{\gamma}\frac{dX}{dt} = \frac{1}{\gamma}\sum_j v_j r_j(\vec{X}) = \sum_j v_j \left[\frac{r_j(X)}{\gamma}\right] f_j(x)$$

$$\boxed{\begin{aligned} K &:= \gamma C \\ C &= \frac{K}{\gamma} \end{aligned}}$$

$$a = \frac{A}{\gamma} \Downarrow A = a \cdot \gamma \qquad f_j(x) := \frac{r_j(\gamma \overset{X}{x})}{\gamma}$$

$A + B \to \emptyset \qquad r(A,B) = c \cdot A \cdot B$

$$f(a,b) = \frac{1}{\gamma} \cdot c \cdot \gamma a \cdot \gamma b = \gamma \cdot c \cdot a \cdot b$$

	MASS ACTION, POP	CONC.
$\emptyset \to ?$ ordine 0	$\gamma \cdot K$	K
$X \to ?$ ordine 1	$K X$	$K \cdot X$
$X + Y \to ?$ ordine 2	$\frac{K}{\gamma} \cdot X \cdot Y$	$K \cdot x \cdot y$

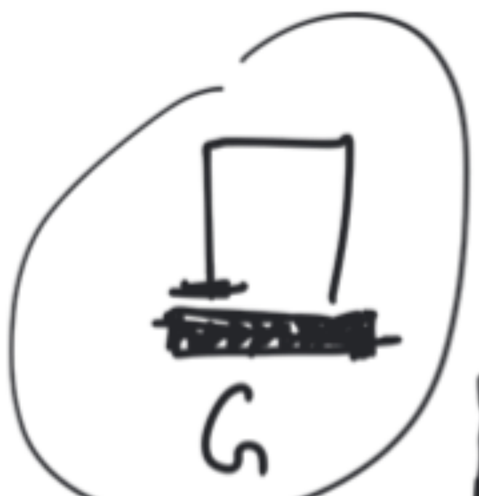
$$K \cdot X = \frac{1}{\gamma} c \cdot X = \frac{1}{\cancel{\gamma}} \cdot c \cdot \cancel{\gamma} \cdot x \Rightarrow K = c$$

Example: gene networks

⊣ repressione

→ attivazione (enhancement)

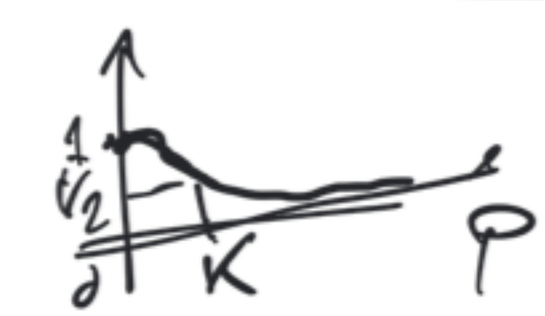
Self repressing gene module



Choices: - explicit/implicit gene
- explicit/implicit mRNA

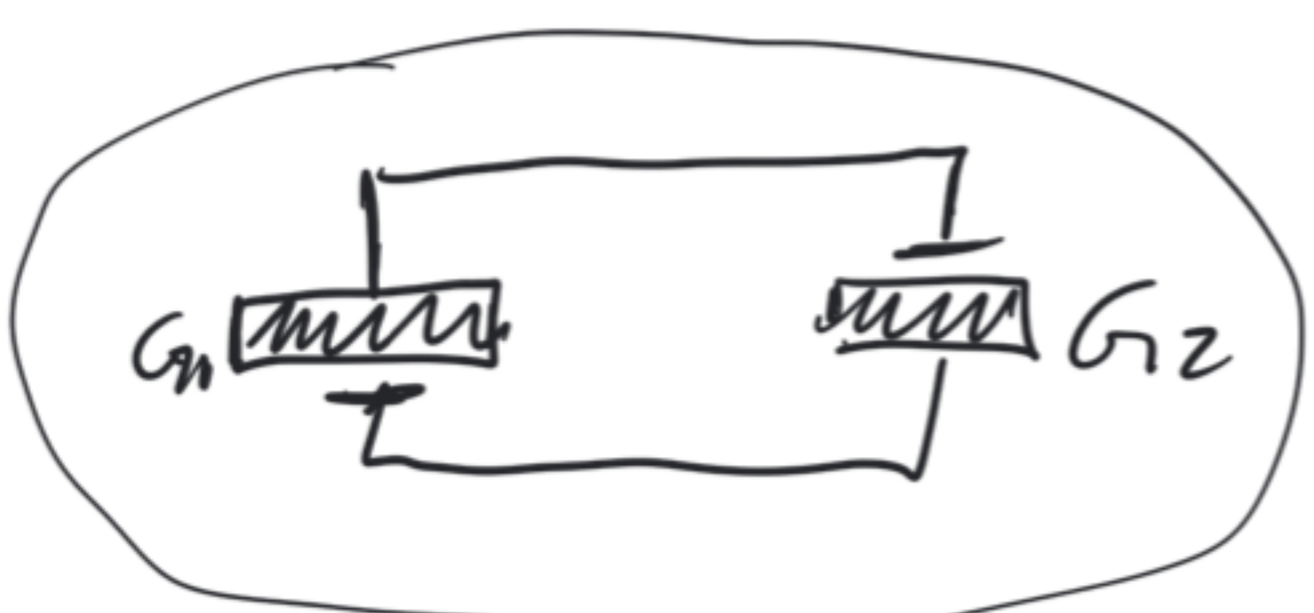
G = gene on
Go: complex G and P
M = mRNA
P = protein

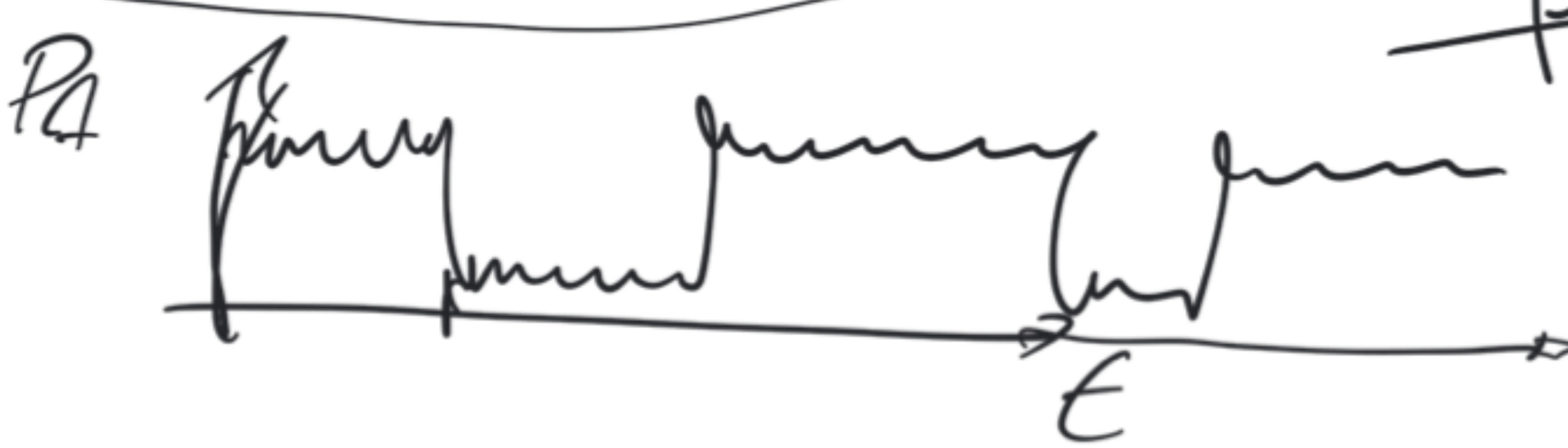
eG, eR mass action	eG, iR, mass action	iG, iR Hill
$G \to G+M$, K_p	$G \to G+P$, K_p	$\emptyset \to P$, $K_p \cdot \frac{1}{K^n+P^n}$
$M \to M+P$, K_t	$P \to \emptyset$, k_d	$P \to \emptyset$, k_d
$M \to \emptyset$, K_{dm}	$G+P \to G_o$, K_b	
$P \to \emptyset$, K_{dp}	$G_o \to G+P$, K_u	
$G+P \to G_o$, K_b		
$G_o \to G+P$, K_u		



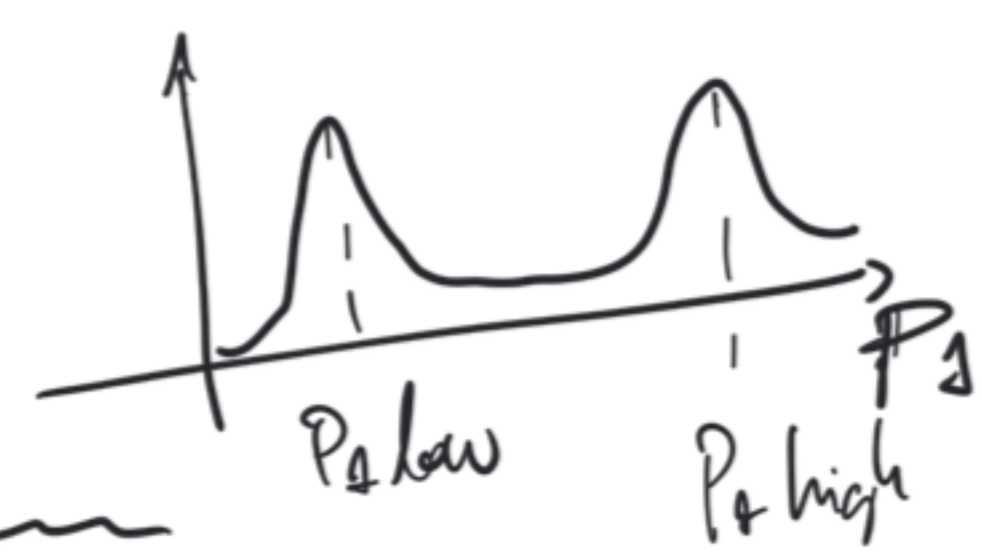
$K_p \frac{P^n}{K^n+P^n}$, activation

Bistable switch



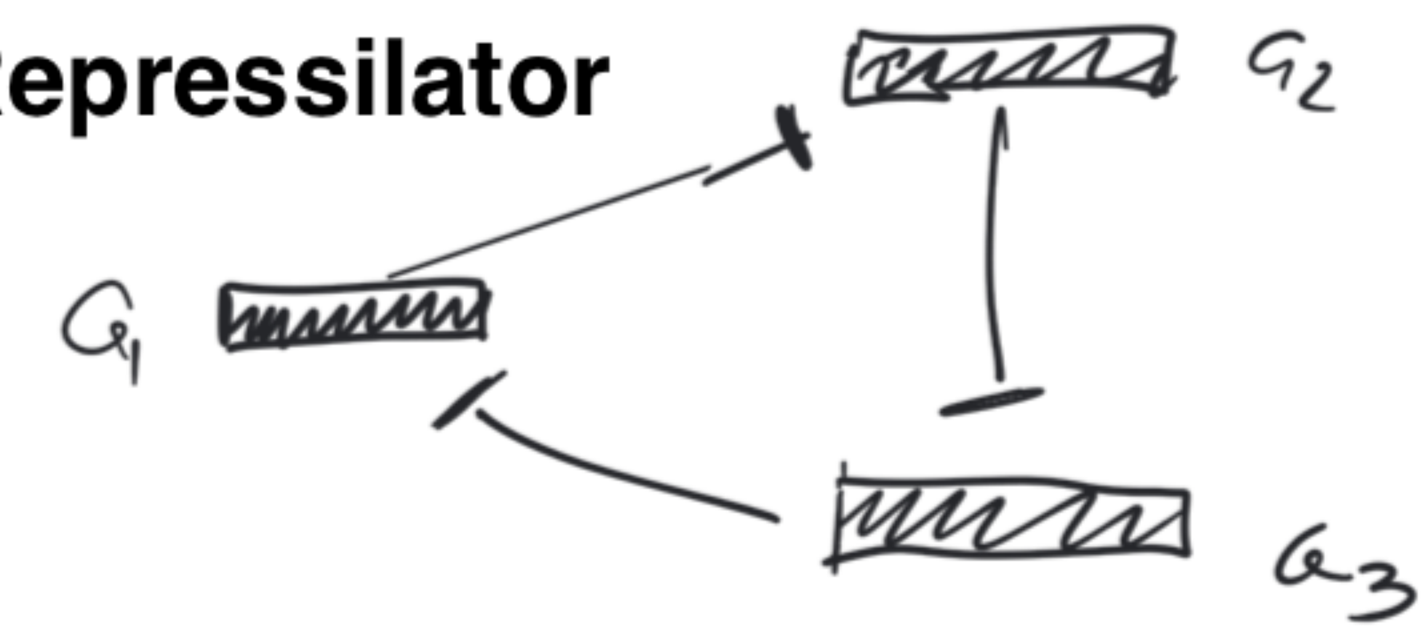


CTMC

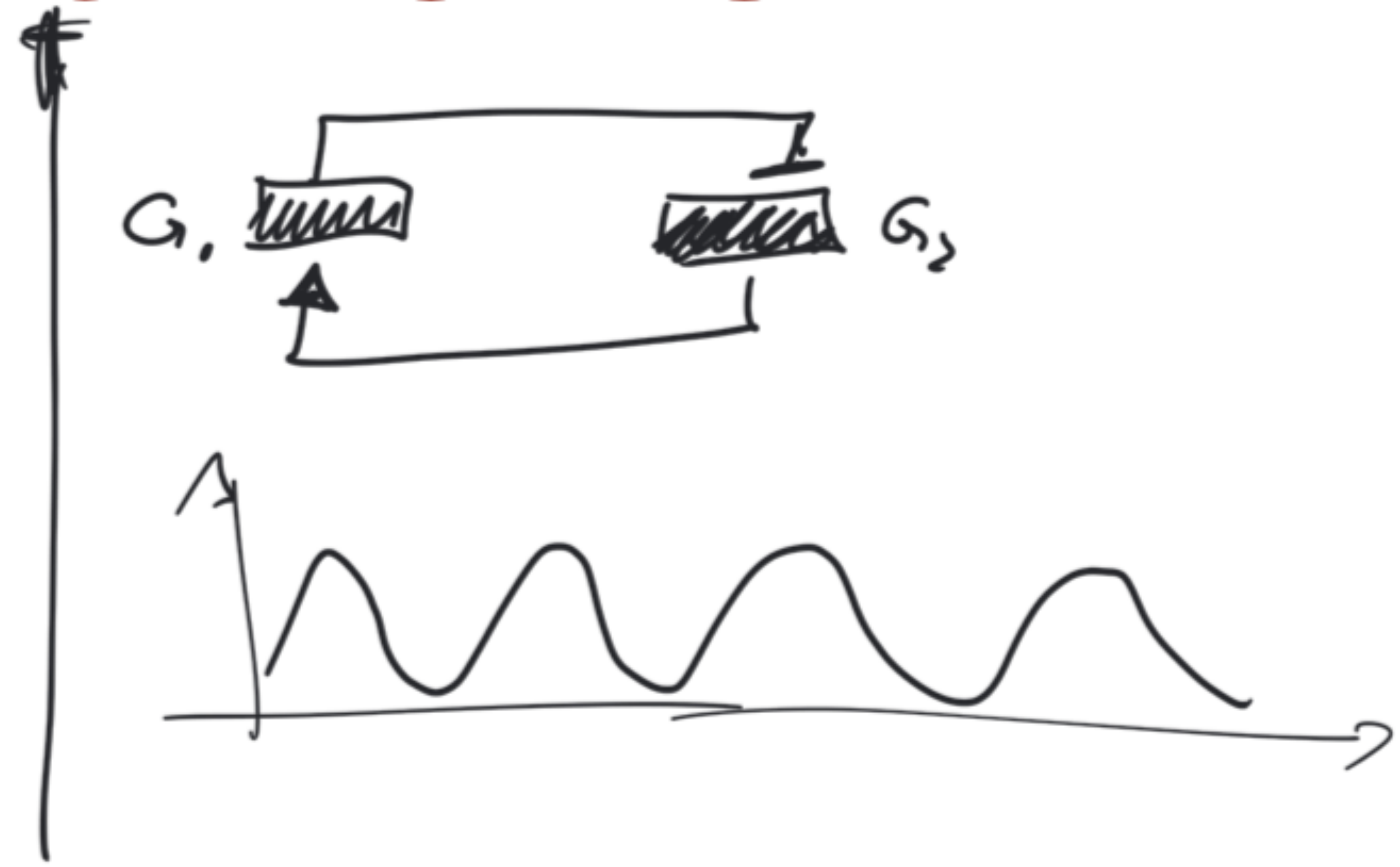


Example: gene networks

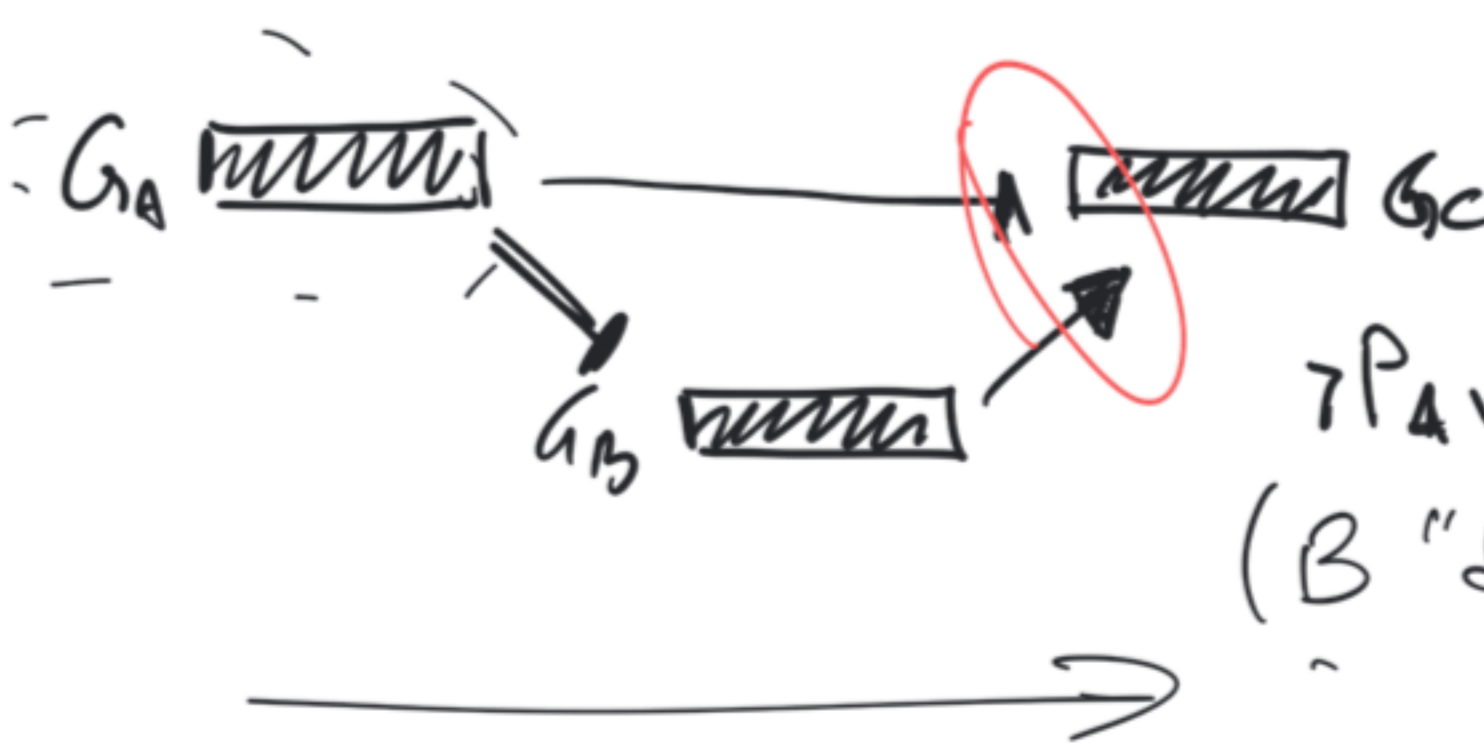
Repressilator



Periodic trajectory

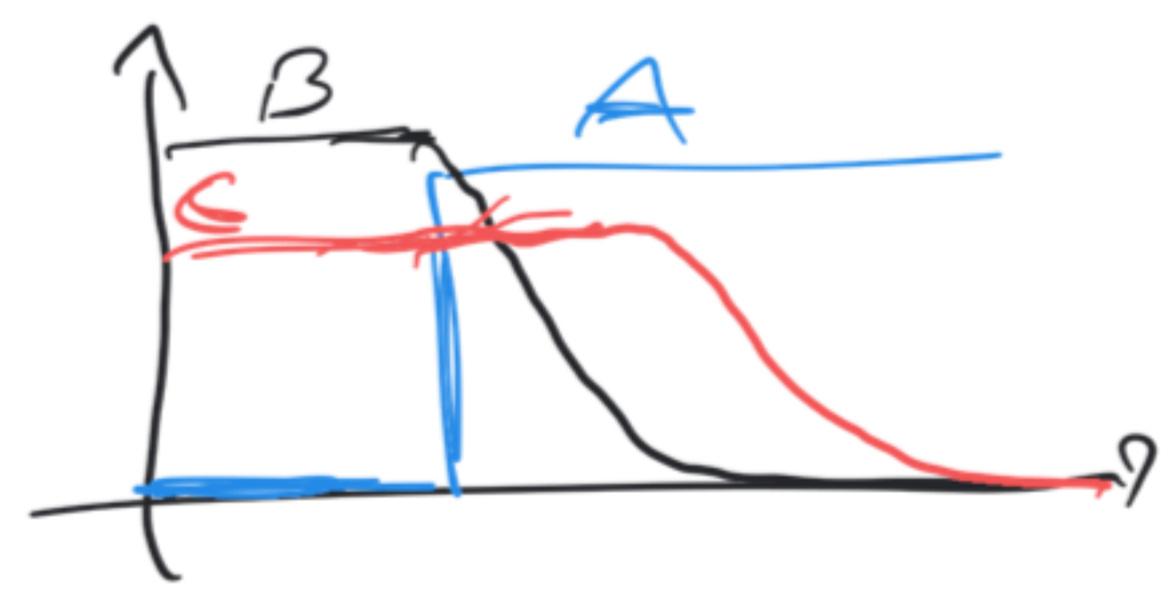


Feed Forward Loops



$\neg P_A \vee P_B \implies$ expression

(B "douwa" A)



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