

# Inverse design for the chromatography system

Nicola De Nitti

Joint work with G. M. Coclite, C. Donadello, and F. Peru

FAU Erlangen-Nürnberg (Germany)

August 2, 2023

$$(C) \quad \begin{cases} \partial_t u_1 + \partial_x \left( \frac{u_1}{1 + u_1 + u_2} \right) = 0, & t > 0, x \in \mathbb{R}, \\ \partial_t u_2 + \partial_x \left( \frac{u_2}{1 + u_1 + u_2} \right) = 0, & t > 0, x \in \mathbb{R}, \\ u_1(0, x) = \bar{u}_1(x), & x \in \mathbb{R}, \\ u_2(0, x) = \bar{u}_2(x), & x \in \mathbb{R}, \end{cases}$$

where  $u_1, u_2 \in \mathbb{R}_+$  are the components' concentrations.

[Bianchini, *SIMA* 2001]: For any initial condition  $\bar{u}_1, \bar{u}_2 \in L^\infty(\mathbb{R})$ , the Cauchy problem (C) admits a unique *entropy admissible solution*.

In particular, the system admits a *continuous semi-group of solutions*

$$\begin{aligned} S^+ : \quad \mathbb{R}_+ \times L^\infty(\mathbb{R}; \mathbb{R}^2) &\rightarrow L^1_{\text{loc}}(\mathbb{R}; \mathbb{R}^2) \\ (t, U_0 = (\bar{u}_1, \bar{u}_2)) &\mapsto S_t^+(U_0). \end{aligned}$$

Using the change of variables

$$v := u_1 + u_2 \quad \text{and} \quad w := u_1 - u_2,$$

the system (C) reduces to the coupling between a scalar conservation law and a linear continuity equation:

$$(T) \quad \begin{cases} \partial_t v + \partial_x \left( \frac{v}{1+v} \right) = 0, & t > 0, x \in \mathbb{R}, \\ \partial_t w + \partial_x \left( \frac{w}{1+v} \right) = 0, & t > 0, x \in \mathbb{R}, \\ v(0, x) = \bar{u}_1(x) + \bar{u}_2(x), & x \in \mathbb{R}, \\ w(0, x) = \bar{u}_1(x) - \bar{u}_2(x), & x \in \mathbb{R}. \end{cases}$$

Triangular system: scalar conservation law + transport equation with OSL velocity.

[Panov, *Springer* 2008]: Let us consider the (more general) problem

$$(P) \quad \begin{cases} \partial_t(A\rho) + \partial_x(B\rho) = 0, & t > 0, x \in \mathbb{R}, \\ A(0, x)\rho(0, x) = A(0, x)\rho_0(x), & x \in \mathbb{R}, \end{cases}$$

under the assumptions

- 1  $A$  and  $B$  in  $L^\infty(\mathbb{R}_+ \times \mathbb{R})$ ;
- 2  $\partial_t A + \partial_x B = 0$  in  $\mathcal{D}'((0, +\infty) \times \mathbb{R})$ ;
- 3 there exists  $N : \mathbb{R} \rightarrow \mathbb{R}$  such that  $\varepsilon N(\varepsilon) \rightarrow 0$  as  $\varepsilon$  tends to zero and for all  $\varepsilon > 0$ ,  $|B| \leq N(\varepsilon)(A + \varepsilon)$  a.e. in  $(0, +\infty) \times \mathbb{R}$ ;
- 4  $\text{ess-lim}_{t \rightarrow 0^+} A(t, \cdot) = A(0, \cdot)$  in  $L^1_{\text{loc}}(\mathbb{R})$  and  $A(0, \cdot) \in L^\infty(\mathbb{R})$ .

For any given bounded initial condition  $\rho_0$ , there exists a bounded function  $\rho$ , called *generalized solution* of (P), such that, for any test function  $\varphi$  in  $C_0^\infty([0, +\infty) \times \mathbb{R})$ ,

$$\int_0^{+\infty} \int_{\mathbb{R}} \left( (A\rho)\partial_t\varphi + (B\rho)\partial_x\varphi \right) dx dt + \int_{\mathbb{R}} A(0, x)\rho_0(x)\varphi(0, x) dx = 0.$$

Moreover, every generalized solution  $\rho$  enjoys the following properties.

**Strong traces** The initial condition is satisfied in the sense that in  $L^1_{\text{loc}}(\mathbb{R})$

$$\text{ess-}\lim_{t \rightarrow 0^+} A(t, x)\rho(t, x) = A(0, x)\rho_0(x),$$

and for all  $T > 0$ , there exists  $\text{ess-}\lim_{t \rightarrow T^-} A(t, x)\rho(t, x)$  in  $L^1_{\text{loc}}(\mathbb{R})$ .

**Reversibility** If  $\rho$  is a generalized solution of problem (P) and the identity  $A(T, x)\rho(T, x) = A(0, x)\rho_0(x)$  holds in the sense of strong traces, then  $t \mapsto \rho(T-t)$  is a generalized solution of

$$(P1) \quad \begin{cases} \partial_t(A\rho) - \partial_x(B\rho) = 0, & t > 0, x \in \mathbb{R}, \\ A(0, x)\rho(0, x) = A(0, x)\rho_0(x), & x \in \mathbb{R}. \end{cases}$$

**Uniqueness** If  $A(0, x)\rho_0(x) = 0$  a.e. on  $\mathbb{R}$  then  $A(t, x)\rho(t, x) = 0$  a.e. on  $\mathbb{R}_+ \times \mathbb{R}$ .

**Renormalization** for any function  $\mu$  in  $C(\mathbb{R})$  the function  $\mu \circ \rho$  satisfies

$$(P2) \quad \begin{cases} \partial_t(A(\mu(\rho))) + \partial_x(B(\mu(\rho))) = 0, & t > 0, x \in \mathbb{R}, \\ (\mu(\rho))(0, x) = \mu(\rho_0(x)), & x \in \mathbb{R}, \end{cases}$$

in the sense of distributions.

In the case of system (T), the scalar equation

$$(CS) \quad \partial_t v + \partial_x \left( \frac{v}{1+v} \right) = 0, \quad t > 0, x \in \mathbb{R},$$

admits a unique entropy solution in  $L^\infty(\mathbb{R}_+ \times \mathbb{R})$  starting from any initial condition  $v_0 \in L^\infty(\mathbb{R})$ .

This allows us to define the divergence-free vector field  $t \mapsto (A(t, x), B(t, x))$ , for  $A(t, x) = v(t, x)$  and  $B(t, x) = \frac{v(t, x)}{1+v(t, x)}$ , satisfying all of the hypothesis above.

Then Panov's theorem guarantees that, for any given  $z_0 \in L^\infty(\mathbb{R})$ , there exists a unique generalized solution in  $L^\infty(\mathbb{R}_+ \times \mathbb{R})$  of

$$(TP) \quad \begin{cases} \partial_t(vz) + \partial_x \left( \frac{vz}{1+v} \right) = 0, & t > 0, x \in \mathbb{R}, \\ z(0, x) = z_0(x), & x \in \mathbb{R}. \end{cases}$$

From this, we can recover the solution for the chromatography system in the form (T) and (C):

- the solution  $w$  of the transport equation appearing in (T) can be seen as  $w = vz$  if we set  $z_0 = (\bar{u}_1 - \bar{u}_2)/v_0$ ;
- the solution  $(u_1, u_2)$  of (C) can be seen as  $(u_1 = vz_1, u_2 = vz_2)$  if  $z_i$  (for  $i \in \{1, 2\}$ ) is the solution of (TP) corresponding to the initial condition  $z_{0,i} = \bar{u}_i/v_0$ .

In both cases, since the  $z$  satisfies the maximum principle and we consider  $v_0 = \bar{u}_1 + \bar{u}_2$  with  $\bar{u}_i \geq 0$ , we have that  $\|z\|_{L^\infty(\mathbb{R})} \leq 1$ .

## Definition 1 (Solution of the chromatography system in the form (C))

Let  $\bar{U} = (\bar{u}_1, \bar{u}_2) \in L^\infty(\mathbb{R}; \mathbb{R}^2)$  be the initial conditions imposed to the system (C). A function  $U = (u_1, u_2) \in L^\infty((0, T) \times \mathbb{R}; \mathbb{R}^2)$  is a *strong generalized entropy solution* for the system (C) if

$$U = \left( \frac{v+w}{2}, \frac{v-w}{2} \right), \text{ where}$$

- the function  $v$  is the Kruřkov entropy solution of

$$(CS) \quad \begin{cases} \partial_t v + \partial_x \left( \frac{v}{1+v} \right) = 0, & t \in (0, T), x \in \mathbb{R}, \\ v(0, x) = \bar{u}_1(x) + \bar{u}_2(x), & x \in \mathbb{R} :=; \end{cases}$$

- the function  $w$  is given by  $w = vz$ , where  $z$  is the solution of (TP) in the weak sense with initial datum  $z_0(x) = \frac{\bar{u}_1(x) - \bar{u}_2(x)}{\bar{u}_1(x) - \bar{u}_2(x)}$  and coefficients  $A = v$  and  $B = \frac{v}{1+v}$ .

In the above definition, the value of  $\frac{\bar{u}_1(x) - \bar{u}_2(x)}{\bar{u}_1(x) - \bar{u}_2(x)}$  can be taken arbitrary  $\pm 1$  at points where  $\bar{U} = 0$ .



## Definition 2 (Renormalized entropy solution of the chromatography system in the form (C))

The function  $U \in L^\infty((0, T) \times \mathbb{R}; \mathbb{R}^2)$  is a renormalized entropy solution for the system (T) if

- the function  $v$  is the Kružkov entropy solution of (CS);
- the function  $w$  is given by  $w = zv$  where, for any test function  $\varphi \in C_0^\infty([0, T) \times \mathbb{R})$  and any continuous function  $\mu$ ,  $z$  satisfies

$$\int_0^T \int_{\mathbb{R}} \left( v\mu(z)\partial_t\varphi + \frac{1}{1+v}\mu(w)\partial_x\varphi \right) dx dt + \int_{\mathbb{R}} v(0, x)\mu(z_0(x))\varphi(0, x) dx = 0.$$

## Entropy/entropy-flux pairs

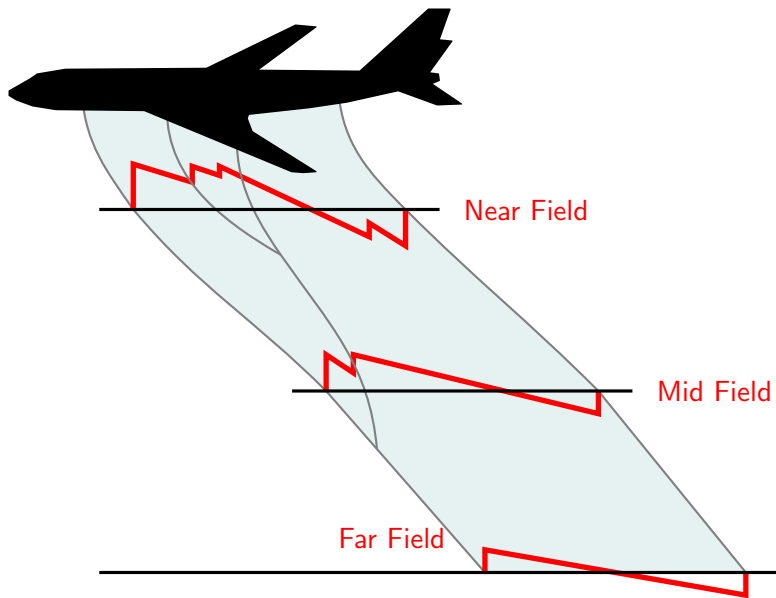
The entropy/entropy-flux pairs for the systems (T) take the following form:

$$\begin{aligned}\mathcal{E}(v, w) &:= \eta(v) + v\mu\left(\frac{w}{v}\right), \\ \mathcal{Q}(v, w) &:= q(v) + \frac{v}{1+v}\mu\left(\frac{w}{v}\right),\end{aligned}$$

where  $\eta$  is any entropy function for (CS) and  $\mu \in C(\mathbb{R})$ . Therefore, the strong generalized entropy solutions coincide with the entropy solutions for the system.

- 1 for any given  $T > 0$ , characterize the set of profiles  $U_T = (u_1^T, u_2^T) \in L^\infty(\mathbb{R}; \mathbb{R}^2)$  for which there exists at least one initial condition  $(\bar{u}_1, \bar{u}_2) \in L^\infty(\mathbb{R}; \mathbb{R}^2)$  such that  $S_T^+(\bar{u}_1, \bar{u}_2) = (u_1^T, u_2^T)$ ;
- 2 for each of such attainable profiles, characterize the set of initial data leading to them,  $\mathfrak{I}(U_T)$ ;
- 3 for profiles that cannot be attained by a trajectory of the system, recover the initial data leading to their “best possible approximation”.

# Sonic-boom minimization and inverse design for the Burgers' equation



The set of states in  $L^\infty(\mathbb{R})$  attainable by Kružkov entropy solutions at time  $T > 0$  to scalar conservation laws with strictly convex flux was characterized in [Ancona–Marson, *SICON* 1998] as follows:

$$(AS) \quad \mathcal{A}_T(\mathbb{R}, f) = \left\{ u \in L^\infty(\mathbb{R}) : \exists \rho : \mathbb{R} \rightarrow \mathbb{R}, \text{ right continuous,} \right. \\ \left. \text{non-decreasing such that } f'(u) = \frac{x - \rho(x)}{T} \right\}$$

### Oleinik's condition

Furthermore, for every  $u_T \in \mathcal{A}_T(\mathbb{R}, f)$ , there exists a unique *isentropic solution*  $u : [0, T] \times \mathbb{R} \rightarrow \mathbb{R}$  that verifies  $u(T, \cdot) = u_T$ .

# Scalar problem: backward reconstruction

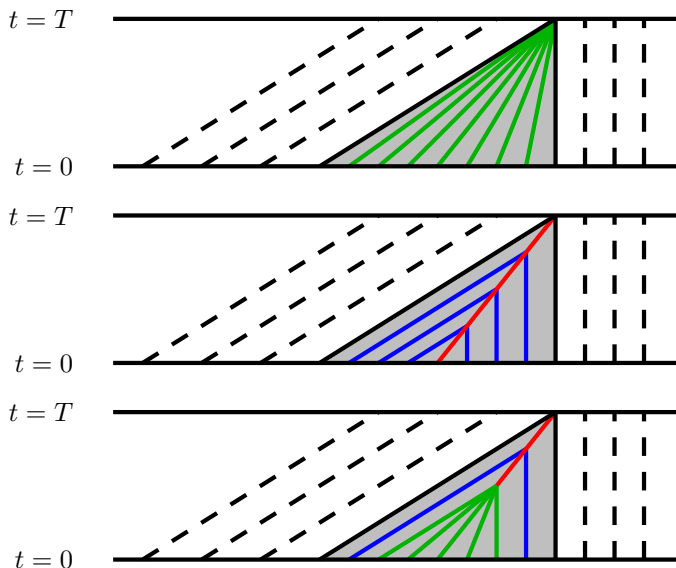


Figure: Multiple initial data may lead to the same target profile.

[Colombo–Perrollaz, *JMPA* 2020] & [Liard–Zuazua, *IEEE* 2021] characterized the set of inverse designs as follows.

## Theorem 3 (Inverse design for scalar conservation laws)

Let us consider a strictly convex scalar conservation law, fix  $T > 0$ , and let  $v_T \in \mathcal{A}_T(\mathbb{R}, f)$ . Then, the initial data  $\tilde{u}_0 \in L^\infty(\mathbb{R})$  verifies  $\mathcal{S}_T^+(\tilde{u}_0) = u_T$  if and only if the following statement holds:

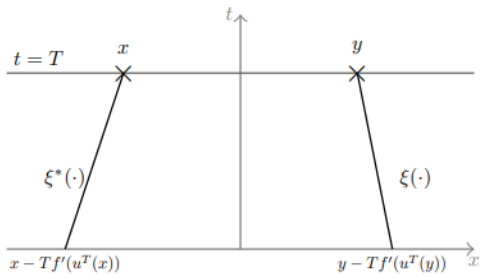
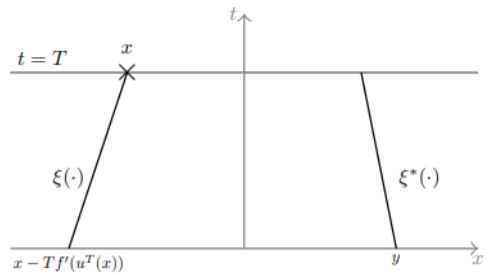
1) for any  $(x, y) \in X(u_T) \times \mathbb{R}$

$$(1) \quad \int_{x-Tf'(u_T(x))}^y \mathcal{S}_T^-(u_T)(s) \, ds \leq \int_{x-Tf'(u_T(x))}^y \tilde{u}_0(s) \, ds,$$

2) for any  $(x, y) \in X(u_T)^2$

$$(2) \quad \int_{x-Tf'(u_T(x))}^{y-Tf'(u_T(y))} \mathcal{S}_T^-(u_T)(s) \, ds = \int_{x-Tf'(u_T(x))}^{y-Tf'(u_T(y))} \tilde{u}_0(s) \, ds,$$

where  $X(u_T)$  is the set of points of approximate continuity of  $u_T$ .



[Andreianov–Donadello–Ghoshal–Shyam–Razafison, *J. Evol. Eq.* 2015]: The set of states in  $L^\infty(\mathbb{R})$  that are attainable by entropy solutions of system (T) is given by

$$(AT) \quad \mathfrak{A}_T(\mathbb{R}) = \mathcal{A}_T(\mathbb{R}, f) \times L^\infty(\mathbb{R}).$$

**NB:** A generic element of the set of the attainable profiles for (T) at time  $T > 0$ ,

$$\mathfrak{A}_T(\mathbb{R}) = \left\{ (v_T, w_T) : v_T \in \mathcal{A}_T \left( \mathbb{R}, v \mapsto \frac{v}{1+v} \right) \text{ and } w_T \in L^\infty(\mathbb{R}) \right\},$$

does not correspond to an attainable profile for the system (C) because it might happen that  $((v_T + w_T)(x), (v_T - w_T)(x))$  is not in  $\mathbb{R}_+^2$  for almost every  $x \in \mathbb{R}$ , while all physically relevant solutions of (C) are in  $L^\infty(\mathbb{R}_+ \times \mathbb{R}; \mathbb{R}_+^2)$ .

Therefore, we define

$$\mathcal{A}_T(\mathbb{R}) = \left\{ (v_T, w_T) : v_T \in \mathcal{A}_T \left( \mathbb{R}, v \mapsto \frac{v}{1+v} \right) \text{ and there exists } z \in L^\infty(\mathbb{R}_+ \times \mathbb{R}; [-1, 1]) \text{ such that } w_T = zv_T \right\}$$

and we say that  $U_T = (u_1^T, u_2^T)$  is attainable for system (C) if and only if  $(v_T := u_1^T + u_2^T, w_T = u_1^T - u_2^T) \in \mathcal{A}_T$ .



## Theorem 4 (Characterization and properties of the set of inverse designs)

- 1) Given  $U_T = (u_1^T, u_2^T) \in L^\infty(\mathbb{R}; \mathbb{R}_+^2)$  such that  $V_T = (v_T = u_1^T + u_2^T, w_T = u_1^T - u_2^T) \in \mathfrak{A}_T(\mathbb{R})$ , the set of inverse design

$$\mathfrak{i}(U_T) = \{U_0 = (u_1^0, u_2^0) \in L^\infty(\mathbb{R}; \mathbb{R}_+) \times L^\infty(\mathbb{R}; \mathbb{R}_+) : S_T^+(U_0) = U_T\}$$

can be characterized as follows:

$$\mathfrak{i}(U_T) = \left\{ U_0 = (u_1^0, u_2^0) \in L^\infty(\mathbb{R}; \mathbb{R}_+) \times L^\infty(\mathbb{R}; \mathbb{R}_+) : \begin{array}{l} u_1^0 + u_2^0 \in \mathcal{I}(v_T) \text{ and } u_i^0 = v_0 \mathcal{S}_T^-[\mathcal{S}_*(v_0)](u_i^T / v^T), := i = 1, 2 \end{array} \right\}.$$

- 2) Given  $V_T = (v_T, w_T) \in \mathfrak{A}_T(\mathbb{R})$ , the set of inverse design

$$\mathfrak{J}(V_T) = \{V_0 \in L^\infty(\mathbb{R}) \times L^\infty(\mathbb{R}) : \mathfrak{S}_T^+(V_0) = V_T\}$$

can be characterized as follows:

$$\mathfrak{J}(V_T) = \{(v_0, w_0) \in L^\infty(\mathbb{R}) \times L^\infty(\mathbb{R}) : v_0 \in \mathcal{I}(v_T) \text{ and } w_0 = \mathcal{S}_T^-[\mathcal{S}_*(v_0)](w_T)\}.$$

In both of the above cases, the 1-to-1 correspondence between the elements of  $\mathcal{I}(v_T)$  and the elements of  $i(U_T)$  and  $\mathcal{J}(V_T)$ , together with the results on  $\mathcal{I}(v_T)$  proved in [Colombo–Perrollaz, *JMPA* 2020] yield the following properties:

- (T1) the set  $\mathcal{J}(V_T)$  is closed with respect to the  $L_{\text{loc}}^1 \times L_{\text{loc}}^1$  topology;
- (T2) the set  $\mathcal{J}(V_T)$  has empty interior with respect to the  $L_{\text{loc}}^1 \times L_{\text{loc}}^1$  topology;
- (G1) the sets  $\mathcal{J}(V_T)$  and  $i(U_T)$  reduce to a singleton if and only if  $v_T \in C(\mathbb{R})$ .

Let us describe the numerical method:

- 1 first, we use the entropic solver to get the isentropic solution of the first equation;
- 2 then, the numerical backward resolution of the transport equation is based on considering the auxiliary forward problem

$$\partial_t w + \partial_x (-g(v)w) = 0, \quad t > 0, x \in \mathbb{R},$$

where  $v$  is an entropic solution of the first equation.

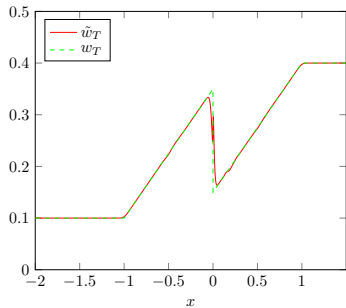
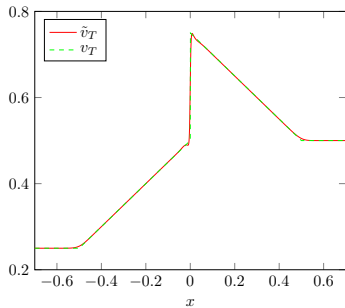
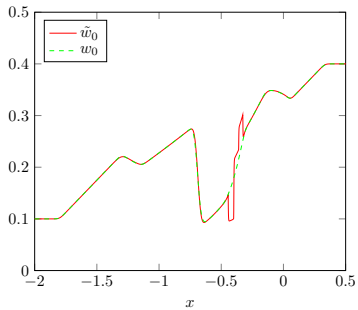
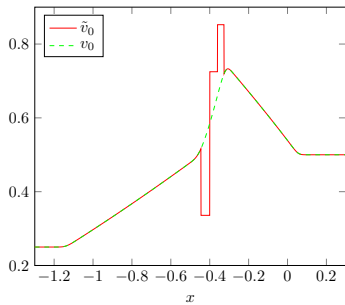
We consider

$$v_T(x) = \begin{cases} 0.25, & \text{if } x < -0.5, \\ 0.25 + 0.5(x + 0.5), & \text{if } -0.5 \leq x < 0, \\ 0.75 - 0.5, & \text{if } 0 \leq x < 0.5, \\ 0.5, & \text{if } 0.5 \leq x, \end{cases}$$

as a final state for the conservation law and

$$w_T(x) = \begin{cases} 0.1, & \text{if } x \leq -1, \\ 0.25(x + 1) + 0.1, & \text{if } -1 < x \leq 0, \\ 0.25(x - 1) + 0.4, & \text{if } 0 < x \leq 1, \\ 0.4, & \text{if } 1 < x, \end{cases}$$

as a final state for the transport equation. We choose  $\Delta x = 7.8 \times 10^{-4}$  and  $\Delta t = \Delta x/2$ .



# Unreachable profiles and an optimization problem

we fix  $T > 0$  and consider a target profile  $v_{\text{tar}} = (v_{\text{tar}}, w_{\text{tar}})$  which is *not attainable* in time  $T$  for the system (T). We assume that

$$v_{\text{tar}}(x) = \begin{cases} v^-, & \text{for } x < a, \\ \bar{v}(x), & \text{for } x \in [a, b], \\ v^+, & \text{for } x > b, \end{cases} \quad w_{\text{tar}}(x) = \begin{cases} w^-, & \text{for } x < a, \\ \bar{w}(x), & \text{for } x \in [a, b], \\ w^+, & \text{for } x > b, \end{cases}$$

for some essentially bounded functions  $\bar{v}, \bar{w}$ .

We want to characterize the initial conditions which drive the system as close as possible to  $v_{\text{tar}}$  with respect to the  $L^2$  norm. These are the minima of

$$J_0(Q_0) = \|\mathfrak{S}_T^+(Q_0) - v_{\text{tar}}\|_{L^2(\mathbb{R}; \mathbb{R}^2)},$$

where  $\mathfrak{S}_T^+(Q_0)$  belongs to the subset of  $\mathfrak{A}_T(\mathbb{R})$  defined as

$$\mathcal{U}^T(v_{\text{tar}}) = \left\{ Q = (q_1, q_2) \in L^\infty(\mathbb{R}; \mathbb{R}^2) : \right. \\ \left. q_1 \in \mathcal{A}_T(\mathbb{R}, f), \|Q\|_{L^\infty(\mathbb{R})} \leq C, \text{ and } Q - v_{\text{tar}} \in L^1(\mathbb{R}) \right\}.$$

Due to the definition of  $\mathfrak{A}_T$ , this optimization problem is equivalent to finding  $q_{1, \text{opt}}$  such that

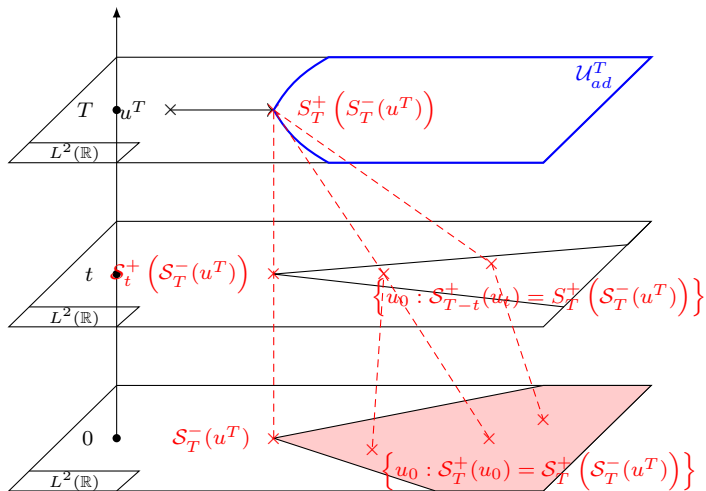
$$\text{(Opt)} \quad \|q_{1, \text{opt}} - v_{\text{tar}}\|_{L^2(\mathbb{R})} = \min_{q \in \mathcal{U}_1^T(v_{\text{tar}})} \|q - v_{\text{tar}}\|_{L^2(\mathbb{R})},$$

where the admissible set  $\mathcal{U}_1^T(v_{\text{tar}})$  is defined by

$$\mathcal{U}_1^T(v_{\text{tar}}) = \left\{ q \in L^\infty(\mathbb{R}) : q \in \mathcal{A}_T \left( \mathbb{R}, v \mapsto \frac{v}{1+v} \right), \|q\|_{L^\infty(\mathbb{R})} \leq C, \text{ and } \text{supp}(q - v_{\text{tar}}) \subset K \right\}.$$

# Backward–forward formulation

[Liard–Zuazua, *SIMA* 2023]:  $q_{1, \text{opt}} = \mathcal{S}_T^+(\mathcal{S}_T^-(v_{\text{tar}}))$ .





However,  $(q_{1, \text{opt}}, w_{\text{tar}})$  does not necessarily belong to  $\mathcal{A}_T(\mathbb{R})$  as  $q_{1, \text{opt}} - w_{\text{tar}}$  is not everywhere positive.

### Modified strategy.

- First, we associate to  $U_{\text{tar}}$  the profile  $v_{\text{tar}} = (v_{\text{tar}} = u_1^{\text{tar}} + u_2^{\text{tar}}, w_{\text{tar}} = u_1^{\text{tar}} - u_2^{\text{tar}})$ .
- Then we apply the strategy above to find  $q_{1, \text{opt}}$ .
- Finally, we consider  $q_{2, \text{opt}} = \min \{q_{1, \text{opt}}, w_{\text{tar}}\}$  so to obtain a second component which is as close as possible to  $w_{\text{tar}}$ , under the constraint that  $q_{1, \text{opt}} - q_{2, \text{opt}} \geq 0$ .

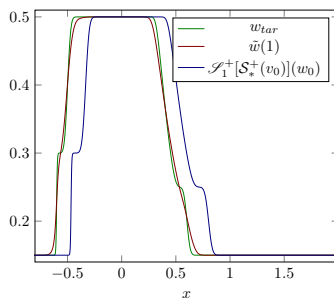
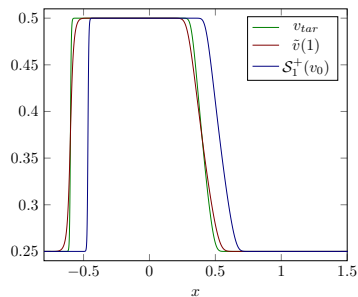
The couple  $Q_{\text{opt}} = (q_{1, \text{opt}}, q_{2, \text{opt}})$  is in  $\mathcal{A}_T(\mathbb{R})$ , so that the profile attainable at time  $T$  for (C) which is the closest to  $U_{\text{tar}}$  in  $L^2$  is

$$U_{\text{opt}} = \left( \frac{1}{2}(q_{1, \text{opt}} + q_{2, \text{opt}}), \frac{1}{2}(q_{1, \text{opt}} - q_{2, \text{opt}}) \right).$$

Given the initial conditions  $V_0 = (v_0, w_0)$ , with

$$v_0(x) = \begin{cases} 0.5, & \text{if } -1 < x < 0, \\ 0.25, & \text{otherwise,} \end{cases}$$

$$w_0(x) = \begin{cases} 0.5, & \text{if } -1 < x < 0, \\ 0.15, & \text{otherwise,} \end{cases}$$



Thank you for your attention!

- [1] G. M. Coclite, N. De Nitti, C. Donadello, and F. Peru. *Inverse design and boundary controllability for the chromatography system*. HAL-04164795, 2023.