

Classical Optimal Designs for Stationary Diffusion with Multiple Phases

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Funded by
the European Union
NextGenerationEU



Setting

$\Omega \subset \mathbb{R}^d$ is occupied by N materials - conductivities described by symmetric positive-definite matrices

$$\mathbf{M}_1, \dots, \mathbf{M}_N \in \text{Sym}_d.$$

If χ_j is the characteristic function of phase j and $\mathbf{R} \in L^\infty(\Omega; SO(d))$ is a rotation field, overall conductivity field is

$$\mathbf{A}(\mathbf{x}) = \sum_{j=1}^N \chi_j(\mathbf{x}) \mathbf{R}(\mathbf{x})^\top \mathbf{M}_j \mathbf{R}(\mathbf{x}), \quad \sum_{j=1}^N \chi_j = 1.$$

For heat sources $f_1, \dots, f_m \in H^{-1}(\Omega)$, the corresponding temperatures satisfy

$$-\text{div}(\mathbf{A} \nabla u_i) = f_i, \quad u_i \in H_0^1(\Omega), \quad i = 1, \dots, m.$$

The optimal design problem

For every state equation, the energy equals

$$E_i(\mathbf{A}) = \int_{\Omega} \mathbf{A} \nabla u_i \cdot \nabla u_i \, dx = \langle f_i, u_i \rangle.$$

We maximize the weighted sum

$$J(\mathbf{A}) = \sum_{i=1}^m \mu_i \langle f_i, u_i \rangle \longrightarrow \max, \quad \mu_i > 0,$$

among all material arrangements satisfying the prescribed quantities

$$\int_{\Omega} \chi_j \, d\mathbf{x} = q_j, \quad j = 1, \dots, N.$$

Why the problem must be relaxed

Even for one state equation and two isotropic materials, the classical problem may fail to attain its maximum.

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- ▶ Maximizing sequences can develop oscillations on increasingly fine scales.
- ▶ Their characteristic functions converge only to local proportions $\theta = (\theta_1, \dots, \theta_N)$.
- ▶ Their conductivity fields converge, in the sense of H -convergence, to an effective conductivity $\mathbf{A}^\infty$.

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Thus homogenization replaces pure arrangements by composite materials:

$$\chi^n \xrightarrow{*} \theta, \quad \mathbf{A}^n \xrightarrow{H} \mathbf{A}^\infty, \quad \mathbf{A}^\infty(\mathbf{x}) \in \mathcal{K}(\theta(\mathbf{x})) \quad \text{a.e.}$$

The relaxed problem admits the effective limits of all fine-scale mixtures.

Three related admissible classes

For local proportions $\boldsymbol{\theta}$, define

$$\frac{1}{\lambda_{-}(\boldsymbol{\theta})} = \sum_{j=1}^N \frac{\theta_j}{\underbrace{\lambda_1(\mathbf{M}_j)}_{\text{smallest eigenvalue}}}, \quad \lambda_{+}(\boldsymbol{\theta}) = \sum_{j=1}^N \theta_j \underbrace{\lambda_d(\mathbf{M}_j)}_{\text{largest eigenvalue}} \rightarrow \text{bounds on eigenvalues of admissible tensors}$$

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All three formulations impose $\sum_j \theta_j = 1$ and $\int_{\Omega} \theta_j dx = q_j$.

$\mathcal{A}$: homogenized designs	$\mathcal{B}$: bounded tensors	$\mathcal{T}$: proportions
$\mathbf{A}(\mathbf{x}) \in \mathcal{K}(\boldsymbol{\theta}(\mathbf{x}))$	$\lambda_-(\boldsymbol{\theta})\mathbf{I} \leq \mathbf{A} \leq \lambda_+(\boldsymbol{\theta})\mathbf{I}$	$\mathbf{A} = \lambda_-(\boldsymbol{\theta})\mathbf{I}$

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Question

When is an optimizer classical (bang–bang), meaning that it uses only the original pure materials?

The problem on $\mathcal{T} = \{\vartheta \in L^\infty(\Omega; [0, 1]^N) : \sum_j \vartheta_j = 1, \int_\Omega \vartheta_j = q_j\}$

For $\theta \in \mathcal{T}$, let u_i solve

$$-\operatorname{div}(\lambda_-(\theta)\nabla u_i) = f_i, \quad I(\theta) = \sum_{i=1}^m \mu_i \langle f_i, u_i \rangle.$$

Our main task is

$$\max_{\theta \in \mathcal{T}} I(\theta).$$

Introduce

$$\mathcal{S} = \{\sigma = (\sigma_1, \dots, \sigma_m) \in L^2(\Omega; \mathbb{R}^d)^m : -\operatorname{div} \sigma_i = f_i\}.$$

The dual variational formulation gives

$$I(\theta) = \min_{\sigma \in \mathcal{S}} \sum_{i=1}^m \mu_i \int_\Omega \frac{|\sigma_i|^2}{\lambda_-(\theta)} dx,$$

which leads directly to the saddle-point formulation.

The saddle-point structure

Set

$$H(\boldsymbol{\theta}, \boldsymbol{\sigma}) = \sum_{i=1}^m \mu_i \int_{\Omega} \frac{|\boldsymbol{\sigma}_i|^2}{\lambda_{-}(\boldsymbol{\theta})} dx.$$

Then

$$\max_{\boldsymbol{\theta} \in \mathcal{T}} I(\boldsymbol{\theta}) = \max_{\boldsymbol{\theta} \in \mathcal{T}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} H(\boldsymbol{\theta}, \boldsymbol{\sigma}).$$

- ▶ H is linear in $\boldsymbol{\theta}$;
- ▶ H is strictly convex in $\boldsymbol{\sigma}$;
- ▶ $\mathcal{T}$ is weak-* compact.

There is a saddle point $(\boldsymbol{\theta}^*, \boldsymbol{\sigma}^*)$:

$$H(\boldsymbol{\theta}, \boldsymbol{\sigma}^*) \leq H(\boldsymbol{\theta}^*, \boldsymbol{\sigma}^*) \leq H(\boldsymbol{\theta}^*, \boldsymbol{\sigma}).$$

The optimal flux $\boldsymbol{\sigma}^*$ is unique.

Optimality splits into two conditions

A design θ^* solves the reduced problem if and only if

1. it maximizes $H(\cdot, \sigma^*)$:

$$\max_{\theta \in \mathcal{T}} \int_{\Omega} \sum_{j=1}^N \frac{\theta_j}{\lambda_1(\mathbf{M}_j)} \underbrace{\sum_{i=1}^m \mu_i |\sigma_i^*|^2}_{\psi} dx;$$

2. the flux and state are compatible:

$$\sigma_i^* = \lambda_-(\theta^*) \nabla u_i^*, \quad i = 1, \dots, m.$$

Interpretation

First solve a linear allocation problem driven by ψ ; then verify that the allocated design generates the same optimal flux.

The allocation principle

Assumption

$$\lambda_1(\mathbf{M}_1) < \lambda_1(\mathbf{M}_2) < \cdots < \lambda_1(\mathbf{M}_N).$$

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Objective

$$\max_{\boldsymbol{\theta} \in \mathcal{T}} \int_{\Omega} \sum_{j=1}^N \frac{\theta_j}{\lambda_1(\mathbf{M}_j)} \underbrace{\sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2}_{\psi \geq 0} dx = \max_{\boldsymbol{\theta} \in \mathcal{T}} \int_{\Omega} \sum_{j=1}^N \frac{\theta_j}{\lambda_1(\mathbf{M}_j)} \psi$$

The allocation principle

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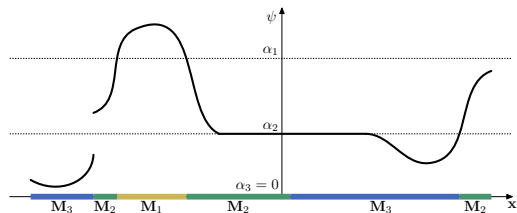
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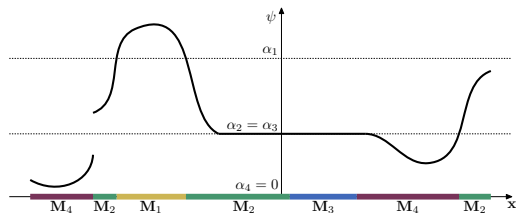
$$\max_{\boldsymbol{\theta} \in \mathcal{T}} \int_{\Omega} \sum_{j=1}^N \frac{\theta_j}{\lambda_1(\mathbf{M}_j)} \underbrace{\sum_{i=1}^m \mu_i |\boldsymbol{\sigma}_i^*|^2}_{\psi \geq 0} dx = \max_{\boldsymbol{\theta} \in \mathcal{T}} \int_{\Omega} \sum_{j=1}^N \frac{\theta_j}{\lambda_1(\mathbf{M}_j)} \psi$$

Since $1/\lambda_1(\mathbf{M}_1)$ is largest, material $\mathbf{M}_1$ should occupy the region where ψ is largest; then $\mathbf{M}_2$, and so on.

Visual representation of allocation via horizontal level sets of ψ

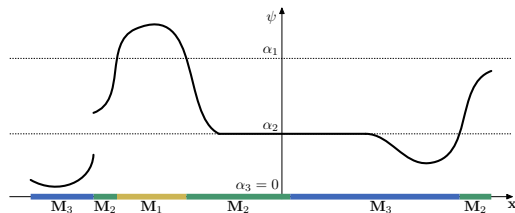


(a) Unique solution

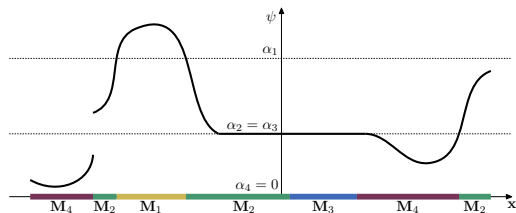


(b) Arbitrary mixture on certain level sets

Visual representation of allocation via horizontal level sets of ψ



(a) Unique solution



(b) Arbitrary mixture on certain level sets

Let $\lambda_\psi(\alpha) = |\{\mathbf{x} : \psi(\mathbf{x}) > \alpha\}|$ and choose thresholds

$$\alpha_k = \min \left\{ \alpha \geq 0 : \lambda_\psi(\alpha) \leq \sum_{j=1}^k q_j \right\}, \quad \alpha_N = 0.$$

Complete characterization of the auxiliary problem

Theorem

$\theta^* \in \mathcal{T}$ is optimal for the allocation problem if and only if, for every k ,

$$\text{ess sup } \theta_k^* \subset \{\alpha_k \leq \psi \leq \alpha_{k-1}\}, \quad \theta_k^* = 1 \text{ on } \{\alpha_k < \psi < \alpha_{k-1}\},$$

with $\alpha_0 = +\infty$.

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with $\alpha_0 = +\infty$.

- ▶ A bang–bang optimizer always exists.
- ▶ Non-uniqueness occurs only on threshold level sets $\{\psi = \alpha_k\}$ of positive measure
- ▶ On open strips between thresholds, the material is uniquely determined.

Extensions of the allocation result

Equal minimal eigenvalues

If

$$\lambda_1(M_1) = \cdots = \lambda_1(M_k),$$

then $M_1, \dots, M_k$ are interchangeable and may be treated as one material of quantity $q_1 + \cdots + q_k$. In this case, uniqueness may fail.

Upper bounds on material quantities

If

$$\int_{\Omega} \theta_j \, dx \leq q_j, \quad \sum_{j=1}^N q_j \geq |\Omega|,$$

allocate materials successively in increasing order of $\lambda_1(M_j)$. Each material is used to full capacity until Ω is filled; the remaining materials are discarded.

What this says about the relaxed tensor problem

For every maximizer θ^* of the reduced problem,

$$(\theta^*, \lambda_-(\theta^*)I)$$

maximizes the problem over the larger class $\mathcal{B}$. More generally, $(\theta^*, \mathbf{A})$ is optimal over $\mathcal{B}$ exactly when

$$\mathbf{A}^{-1}\sigma_i^* = \frac{1}{\lambda_-(\theta^*)}\sigma_i^*, \quad i = 1, \dots, m.$$

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The remaining issue

For several states, such an $\mathbf{A}$ need not lie in the true G -closure $\mathcal{K}(\theta^*)$.

Case of spherical symmetry

Let Ω be a ball and all f_i radial. Uniqueness of optimal flux yields

$$\sigma_i^*(\mathbf{x}) = \sigma_i^*(r) \underbrace{\mathbf{e}_r}_{\substack{\text{unit} \\ \text{radial} \\ \text{direction}}}.$$

The divergence constraint becomes

$$-\frac{1}{r^{d-1}}(r^{d-1}\sigma_i^*(r))' = f_i(r),$$

hence

$$\sigma_i^*(r) = -\frac{1}{r^{d-1}} \int_0^r \rho^{d-1} f_i(\rho) d\rho$$

and therefore $\psi(r) = \sum_i \mu_i |\sigma_i^*(r)|^2$ is explicit.

Why radial allocation solves the true relaxation

Choose a radial maximizer $\theta^*(r)$ of the allocation problem. Define

$$u_i^*(r) = - \int_r^R \frac{\sigma_i^*(\rho)}{\lambda_-(\theta^*(\rho))} d\rho.$$

Then

$$\sigma_i^* = \lambda_-(\theta^*) \nabla u_i^*,$$

so the compatibility condition holds automatically.

- ▶ The radial proportions θ^* can be realized by a simple laminate whose layers are orthogonal to the radial direction; its effective conductivity belongs to the true G -closure and satisfies the tensor optimality condition for every radial optimal flux.
- ▶ Since the allocation problem admits a radial bang–bang maximizer, the original problem also admits a radial classical solution.

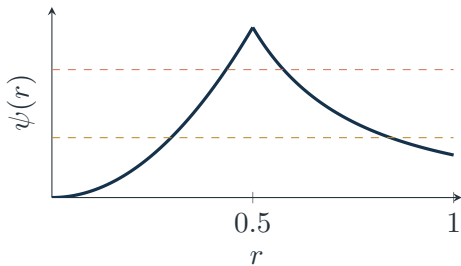
Every radial maximizer solves the true relaxed problem $(\mathcal{A})$, and at least one such maximizer solves the original classical problem.

Example 1: three materials, one state - unique classical design

In $\Omega = B(0, 1) \subset \mathbb{R}^2$, take

$$f = \chi_{B(0,1/2)}, \quad \sigma^*(r) = \begin{cases} -r/2, & 0 \leq r \leq 1/2, \\ -1/(8r), & 1/2 < r \leq 1. \end{cases}$$

Hence $\psi = (\sigma^*)^2$ has no level set of positive measure.



- thresholds cut the graph at finitely many radii;
- each phase occupies radial shells;
- the optimizer is unique, radial, and bang–bang.

Example 2: three materials, one state - flat levels create non-uniqueness

In $\Omega = B(0, 2) \subset \mathbb{R}^2$, choose

$$f(r) = \begin{cases} -2, & 0 \leq r \leq 1, \\ -1/r, & 1 < r \leq 2, \end{cases} \quad \psi(r) = \begin{cases} r^2, & 0 \leq r \leq 1, \\ 1, & 1 < r \leq 2. \end{cases}$$

The outer annulus has constant ψ and occupies $3/4$ of the area.

Volume regime

$(q_j = \eta_j |\Omega|)$

Structure of optimal designs

$\eta_1 > 3/4$

unique radial classical design

$\eta_1 \leq 3/4 < \eta_1 + \eta_2$

$\mathbf{M}_1$ and $\mathbf{M}_2$ may be rearranged arbitrarily in the outer annulus

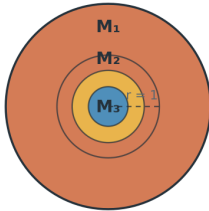
$\eta_1 + \eta_2 \leq 3/4$

arbitrary admissible mixtures of all three phases may occur in the outer annulus

Example 2: optimal designs in the three volume regimes

Case 1

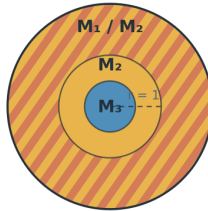
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Unique radial design

Case 2

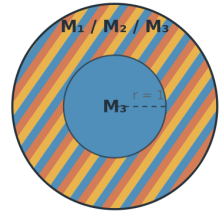
$$\eta_1 \leq 3/4 < \eta_1 + \eta_2$$



Non-unique outer annulus

Case 3

$$\eta_1 + \eta_2 \leq 3/4$$



Non-unique outer annulus



Striped regions represent arbitrary admissible arrangements subject to the volume constraints.

Thank you.