Some optimization problems in an algal raceway pond

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Introduction

- Motivation: High potential on commercial applications, e.g., cosmetics, pharmaceuticals, food complements, wastewater treatment, green energy, etc.
- Raceway ponds

Figure: A typical raceway for cultivating microalgae. Notice the paddle-wheel which mixes the culture suspension. Picture from INRA (ANR Symbiose project) [1].

1D Illustration

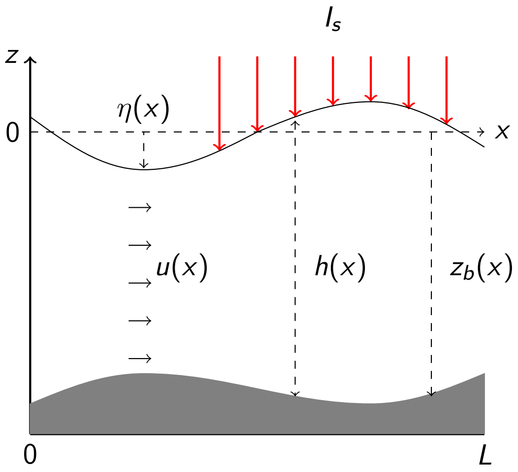

Figure: Representation of the hydrodynamic model.

Saint-Venant Equations

- 1D steady state Saint-Venant equations

$$\partial_x(hu) = 0, \tag{1}$$

$$\partial_x(hu^2 + g\frac{h^2}{2}) = -gh\partial_x z_b. \tag{2}$$

Saint-Venant Equations

- u, z_b as a function of h

$$u = \frac{Q_0}{h}, \tag{1}$$

$$z_b = \frac{M_0}{g} - \frac{Q_0^2}{2gh^2} - h, \tag{2}$$

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- Froude number:

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$Fr < 1$: subcritical case (i.e. the flow regime is fluvial)
$Fr > 1$: supercritical case (i.e. the flow regime is torrential)

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- Given a smooth topography z_b, there exists a unique positive smooth solution of h which satisfies the subcritical flow condition [5, Lemma 1].

Lagrangian Trajectories

- Incompressibility of the flow: $\nabla \cdot \underline{\mathbf{u}} = 0$ with $\underline{\mathbf{u}} = (u(x), w(x,z))$

$$\partial_x u + \partial_z w = 0. \tag{3}$$

- Integrating (3) from z_b to z and using the kinematic condition at bottom ($w(x, z_b) = u(x)\partial_x z_b$) gives:

$$w(x,z) = (\frac{M_0}{g} - \frac{3u^2(x)}{2g} - z)u'(x).$$

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$$\begin{pmatrix} \dot{x}(t) \\ \dot{z}(t) \end{pmatrix} = \begin{pmatrix} u(x(t)) \\ w(x(t), z(t)) \end{pmatrix}.$$

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- A time free formulation of the Lagrangian trajectory:

$$z(x) = \color{red}{\eta(x)} + \frac{\color{red}{h(x)}}{\color{blue}{h(0)}}(\color{blue}{z(0)} - \color{blue}{\eta(0)}). \tag{4}$$

Han model [4]

- A: open and ready to harvest a photon,
  B: closed while processing the absorbed photon energy,
  C: inhibited if several photons have been absorbed simultaneously.
- $$\begin{cases} \dot{A} = -\sigma I A + \frac{B}{\tau}, \\ \dot{B} = \sigma I A - \frac{B}{\tau} + k_r C - k_d \sigma I B, \\ \dot{C} = -k_r C + k_d \sigma I B. \end{cases} \quad (5)$$
- A, B, C are the relative frequencies of the three possible states with $A + B + C = 1$.

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- Using their sum equals to one to eliminate B

$$\begin{cases} \dot{A} = -(\sigma I + \frac{1}{\tau})A + \frac{1-C}{\tau}, \\ \dot{C} = -(k_r + k_d \sigma I)C + k_d \sigma I(1 - A), \end{cases}$$

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- The net growth rate:

$$\mu(C, I) := k \sigma I A - R = k \sigma I \frac{(1 - C)}{\tau \sigma I + 1} - R,$$

- The Beer-Lambert law describes how light is attenuated with depth

$$I(x,z) = I_s \exp\Big(- \varepsilon(\eta(x) - z)\Big), \tag{6}$$

where ε is the light extinction defined by:

$$\varepsilon(X) = \alpha_0 X + \alpha_1, \tag{7}$$

with α_0 light extinction coefficient, α_1 background turbidity and X biomass concentration.

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$$\bar{\mu}_\infty := \frac{1}{V} \int_0^L \int_{z_b(x)}^{\eta(x)} \mu\big(C(x,z), I(x,z)\big) \mathrm{d}z \mathrm{d}x,$$

$$\bar{\mu}_{N_z} := \frac{1}{V N_z} \sum_{i=1}^{N_z} \int_0^L \mu(C_i, I_i) h \mathrm{d}x.$$

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- Volume of the system

$$V = \int_0^L h(x)\mathrm{d}x. \tag{8}$$

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- Parameterize h by a vector $a := [a_1, \cdots, a_N] \in \mathbb{R}^N$.
- The computational chain:

$$a \to h \to z_i \to I_i \to C_i \to \bar{\mu}_{N_z}.$$

- Optimization Problem: $\bar{\mu}_{N_z}(a) = \frac{1}{VN_z}\sum_{i=1}^{N_z}\int_0^L \mu(C_i, I_i(a))h(a)\mathrm{d}x$, where C_i satisfy

$$C_i' = \left(-\alpha\left(I_i(a)\right)C_i + \beta\left(I_i(a)\right)\right)\frac{h(a)}{Q_0}.$$

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- Lagrangian

$$\begin{aligned}\mathcal{L}(C_i, a, p_i) = \frac{1}{VN_z}\sum_{i=1}^{N_z}\int_0^L \Big(-\gamma(I_i(a))C_i + \zeta(I_i(a))\Big)h(a)\mathrm{d}x \\ -\sum_{i=1}^{N_z}\int_0^L p_i\Big(C_i' + \frac{\alpha(I_i(a)) - \beta(I_i(a))}{Q_0}h(a)\Big)\mathrm{d}x.\end{aligned}$$

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- The gradient $\nabla\bar{\mu}_{N_z}(a) = \partial_a\mathcal{L}$ is given by

$$\partial_a\mathcal{L} = \sum_{i=1}^{N_z}\int_0^L \Big(\frac{-\gamma'\left(I_i\right)C_i + \zeta'\left(I_i\right)}{VN_z} + p_i\frac{-\alpha'(I_i)C_i + \beta'(I_i)}{Q_0}\Big)h\partial_a I_i\mathrm{d}x \\ +\sum_{i=1}^{N_z}\int_0^L \Big(\frac{-\gamma\left(I_i\right)C_i + \zeta\left(I_i\right)}{VN_z} + p_i\frac{-\alpha(I_i)C_i + \beta(I_i)}{Q_0}\Big)\partial_a h\mathrm{d}x.$$

Numerical settings

Parameterization of h: Truncated Fourier

$$h(x) = a_0 + \sum_{n=1}^{N} a_n \sin(2n\pi \frac{x}{L}). \tag{9}$$

Parameter to be optimized: Fourier coefficients $a := [a_1, \dots, a_N]$. We use this parameterization based on the following reasons :

- We consider a hydrodynamic regime where the solutions of the shallow water equations are smooth and hence the water depth can be approximated by (9).
- One has naturally $h(0) = h(L)$ under this parameterization, which means that we have accomplished one lap of the raceway pond.
- We assume a constant volume of the system V, which can be achieved by fixing a_0. Indeed, under this parameterization and using (8), one finds $V = a_0 L$.

Convergence on vertical discretization number

We fix $N = 5$ and take 100 random vector a. For N_z varying from 1 to 80, we compute the average value of $\bar{\mu}_{N_z}$ for each N_z.

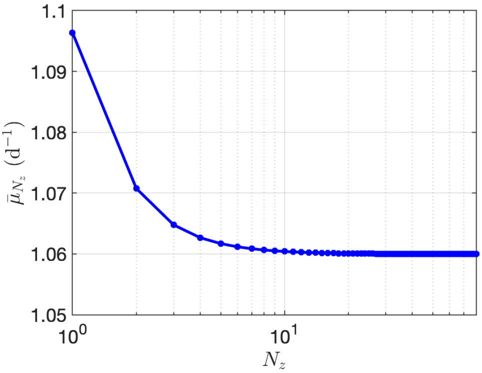
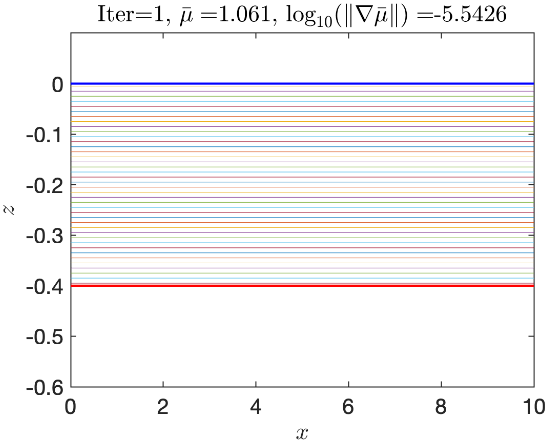


Figure: The value of $\bar{\mu}_{N_z}$ for $N_z = [1, 80]$.

Optimal Topography

We keep $N = 5$ and take $N_z = 40$. As an initial guess, we consider the flat topography, meaning that a is set to 0.



Periodic case

Assumption

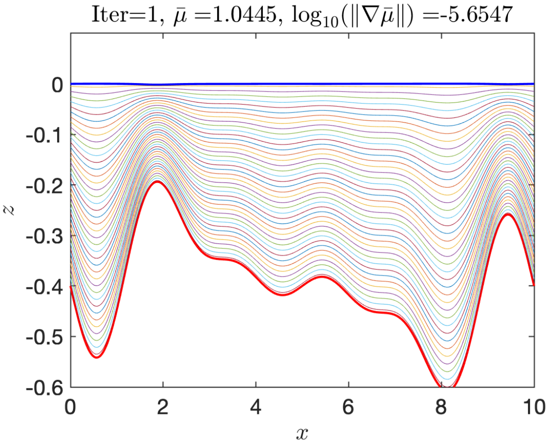
Photoinhibition state C is periodic meaning that $C_i(L) = C_i(0)$

Theorem (Flat topography [2])

Assume the volume of the system V is constant. Then $\nabla \bar{\mu}_{N_z}(0) = 0$.

Optimal topography (C periodic)

We keep $N = 5$ and $N_z = 40$. As an initial guess, we consider a random topography.



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- In the case C periodic, the flat topography is actually the optimal topography.
- What do we do next?

Mixing devices

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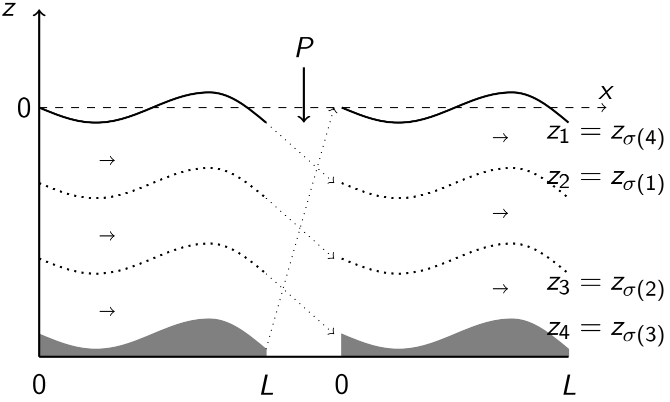


Test with a permutation

We keep $N = 5$, $N_z = 40$ and choose $\sigma = Id$

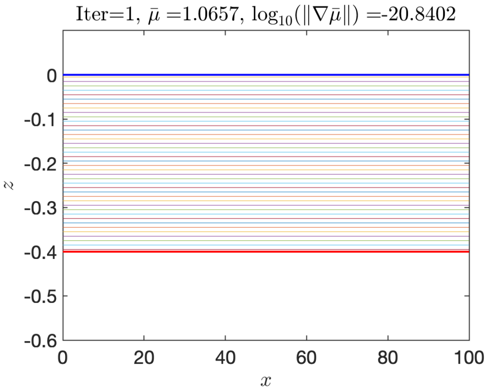
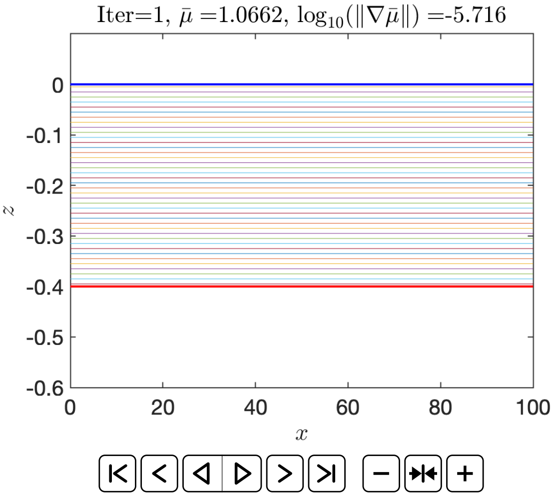


Figure: The optimal topography.

Test with a permutation

We keep $N = 5$, $N_z = 40$ and choose $\sigma = (1\ N_z)(2\ N_z - 1)\dots$



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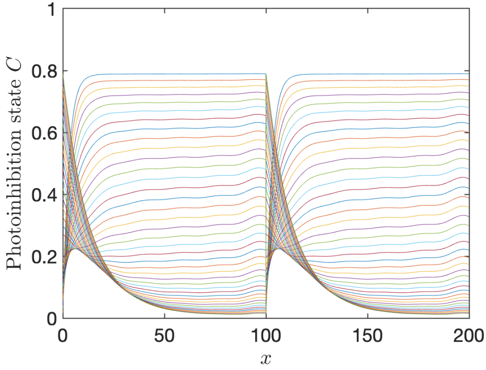

Figure: The evolution of the photo-inhibition state C for two laps.

We can observe that the period of C equals to one.

General problem

Given a period T, and initial time T_0 and a sequence $(T_k)_{k\in\mathbb{N}}$, with $T_k = kT + T_0$, we consider the following resource allocation problem:

Periodic dynamical resource allocation problem

Consider N resources denoted by $(I_n)_{n=1}^N \in \mathbb{R}^N$ which can be allocated to N activities denoted by $(x_n)_{n=1}^N$ where x_n consists of a real function of time. On a time interval $[T_k, T_{k+1})$, each activity uses the assigned resource and evolves according to a linear dynamics

$$\dot{x}_n = -\alpha(I_n)x_n + \beta(I_n), \tag{10}$$

where $\alpha : \mathbb{R} \to \mathbb{R}_+$ and $\beta : \mathbb{R} \to \mathbb{R}_+$ are given. At time T_{k+1}, the resources is re-assigned, meaning that $x(T_{k+1}) = Px(T_{k+1}^-)$ for some $P \in \mathcal{P}$. In this way, $k \in \mathbb{N}$ represents the number of re-assignments and T_k^- represents the moment just before re-assignment.

Assumption

Resources $(I_n)_{n=1}^N$ are constant with respect to time.

Consequence

For a given initial vector of states $(x_n(T_0))_{n=1}^N$, we have

$$x(t) = D(t)x(T_k) + v(t), \quad t \in [T_k, T_{k+1}), \tag{11}$$

where $D(t)$ and $v(t)$ are time dependent.

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where $D(t)$ and $v(t)$ are time dependent.

Let $u \in \mathbb{R}^N$ an arbitrary vector. Define

$$f^k := \langle u, \frac{1}{T} \int_{T_k}^{T_{k+1}} x(t)\mathrm{d}t \rangle, \tag{12}$$

the benefit attached to the time period $[T_k, T_{k+1})$ after k times of re-assignment. Then the average benefit after K operations is given by

$$\frac{1}{K} \sum_{k=0}^{K} f^k.$$

According to (11) and by the definition of P, we have

$$x(T_{k+1}) = Px(T_{k+1}^-) = P(Dx(T_k) + v). \tag{13}$$

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Lemma

Given $k \in \mathbb{N}$ and $P \in \mathcal{P}$, the matrix $\mathcal{I}_N - (PD)^k$ is invertible.

Theorem (One periodic [3])

$(x(T_k))_{k\in\mathbb{N}}$ *is a constant sequence and we have for all* $k \in \mathbb{N}$

$$x(T_k) = (\mathcal{I}_N - PD)^{-1}Pv.$$

The result shows that every $KT-$periodic evolution will actually be $T-$periodic.

Optimization problem

$$\max_{P \in \mathcal{P}} J(P) := \max_{P \in \mathcal{P}} \langle u, (\mathcal{I}_{N_z} - PD)^{-1} P v \rangle, \quad (14)$$

Remark

Since $\#\mathfrak{S} = N!$, this problem cannot be tackled in realistic cases where large values of N must be considered, e.g., to keep a good numerical accuracy.

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Expand the functional (14) as follows

$$\langle u, (\mathcal{I}_{N_z} - PD)^{-1} Pv \rangle = \sum_{l=0}^{+\infty} \langle u, (PD)^l Pv \rangle = \langle u, Pv \rangle + \sum_{l=1}^{+\infty} \langle u, (PD)^l Pv \rangle,$$

Approximation problem

$$\max_{P\in\mathcal{P}} J^{\text{approx}}(P) := \max_{P\in\mathcal{P}} \langle u, Pv \rangle. \tag{15}$$

Lemma

Let $\sigma_+, \ \sigma_- \in \mathfrak{S}$ *such that* $v_{\sigma_+(1)} \leq v_{\sigma_+(2)} \cdots \leq v_{\sigma_+(N)}$ *and* $v_{\sigma_-(N)} \leq v_{\sigma_-(N-1)} \leq \cdots \leq v_{\sigma_-(1)}$ *and* $P_+, \ P_- \in \mathcal{P}$*, the corresponding permutation matrices. Then*

$$P_+ = \mathrm{argmax}_{P \in \mathcal{P}} J^{approx}(P), \quad P_- = \mathrm{argmin}_{P \in \mathcal{P}} J^{approx}(P).$$

Remark (Optimal matrix)

- P_+: *associates the largest coefficient of* u *with the largest coefficient of* v*, the second largest coefficient with the second largest, and so on.*
- P_-: *associates the largest coefficient of* u *with the smallest coefficient of* v*, the second largest coefficient with the second smallest, and so on.*

Theorem (Criterion [3])

Assume that u and v have positive entries and define

$$\phi(m_1) := \frac{1}{s_{\lceil \frac{m_1}{2} \rceil}} \Big(\sum_{l=1}^{+\infty} d_{\max}^{l} F^{+}_{(l+1)m_1} - d_{\min}^{l} F^{-}_{(l+1)m_1} \Big), \tag{16}$$

where $m_1 := \# \{n = 1, \dots, N \mid \sigma(n) \neq \sigma_+(n)\}$, $d_{\max} := \max_{n=1,\dots,N}(d_n)$ *and* $d_{\min} := \min_{n=1,\dots,N}(d_n)$. *Assume that:*

$$\max_{m_1 \geq 2} \phi(m_1) \leq 1. \tag{17}$$

Then the problem $\max_{P \in \mathcal{P}} \langle u, (\mathcal{I}_{N_z} - PD)^{-1} Pv \rangle$ *(resp.* $\min_{P \in \mathcal{P}} \langle u, (\mathcal{I}_{N_z} - PD)^{-1} Pv \rangle$*) and the problem* $\max_{P \in \mathcal{P}} \langle u, Pv \rangle$ *(resp.* $\min_{P \in \mathcal{P}} \langle u, Pv \rangle$*) have the same solution.*

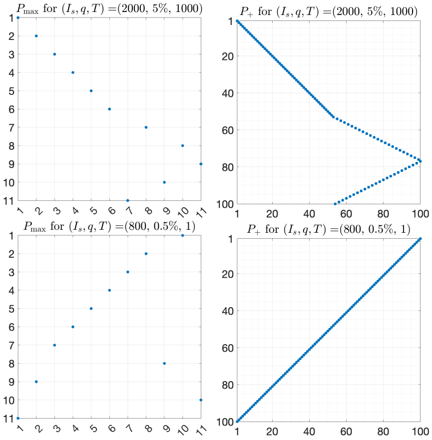

Figure: Optimal matrix $P_{\max}$ for Problem (14) and $N = 11$ (Left) and P_+ for Problem (15) and $N = 100$ (Right) for the two parameters triplets. The blue points represent non-zero entries, i.e., entries equal to 1.

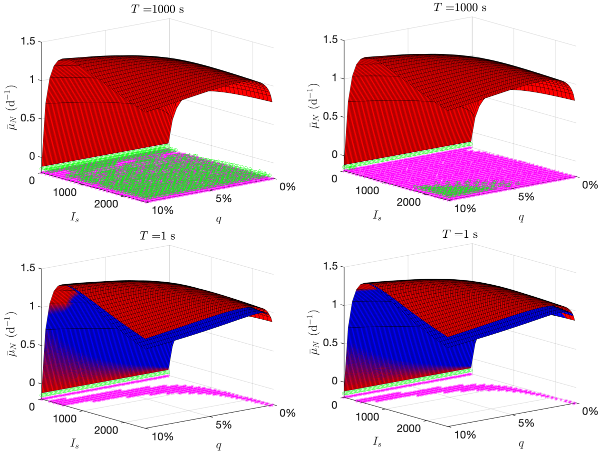

Figure: Average net specific growth rate $\bar{\mu}_N$ for $T = 1\,\mathrm{s}$ (Top) and for $T = 1000\,\mathrm{s}$ (Bottom). Left: $N = 5$. Right: $N = 9$. The red surface is obtained with P_{max} and the blue surface is obtained with P_{+}. The purple stars represent the cases where $P_{\mathrm{max}} = P_{+}$ or, in case of multiple solution, $\bar{\mu}_N(P_{\mathrm{max}}) = \bar{\mu}_N(P_{+})$. The green circle represent the cases where the criterion (17) is satisfied.

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Variable volume

- Volume related parameter a_0 as the average depth of the raceway system:

$$a_0 := \bar{h} = \frac{1}{L}\int_0^L h(x)\mathrm{d}x = \frac{V}{L}. \tag{18}$$

New parameter $\tilde{a} = [a_0, a_1, \ldots, a_N]$.

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- Optimization Problem:

$$\Pi_{N_z}(\tilde{a}) := \bar{\mu}_{N_z}(\tilde{a})Xh(\tilde{a}) = \frac{Y_{\mathrm{opt}} - \alpha_1 a_0}{VN_z\alpha_0}\sum_{i=1}^{N_z}\int_0^L \mu(C_i^P, I_i(\tilde{a}))h(\tilde{a})\mathrm{d}x$$

where C_i^P satisfy

$$C_i^{P\prime} = \left(-\alpha\left(I_i(\tilde{a})\right)C_i^P + \beta\left(I_i(\tilde{a})\right)\right)\frac{h(\tilde{a})}{Q_0},$$
$$PC^P(L) = C^P(0).$$

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- Extra element in gradient: $\nabla\Pi_{N_z}(\tilde{a}) = [\partial_{a_0}\mathcal{L}, \partial_a\mathcal{L}]$.

Optimal Topography (Variable volume)

We keep $N_z = 7$. As an initial guess, we consider the flat topography with $a_0 = 0.4$.

$$P_{\max}^{100} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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