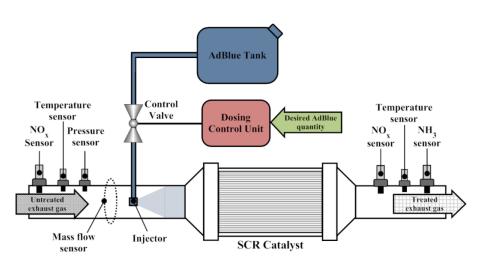
Systematic Catalytic Reduction by Reinforcement Learning

Chris Guiver, Baruch Gutierrez, Allen Hart, James Hook, Uwe Martin, Jordan Taylor

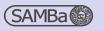
June 14, 2019

The Problem





Original Model



$$\frac{d}{dt}c_{NO,k} = \frac{n}{V_c \cdot \varepsilon_g} \cdot \frac{\hat{m}_{EG} \cdot R}{p_{EG} \cdot M_{EG}} \left(T_{EG,k-1} \cdot c_{NO,k-1} - T_{c,k} \cdot c_{NO,k} \right) + \\ + a_R \left(-4 \cdot r_{std,k} - 2 \cdot r_{fst,k} - r_{NO,g,k} \right)$$

$$\frac{d}{dt}c_{NO_2,k} = \frac{n}{V_c \cdot \varepsilon_g} \cdot \frac{\hat{m}_{EG} \cdot R}{p_{EG} \cdot M_{EG}} \left(T_{EG,k-1} \cdot c_{NO_2,k-1} - T_{c,k} \cdot c_{NO_2,k} \right) + \\ + a_R \left(-2 \cdot r_{fst,k} - 6 \cdot r_{slw,k} + r_{NO,g,k} \right)$$

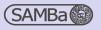
$$\frac{d}{dt}c_{NH_3,k} = \frac{n}{V_c \cdot \varepsilon_g} \cdot \frac{\hat{m}_{EG} \cdot R}{p_{EG} \cdot M_{EG}} \left(T_{EG,k-1} \cdot c_{NH_3,k-1} - T_{c,k} \cdot c_{NH_3,k} \right) + \\ + a_R \left(-r_{ad,k} + r_{de,k} - 4 \cdot r_{ox,g,k} \right)$$

$$\frac{d}{dt}c_{O_2,k} = \frac{n}{V_c \cdot \varepsilon_g} \cdot \frac{\hat{m}_{EG} \cdot R}{p_{EG} \cdot M_{EG}} \left(T_{EG,k-1} \cdot c_{O_2,k-1} - T_{c,k} \cdot c_{O_2,k} \right) + \\ + a_R \left(-0.5 \cdot r_{NO,g,k} \right)$$

$$\frac{d}{dt}\theta_{NH_3,k} = \frac{1}{\Theta_{NH_3}} \left(r_{ad,k} - r_{de,k} - 4 \cdot r_{std,k} - 4 \cdot r_{fst,k} - 8 \cdot r_{slw,k} - 4 \cdot r_{ox,k} \right)$$

$$\frac{d}{dt}T_{c,k} = \frac{n}{m_c \cdot c_{p,c}} \left(\hat{m}_{EG} \cdot c_{p,EG} \cdot \left(T_{EG,k-1} - T_{c,k} \right) + \alpha_c \cdot a_c \cdot \left(T_{Amb} - T_{c,k} \right) \right)$$

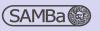
Simplified Model

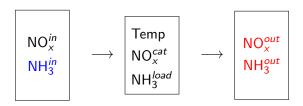


$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}t}\mathsf{T} &= -a(\mathsf{T}-200) + b\mathsf{NO}_x^{in} \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathsf{NO}_x^{cat} &= \mathsf{NO}_x^{in} - \mathsf{NO}_x^{out} - \alpha R(\mathsf{T},\mathsf{NO}_x^{cat},\mathsf{NH}_3^{load}) \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathsf{NH}_3^{load} &= \mathsf{NH}_3^{in} - \mathsf{NH}_3^{out} - R(\mathsf{T},\mathsf{NO}_x^{cat},\mathsf{NH}_3^{load}) \end{split}$$

$$R(\mathsf{T},\mathsf{NO}_{\scriptscriptstyle X}^{\mathit{cat}},\mathsf{NH}_{3}^{\mathit{load}}) = f(\mathsf{T})\mathsf{NO}_{\scriptscriptstyle X}^{\mathit{cat}}\mathsf{NH}_{3}^{\mathit{load}}$$

Simplified Model





Challenge: Correctly control the amount of NH_3^{in} injected into the system at every time step t.

Challenge



Challenge: Correctly control the amount of NH_3^{in} injected into the system at every time step t.

Idea: Use Reinforcement-Learning to train a controller capable of correctly deciding the optimal amount.

Q-Learning

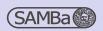


Reinforcement Learning involves an agent, moving through a state space, \mathcal{S} , by selecting an action from an action space, \mathcal{A} , at each state.

Given we are at some state $s_t \in \mathcal{S}$, taking an action $a_t \in \mathcal{A}$ provides the agent with the reward r = r(s, a) and new state s_{t+1} .

The aim of the agent is to maximise the total (future) reward.

Chess Example



Q-Learning



Idea:

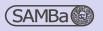
$$Q(s,a) \approx \mathbb{E} \left[\text{future discounted sum of rewards if we start at state} \\ \text{and then follow current policy for the rest of time} \\ \text{Ideally:} \right]$$

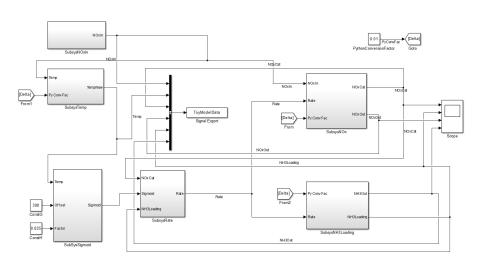
$$Q(s_t, a_t) = r_t + \gamma \max_{a} \mathbb{E}[Q(s_{t+1}, a)]$$

The objective of the training is to update Q iteratively to take into account future values of Q, i.e. to correctly reflect the value of rewards available after multiple actions.

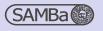
$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) - \alpha \left(Q(s_t, a_t) - r_t - \gamma \cdot \max_{a} \mathbb{E}[Q(s_{t+1}, a)] \right)$$

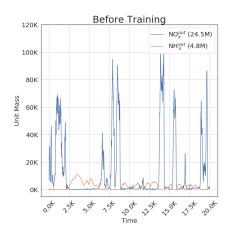
Toy Model in Simulink

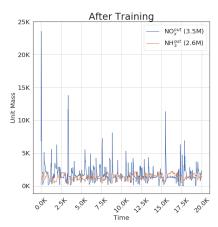




Results I - Output Gases

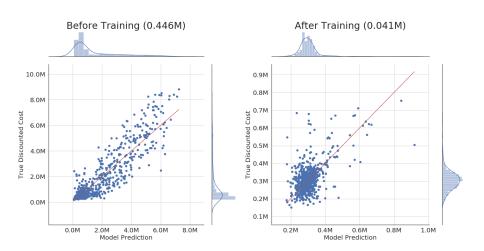




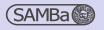


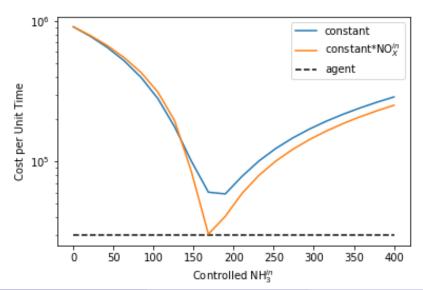
Results II - Predicted vs True Discounted Cost (SAMBa



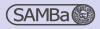


Results III - Comparison of Policies





Remarks



Pros

- Our agent can learn a policy governed by a system of differential equations without seeing them.
- Ability to have "online" learning to cater policy to the user.
- Cheap evaluation to determine appropriate control.

Cons

- A parameter space to search i.e. discount factor γ , learning rate α , and exploration rate ϵ .
- Long training time.

Future

- Tune the toy model to be more realistic.
- Use the original set of differential equations.
- Allow noisy measurements.