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Optimal synthesis of membrane filtration systems

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Introduction

We are interested in :

- membrane filtration systems
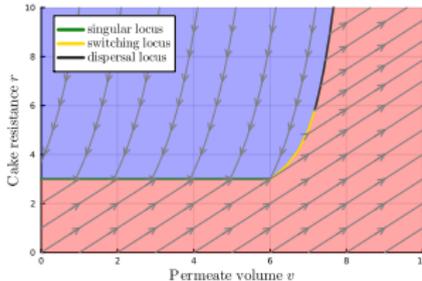- optimal feedback synthesis
- automatic generation

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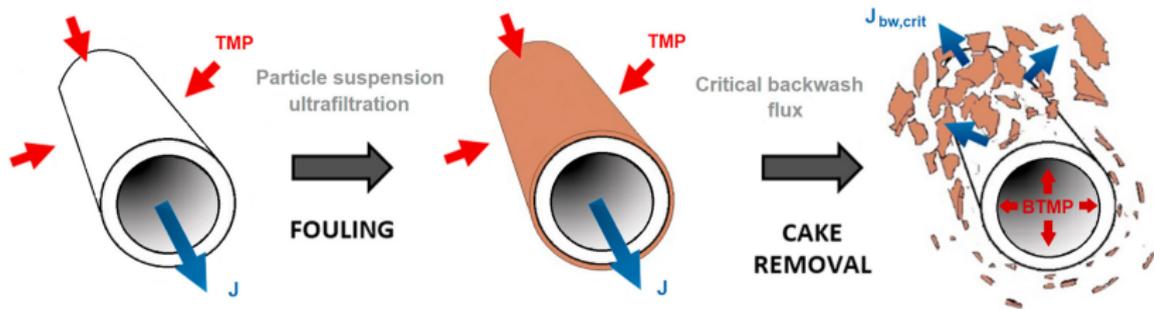
Membrane filtration systems

Figure: Extracted from [Vroman et al., 2021]

State/cost :
- r : resistance of cake layer
- v : permeate volume
- e : energy spend

Control :
- $u = +1$: filtration
- $u = -1$: backwash

Dynamics modeling

The dynamics for filtration and backwash modes are assumed to be given respectively by

- $r_+(r)$ and $r_-(r)$ for $\dot{r}$ (speed of variation of r),
- $v_+(r)$ and $v_-(r)$ for $\dot{v}$ (effective flow rate),
- $e_+(r)$ and $e_-(r)$ for $\dot{e}$ (instantaneous energy consumption).

Considering $u \in [-1, 1]$, the dynamics are modeled by

$$\begin{cases} \dot{r} = \dfrac{1+u}{2}r_+(r) + \dfrac{1-u}{2}r_-(r), \\ \dot{v} = \dfrac{1+u}{2}v_+(r) + \dfrac{1-u}{2}v_-(r), \\ \dot{e} = \dfrac{1+u}{2}e_+(r) + \dfrac{1-u}{2}e_-(r). \end{cases}$$

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Dynamics modeling

Denoting

$$r_0(r) = \frac{1}{2}\big(r_+(r) + r_-(r)\big), \qquad r_1(r) = \frac{1}{2}\big(r_+(r) - r_-(r)\big),$$

$$v_0(r) = \frac{1}{2}\big(v_+(r) + v_-(r)\big), \qquad v_1(r) = \frac{1}{2}\big(v_+(r) - v_-(r)\big),$$

$$e_0(r) = \frac{1}{2}\big(e_+(r) + e_-(r)\big), \qquad e_1(r) = \frac{1}{2}\big(e_+(r) - e_-(r)\big),$$

the dynamic of the system is

$$\begin{cases} \dot{r} = r_0(r) + u\, r_1(r) \\ \dot{v} = v_0(r) + u\, v_1(r) \\ \dot{e} = e_0(r) + u\, e_1(r) \end{cases}$$

Case #1 : Minimum energy

The goal is to minimise the energy to provide a desired volume of filtered water v_f :

$$(\#1) \quad \begin{cases} \min_{r,v,u,t_f} \int_{t_0}^{t_f} e_0(r(t)) + u(t)\, e_1(r(t))\, \mathrm{d}t, \\ \text{s.c. } \dot{r}(t) = r_0(r(t)) + u(t)\, r_1(r(t)), \\ \quad\quad \dot{v}(t) = v_0(r(t)) + u(t)\, v_1(r(t)), \\ \quad\quad u(t) \in [-1, 1], \quad t \in [t_0, t_f], \\ \quad\quad r(t_0) = R_0, \quad v(t_0) = 0, \quad v(t_f) = v_f. \end{cases}$$

Case #2 : Maximum volume

The goal is to maximise the filtered volume on a fixed time interval $[t_0, T]$:

$$(\#2) \quad \begin{cases} \max_{r,u} \int_{t_0}^{T} v_0(r(t)) + u(t)\, v_1(r(t))\, \mathrm{d}t, \\ \text{s.c. } \dot{r}(t) = r_0(r(t)) + u(t)\, r_1(r(t)), \\ \quad u(t) \in [-1, 1], \quad t \in [t_0, T], \\ \quad r(t_0) = R_0 \geq 0. \end{cases}$$

Equivalent formulation

Let us consider the following general formulation

$$(\text{OCP}) \quad \begin{cases} \displaystyle\min_{x,y,u,t_f} \int_{t_0}^{t_f} f_0(x(t)) + u(t)\, g_0(x(t))\, \mathrm{d}t, \\[2mm] \text{s.c. } \dot{x}(t) = f_1(x(t)) + u(t)\, g_1(x(t)), \\[1mm] \qquad \dot{y}(t) = f_2(x(t)) + u(t)\, g_2(x(t)), \\[1mm] \qquad u(t) \in [-1,1], \quad t \in [t_0, t_f], \\[1mm] \qquad x(t_0) = x_0, \quad y(t_0) = y_0, \quad y(t_f) = y_f, \end{cases}$$

and we denote $f = (f_0, f_1, f_2)$ and $g = (g_0, g_1, g_2)$. This problem corresponds to a class of production-regeneration systems where:

- x corresponds to the internal resistance,
- y model a target to reach or a budget constraint.

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Equivalent formulation

Case (#1) can be written as (OCP) :

(OCP)

$$
\begin{cases}
\min_{x,y,u,t_f} \int_{t_0}^{t_f} e_0(x(t)) + u(t)\, e_1(x(t))\, \mathrm{d}t, \\
\mathrm{s.c.}\ \dot{x}(t) = r_0(x(t)) + u(t)\, r_1(x(t)), \\
\quad\ \dot{y}(t) = v_0(x(t)) + u(t)\, v_1(x(t)), \\
\quad\ u(t) \in [-1, 1], \quad t \in [t_0, t_f], \\
\quad\ x(t_0) = R_0, \quad y(t_0) = 0, \quad y(t_f) = v_f,
\end{cases}
$$

with $f = (e_0, r_0, v_0)$ and $g = (e_1, r_1, v_1)$. In this case :

- x corresponds to the resistance of the cake layer,
- y corresponds to the produced volume.

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Equivalent formulation

Case (#2) can be written as (OCP) :

$$
\text{(OCP)} \quad
\begin{cases}
\displaystyle \min_{x,y,u,t_f} \int_{t_0}^{t_f} -v_0(x(t)) - u(t)\, v_1(x(t))\, \mathrm{d}t, \\[2mm]
\text{s.c. } \dot{x}(t) = r_0(x(t)) + u(t)\, r_1(x(t)), \\[1mm]
\phantom{\text{s.c. }} \dot{y}(t) = 1, \\[1mm]
\phantom{\text{s.c. }} u(t) \in [-1,1], \quad t \in [t_0, t_f], \\[1mm]
\phantom{\text{s.c. }} x(t_0) = R_0, \quad y(t_0) = t_0, \quad y(t_f) = T,
\end{cases}
$$

with $f = (-v_0, r_0, 1)$ and $g = (-v_1, r_1, 0)$. In this case :

- x corresponds to the resistance of the cake layer,
- y corresponds to the time.

Objectives

Provide optimal synthesis of (OCP) "whatever" inputs functions and initial/final conditions are.
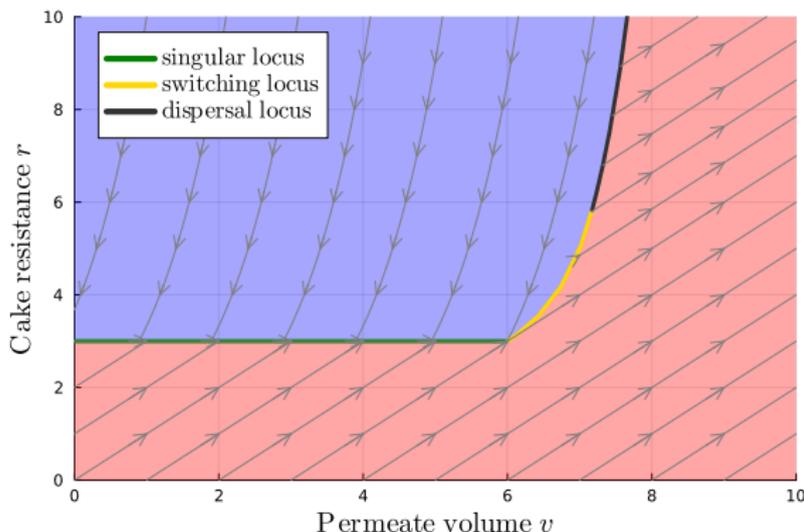

Figure: Example of optimal synthesis with trajectories for Case (#1).

Pontryagin maximum principle

If (x, y, u, t_f) is a solution of (OCP), there exists a costate $p = (-1, p_x, p_y)$ such that $p_x(t_f) = 0$, the *costate dynamic* is satisfied for almost every $t \in [t_0, t_f]$

$$\dot{p}_x(t) = -\frac{\partial H}{\partial x}(x(t), p(t), u(t)), \quad \dot{p}_y(t) = 0,$$

as well as the *maximisation condition* for almost every $t \in [t_0, t_f]$

$$\max_{w \in [-1,1]} H(x(t), p(t), w) = H(x(t), p(t), u(t)) = 0$$

where H is the *hamiltonian* given by

$$H(x, p, u) = H_0(x, p) + u H_1(x, p),$$

$$H_0(x, p) = \langle p \mid f(x) \rangle \quad \text{and} \quad H_1(x, p) = \langle p \mid g(x) \rangle$$

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Optimal control

Using the maximisation condition and the definition of H, for almost all $t \in [t_0, t_f]$, one has

$$
u(t) \begin{cases} = -1 & \text{if} \quad H_1\big(x(t), p(t)\big) < 0 \\ \in [-1, 1] & \text{if} \quad H_1\big(x(t), p(t)\big) = 0 \\ = 1 & \text{if} \quad H_1\big(x(t), p(t)\big) > 0 \end{cases}
$$

Lemma 1

There exists $\bar{t} \in [t_0, t_f[$ such that $u(t) = 1$ for almost every $t \in [\bar{t}, t_f]$.

Singular state and singular control

Let us suppose that there exists $I \subset [t_0, t_f]$ of non-zero mesure such that $H_1(x(t), p(t)) = 0$ for all $t \in I$. One has

$$H_0(x(t), p(t)) = H_1(x(t), p(t)) = 0, \qquad (1)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} H_1(x(t), p(t)) = [H_0, H_1](x(t), p(t)) = 0, \qquad (2)$$

where $[\cdot, \cdot]$ corresponds to the Poisson bracket. From (1), one has $p_x(t) = \alpha(x(t))$ and $p_y(t) = \beta(x(t))$ for all $t \in I$ where

$$\Delta(x)\,\alpha(x) = f_0(x)g_2(x) - f_2(x)g_0(x),$$
$$\Delta(x)\,\beta(x) = f_1(x)g_0(x) - f_0(x)g_1(x),$$
$$\Delta(x) = f_1(x)g_2(x) - f_2(x)g_1(x).$$

Singular state and control

By using (2) and expression of p_x and p_y, the singular state x_s is constant and must be a zero of

$$\psi(x) = -\beta'(x)\Delta(x). \tag{3}$$

Since the singular state is constant, the singular control cancels $\dot{x}$ and is thus given by

$$u_s = -\frac{f_1(x)}{g_1(x)}.$$

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Main theorem

Theorem 2

Under some hypothesis, and denoting

- *σ_- an arc associated to $u = -1$,*
- *σ_+ an arc associated to $u = +1$,*
- *σ_s an arc associated to $u = u_s$,*

the structure of an optimal solution can only be one of

$$\sigma_+, \ \sigma_-\sigma_+, \ \sigma_s\sigma_+, \ \sigma_-\sigma_s\sigma_+ \ \text{or} \ \sigma_+\sigma_s\sigma_+.$$

Use of the Green's theorem

By using the state dynamics, one can construct the 1-form

$$\big(f_0(x) + u(t)g_0(x)\big)\,\mathrm{d}t = \alpha(x)\,\mathrm{d}x + \beta(x)\,\mathrm{d}y$$
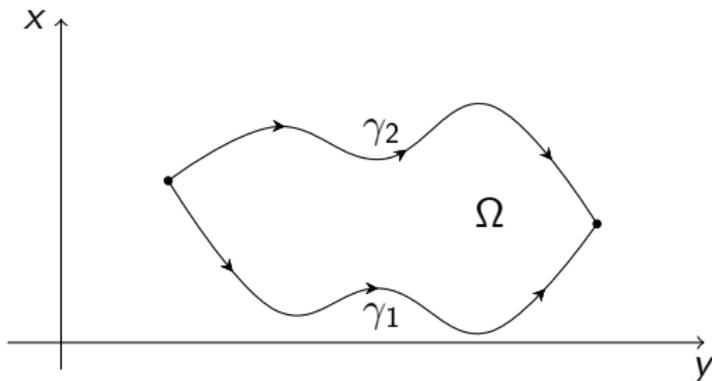
By using the Green's theorem [Miele, 1962], one has

$$J(\gamma_1) - J(\gamma_2) = \oint_{\gamma_1 \cup \gamma_2^{-1}} \alpha(x)\,\mathrm{d}x + \beta(x)\,\mathrm{d}y = \iint_\Omega -\beta'(x)\,\mathrm{d}y\,\mathrm{d}x.$$

Optimal synthesis

By finding zero of ψ, one can compute the singular curve
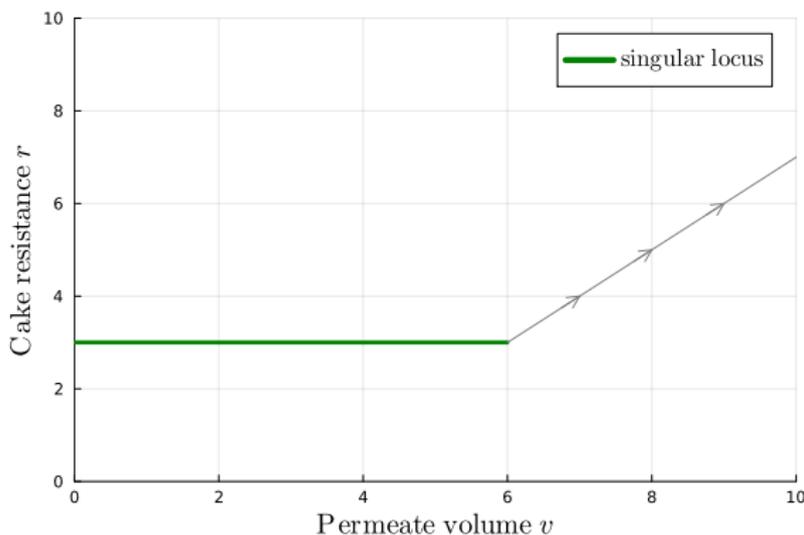
Figure: Optimal synthesis construction

Optimal synthesis
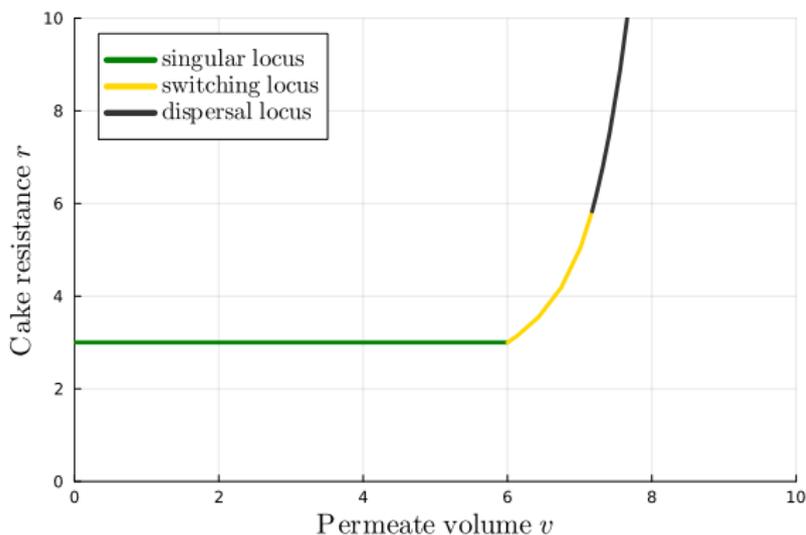
We have to compute the switching curve $\mathcal{S}$

Figure: Optimal synthesis construction

Optimal synthesis

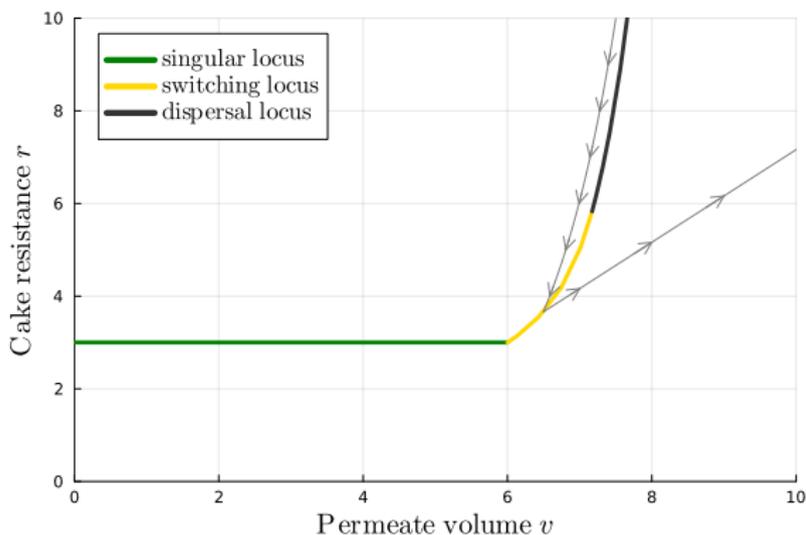We have to compute the switching curve $\mathcal{S}$

Figure: Optimal synthesis construction

Characterization of the switching curve

If $\xi = (x, y) \in \mathcal{S}$ then there exists $p = (-1, p_x, p_y)$ such that

$$H_0(x, p) = H_1(x, p) = 0 \quad \Rightarrow \quad p_x = \alpha(x) \quad \text{and} \quad p_y = \beta(x).$$

Moreover, denoting $\exp_{\vec{H}_+}$ the exponential map associated to the Hamiltonian vector field $\vec{H}_+$ generate by $H_+ = H_0 + H_1$ which stops when $y = y_f$, one has

$$\pi_{p_x}(\exp_{\vec{H}_+}(\xi, p)) = 0.$$

where $\pi_{p_x}(\xi, p) = p_x$. If $(x, y) \in \mathcal{S}$ then it is a zero of the function $S_{\mathcal{S}} \colon \mathbb{R}^2 \to \mathbb{R} = 0$ defined by

$$S_{\mathcal{S}}(x, y) = \pi_{p_x}\big(\exp_{\vec{H}_+}(x, y, p_x(x), p_y(x))\big)$$

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Optimal synthesis

We have to compute the dispersal curve $\mathcal{D}$

Figure: Optimal synthesis construction

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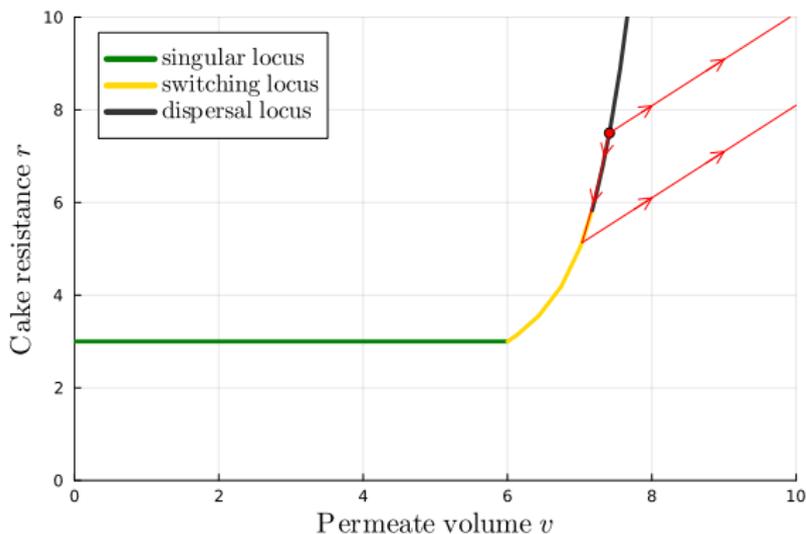000000

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Characterization of the dispersal curve

If $(x, y) \in \mathcal{D}$ then it is a zero of $S_{\mathcal{D}} \colon \mathbb{R}^2 \to \mathbb{R}$ defined by
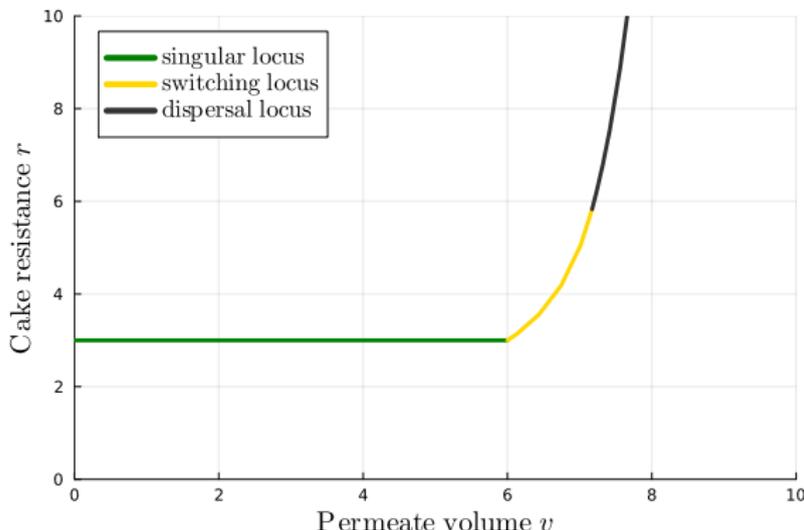
$$S_{\mathcal{D}}(x, y) = J(\gamma_+(x, y)) - J(\gamma_{-+}(x, y))$$

where :

- $\gamma_-(x, y)$ is the trajectory with the structure σ_- starting from (x, y) and stops when $y = y_f$,

- $\gamma_{-+}(x, y)$ is the trajectory with the structure $\sigma_- \sigma_+$ starting from (x, y), stops when $y = y_f$ and switch on the switching curve,

- $J(\gamma)$ correponds to the cost associated to the trajectory γ.

Switching and dispersal curve

The switching and the dispersal curves are the solution of $S(x, y) = 0$, where S is a function $S \colon \mathbb{R}^2 \to \mathbb{R}, (x, y) \mapsto S(x, y)$. Moreover, for both of them, we know an initial point (a, b) such that $S(a, b) = 0$

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Differential continuation method

Let us suppose that there exists a function $\varphi(x)$ such that

$$S(x, \varphi(x)) = 0.$$

Since S is constant, we have

$$\frac{\partial S}{\partial x}(x, \varphi(x)) + \frac{\partial S}{\partial y}(x, \varphi(x))\, \varphi'(x) = 0$$

Function $\varphi(x)$ is the solution of the ODE

$$\varphi'(x) = -\left(\frac{\partial S}{\partial y}(x, \varphi(x))\right)^{-1} \frac{\partial S}{\partial x}(x, \varphi(x)), \quad \varphi(a) = b.$$

Differential continuation method

In Julia, packages **ForwardDiff** and **OrdinaryDiffEq** work
together.

- The gradient of S is computed thanks to the **ForwardDiff**
  package.
- Even if S contains a solution of an ODE, the derivative of S is
  computed properly (it uses variational equations).
- The numerical integration is stopped when a condition is
  satisfied by using **Callback**.

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Conclusion

We can generate automatically optimal feedback map associated to Problems in the form of (OCP), used for membrame filtration systems.
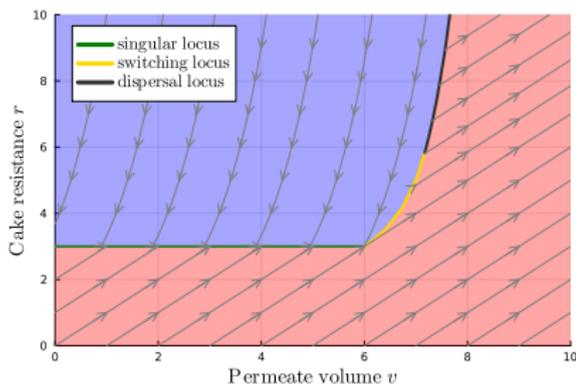
(a) Case (#1)
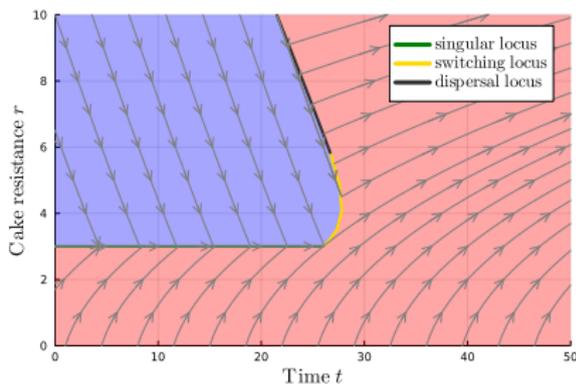
(b) Case (#2)

Conclusion

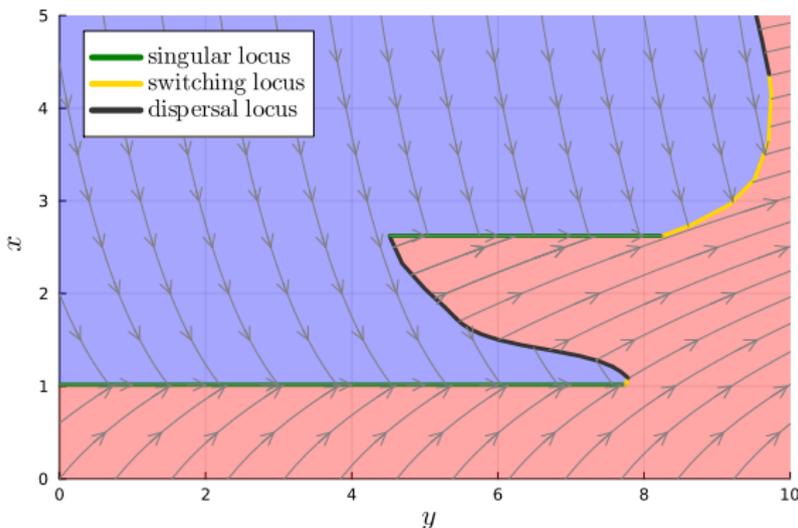This framework can also be applied on more complex example, with non-connected singular locus.

Figure: Toy example with non-connected singular locus.

References

Filtration.jl Package : Documentation and more examples

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Thank you for your attention !

https://remydutto.github.io/