

Some Topics in Mathematical Optimization

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June 9, 2022

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Foreword

A collection of & some personal notes on Mathematical Optimization, especially the 3 major topics: Optimal Control, Shape Optimization, & Topology Optimization.

Keywords. Optimal control; Shape optimization; Topology optimization.

Chapter 1

Wikipedia's

1.1 Wikipedia/Shape Optimization

“*Shape optimization* is part of the field of **optimal control** theory. The typical problem is to find the **shape** which is optimal in that it minimizes a certain cost **functional** while satisfying given **constraints**. In many cases, the functional being solved depends on the solution of a given **PDE** defined on the variable domain.

Topology optimization is, in addition, concerned with the number of connected components/boundaries belonging to the domain. Such methods are needed since typically shape optimization methods work in a subset of allowable shapes which have fixed topological properties, such as having a fixed number of holes in them. Topological optimization techniques can then help work around the limitations of pure shape optimization.” – [Wikipedia/shape optimization](#)

1.1.1 Definition

“Mathematically, shape optimization can be posed as the problem of finding a **bounded set** Ω , **minimizing a functional** $\mathcal{F}(\Omega)$, possibly subject to a **constraint** of the form $\mathcal{G}(\Omega) = 0$. Usually we are interested in sets Ω which are **Lipschitz** or C^1 **boundary** & consist of finite many **components**, which is a way of saying that we would like to find a rather pleasing shape as a solution, not some jumble of rough bits & pieces. Sometimes additional constraints need to be imposed to that end to ensure well-posedness of the problem & uniqueness of the solution.

Shape optimization is an **infinite-dimensional optimization** problem. Furthermore, the space of allowable shapes over which the optimization is performed does not admit a **vector space** structure, making application of traditional optimization methods more difficult.” – [Wikipedia/shape optimization/definition](#)

1.1.2 Examples

- “among all 3D shapes of given volume, find the one which has minimal surface area. Here: $\mathcal{F}(\Omega) = \text{Area}(\partial\Omega)$, with $\mathcal{G}(\Omega) = \text{Volume}(\Omega) = \text{const.}$ The answer, given by the **isoperimetric inequality**, is a **ball**.
- Find the shape of an airplane wing which minimizes **drag**. Here the constraints could be the wing strength, or the wing dimensions.
- Find the shape of various mechanical structures, which can resist a given **stress** while having a minimal mass/volume.
- Given a known 3D object with a fixed radiation source inside, deduce the shape & size of the source based on measurements done on part of the boundary of the object. A formulation of this **inverse problem** using **least squares** fit leads to a shape optimization problem.” – [Wikipedia/shape optimization/examples](#)

1.1.3 Techniques

“Shape optimization problems are usually solved **numerically**, by using **iterative methods**. I.e., one starts with an initial guess for a shape, & then gradually evolves it, until it morphs into the optimal shape.” – [Wikipedia/shape optimization/techniques](#)

1.1.3.1 Keeping track of the shape

Fig. Example: Shape optimization as applied to building geometry. Example provided courtesy of [Formsolver.com](#).

“To solve a shape optimization problem, one needs to find a way to represent a shape in the **computer memory**, & follow its evolution. Several approaches are usually used.

1 approach is to follow the boundary of the shape. For that, one can sample the shape boundary in a relatively dense & uniform manner, i.e., to consider enough points to get a sufficiently accurate outline of the shape. Then, one can evolve the shape by gradually moving the boundary points. This is called the *Lagrangian approach*.

Another approach is to consider a **function** defined on a rectangular box around the shape, which is positive inside of the shape, zero on the boundary of the shape, & negative outside of the shape. One can then evolve this function instead of the shape itself. One can consider a rectangular grid on the box & sample the function at the grid points. As the shape evolves, the grid points do not change; only the function values at the grid points change. This approach, of using a fixed grid, is called the *Eulerian approach*. The idea of using a function to represent the shape is at the basis of the **level set method**.

Fig. Example: Optimization shape families resulting from differing goal parameters. Example provided courtesy of **Formsolver.com**

A 3rd approach is to think of the shape evolution as of a flow problem. I.e., one can imagine that the shape is made of a plastic material gradually deforming s.t. any point inside or on the boundary of the shape can be always traced back to a point of the original shape in a 1-1 fashion. Mathematically, if Ω_0 is the initial shape, & Ω_t is the shape at time t , one considers the **diffeomorphisms** $f_t : \Omega_0 \rightarrow \Omega_t$, for $t \leq t \leq t_0$. The idea is again that shapes are difficult entities to be dealt with directly, so manipulate them by means of a function.” – [Wikipedia/shape optimization/techniques/keeping track of the shape](#)

1.1.3.2 Iterative methods using shape gradients

“Consider a smooth velocity field V & the family of transformations T_s of the initial domain Ω_0 under the velocity field V : $x(0) = x_0 \in \Omega_0$, $x'(s) = V(x(s))$, $T_s(x_0) = x(s)$, $s \geq 0$, & denote $\Omega_0 \mapsto T_s(\Omega_0) = \Omega_s$.

” – [Wikipedia/shape optimization/techniques/iterative methods using shape gradients](#)

1.1.3.3 Geometry parametrization

Chapter 2

Formsolver.com

Chapter 3

Optimal Control

3.1 Introduction

“The mathematical optimization of process governed by PDEs has seen considerable progress in the past decade. Ever faster computational facilities & newly developed numerical techniques have opened the door to important practical applications in fields e.g. fluid flow, microelectronics¹, crystal² growth, vascular³ surgery⁴, & cardiac⁵ medicine, to name just a few. As a consequence, the communities of numerical analysts & optimizers have taken a growing interest in applying their methods to optimal control problems involving PDEs ...” [...] “... the comprehensive text by J.-L. Lions Lions, 1971 covers much of the theory of linear equations & convex cost functionals.” – Tröltzsch, 2010, Preface to the German edition, p. xiii

Tröltzsch, 2010 focuses on basic concepts & notions e.g.:

- Existence theory for linear & semilinear PDEs
- Existence of optimal controls
- Necessary optimality conditions & adjoint equations
- 2nd-order sufficient optimality conditions
- Foundation of numerical methods

Question 3.1. *What is optimal control?*

“The mathematical theory of optimal control has in the past few decades rapidly developed into an important & separate field of applied mathematics. 1 area of application of this theory lies in aviation⁶ & space technology: aspects of optimization come into play whenever the motion of an aircraft or a space vessel⁷ (which can be modeled by ODEs) has to follow a trajectory⁸ that is “optimal” in a sense to be specified.” – Tröltzsch, 2010, Sect. 1.1: *What is optimal control?*, p. 1

All the essential features of an *optimal control problem*:

- a *cost functional* to be minimized,
- an IVP for an ODE in order to determine the *state* y ,
- a *control function* u , &
- various constraints that have to be obeyed.

¹**microelectronics** [n] [uncountable] the design, production & use of very small electronic circuits.

²**crystal** [n] **1.** [countable] a small piece of a substance with many even sides, that is formed naturally when the substance becomes solid; in chemistry, a **crystal** is any solid that has its atoms, ions or molecules arranged in an ordered, symmetrical way; **2.** [uncountable] a clear mineral, e.g. quartz, used in making decorative objects.

³**vascular** [a] [usually before noun] (*medical*) connected with or containing veins.

⁴**surgery** [n] **1.** [uncountable, countable] medical treatment of injuries or diseases that involves cutting open a person’s body, sewing up wounds, etc.; **2.** [countable] (*British English*) a place where a doctor sees patients; **3.** [countable] (*British English*) a time during which a doctor, an MP or another professional person is available to see people.

⁵**cardiac** [a] [only before noun] (*medical*) connected with the heart or heart disease; if somebody has a **cardiac arrest**, their heart suddenly stops temporarily or permanently.

⁶**aviation** [n] [uncountable] the activity of designing, building & flying aircraft.

⁷**vessel** [n] **1.** a tube that carries blood through the body of a person or an animal, or liquid through the parts of a plant; **2.** (*formal*) a large ship or boat; **3.** (*formal*) a container used for holding liquids, e.g. a bowl or cup.

⁸**trajectory** [n] (plural **trajectories**) (*specialist*) **1.** the curved part of something that has been fired, hit or thrown into the air; **2.** the way in which a person, an event or a process develops over a period of time, often leading to a particular result.

“The control u may be freely chosen within the given constraints, while the state is uniquely determined by the differential equation & the initial conditions. We have to choose u in such a way that the cost function is minimized. Such controls are called *optimal*.” [...] “The optimal control of ODEs is of interest not only for aviation & space technology. In fact, it is also important in fields e.g. robotics⁹, movement sequences in sports, & the control of chemical processes & power plants, to name just a few of the various applications. In many cases, however, the processes to be optimized can no longer be adequately modeled by ODEs; instead, PDEs have to be employed for their description. E.g., heat conduction¹⁰, diffusion¹¹, electromagnetic¹² waves, fluid flows, freezing processes, & many other physical phenomenon¹³ can be modeled by PDEs.

In these fields, there are numerous interesting problems in which a given cost functional has to be minimized subject to a differential equation & certain constraints being satisfied. The difference from the above problem “merely” consists of the fact that a PDE has to be dealt with in place of an ordinary one.” – Tröltzsch, 2010, pp. 2–3

Tröltzsch, 2010 discusses, “through examples in the form of mathematically simplified case studies, the optimal control of heating processes, 2-phase problems, & fluid flows”. Tröltzsch, 2010 focuses “on linear & semilinear elliptic & parabolic PDEs, since a satisfactory regularity theory is available for the solutions to such equations. This is not the case for hyperbolic equations. Also, the treatment of quasilinear PDEs is considerably more difficult, & the theory of their optimal control is still an open field in many respects.” [...] “... the Hilbert space setting suffices as a functional analytic framework in the case of linear-quadratic theory.” – Tröltzsch, 2010, p. 3

3.1.1 Examples of Convex Problems

3.1.1.1 Optimal boundary heating

See Tröltzsch, 2010, Subsect. 1.2.1, pp. 3–5.

Example 3.1 (Optimal boundary heating). *Consider a body heated or cooled which occupies the spatial domain $\Omega \subset \mathbb{R}^3$. Apply to its boundary Γ a heat source u (the control), which is constant in time but depends on the location \mathbf{x} on the boundary, i.e., $u = u(\mathbf{x})$. Aim: choose the control in such a way that the corresponding temperature distribution $y = y(\mathbf{x})$ in Ω (the state) is the best possible approximation to a desired stationary temperature distribution $y_\Omega = y_\Omega(\mathbf{x})$:*

$$\min J(y, u) := \frac{1}{2} \int_{\Omega} |y(\mathbf{x}) - y_{\Omega}(\mathbf{x})|^2 d\mathbf{x} + \frac{\lambda}{2} \int_{\Gamma} |u(\mathbf{x})|^2 ds(\mathbf{x}),$$

subject to the state equation:

$$\begin{cases} -\Delta y = 0, & \text{in } \Omega, \\ \partial_{\mathbf{n}} y = \alpha(u - y), & \text{on } \Gamma, \end{cases}$$

and the pointwise control constraints $u_a(\mathbf{x}) \leq u(\mathbf{x}) \leq u_b(\mathbf{x})$ on Γ . “Such pointwise bounds for the control are quite natural, since the available capacities for heating or cooling are usually restricted. The constant $\lambda \geq 0$ can be viewed as a measure of the energy costs needed to implement the control u . From the mathematical viewpoint, this term also serves as a regularization parameter; it has the effect that possible optimal controls show improved regularity properties.” [...] “The function α represents the heat transmission coefficient from Ω to the surrounding medium. The functional J to be minimized is called the cost functional. The factor $\frac{1}{2}$ appearing in it has no influence on the solution of the problem. It is introduced just for the sake of convenience: it will later cancel out a factor 2 arising from differentiation. We seek an optimal control $u = u(\mathbf{x})$ together with the associated state $y = y(\mathbf{x})$. The minus sign in front of the Laplacian Δ appears to be unmotivated at 1st glance. It is introduced because Δ is not a coercive operator, while $-\Delta$ is.” – Tröltzsch, 2010, p. 4

“Observe that in the above problem the cost functional is quadratic, the state is governed by a linear elliptic PDE, & the control acts on the boundary of the domain.”: thus have a *linear-quadratic elliptic boundary control problem*.

Remark 3.1 (Notations used in Tröltzsch, 2010). Denote the element of surface area by ds & the outward unit normal to Γ at $\mathbf{x} \in \Gamma$ by $\nu(\mathbf{x})$ ¹⁴.

Remark 3.2. “The problem is strongly simplified. Indeed, in a realistic model Laplace’s equation $\Delta y = 0$ has to be replaced by the stationary heat conduction equation $\nabla \cdot (a \nabla y) = 0$, where the coefficient a can depend on \mathbf{x} or even on y . If $a = a(y)$ or $a = a(fx, y)$, then the PDE is quasilinear. In addition, it will in many cases be more natural to describe the process by a time-dependent PDE.” – Tröltzsch, 2010, p. 4

⁹robotics [n] [uncountable] the science of designing & operating robots.

¹⁰conduction [n] [uncountable] (physics) the process by which heat or electricity passes along or through a material.

¹¹diffusion [n] [uncountable] 1. the spreading of something more widely; 2. the mixing of substances by the natural movement of their particles; 3. the spreading of elements of culture from 1 region or group to another.

¹²electromagnetic [a] (physics) in which the electrical & magnetic properties of something are related.

¹³phenomenon [n] (plural phenomena a fact or an event in nature or society, especially one that is not fully understood.)

¹⁴NQBH: I prefer to use $\mathbf{n}(\mathbf{x})$, with “n” stands for “normal”, naturally & obviously.

Example 3.2 (Optimal heat source). *Similarly, the control can act as a heat source in the domain Ω . Problems of this kind arise if the body Ω is heated by electromagnetic induction or by microwaves. Assuming at 1st that the boundary temperature vanishes, we obtain the following problem:*

$$\min J(y, u) := \frac{1}{2} \int_{\Omega} |y(\mathbf{x}) - y_{\Omega}(\mathbf{x})|^2 d\mathbf{x} + \frac{\lambda}{2} \int_{\Omega} |u(\mathbf{x})|^2 d\mathbf{x},$$

subject to

$$\begin{cases} -\Delta y = \beta u, & \text{in } \Omega, \\ y = 0, & \text{on } \Gamma, \end{cases}$$

and $u_a(\mathbf{x}) \leq u(\mathbf{x}) \leq u_b(\mathbf{x})$ in Ω . Here, the coefficient $\beta = \beta(\mathbf{x})$ is prescribed. Observe that by the special choice $\beta = \chi_{\Omega_c}$ (where χ_E denotes the characteristic function of a set E), it can be achieved that u acts only in a subdomain $\Omega_c \subset \Omega$. This problem is a linear-quadratic elliptic control problem with distributed control. It can be more realistic to prescribe an exterior temperature y_a rather than assume that the boundary temperature vanishes. Then a better model is given by the state equation

$$\begin{cases} -\Delta y = \beta u, & \text{in } \Omega, \\ \partial_{\mathbf{n}} y = \alpha(y_a - y), & \text{on } \Gamma. \end{cases}$$

3.1.1.2 Optimal nonstationary boundary control

See Tröltzsch, 2010, pp. 5–6. “Let $\Omega \subset \mathbb{R}^3$ represent a potato that is to be roasted over a fire for some period of time $T > 0$.” Denote its temperature by $y = y(t, \mathbf{x})$, with $(t, x) \in [0, T] \times \Omega$. “Initially, the potato has temperature $y_0 = y_0(\mathbf{x})$, & we want to serve it at a pleasant palatable¹⁵ temperature y_{Ω} at the final time T .” Write $Q := (0, T) \times \Omega$, $\Sigma := (0, T) \times \Gamma$. Then problem reads as follows:

$$\min J(y, u) := \frac{1}{2} \int_{\Omega} |y(T, \mathbf{x}) - y_{\Omega}(\mathbf{x})|^2 d\mathbf{x} + \frac{\lambda}{2} \int_0^T \int_{\Gamma} |u(t, \mathbf{x})|^2 d\Gamma dt,$$

subject to

$$\begin{cases} y_t - \Delta y = 0, & \text{in } Q, \\ \partial_{\mathbf{n}} y = \alpha(u - y), & \text{on } \Sigma, \\ y(0, \mathbf{x}) = y_0(\mathbf{x}), & \text{in } \Omega, \end{cases}$$

& $u_a(t, \mathbf{x}) \leq u(t, \mathbf{x}) \leq u_b(t, \mathbf{x})$ on Σ . By continued turning of the spit¹⁶, we produce $u(t, \mathbf{x})$. The heating process has to be described by the *nonstationary heat equation*, which is a parabolic differential equation: thus have to deal with a *linear-quadratic parabolic boundary control problem*.

3.1.1.3 Optimal vibrations

“Suppose that a group of pedestrians crosses a bridge, trying to excite¹⁷ oscillations¹⁸ in it. This can be modeled (strongly abstracted) as follows: let $\Omega \subset \mathbb{R}^2$ denote the domain of the bridge, $y = y(t, \mathbf{x})$ its *transversal*¹⁹ *displacement*²⁰, $u = u(t, \mathbf{x})$ the *force density* acting in the vertical direction, & $y_d = y_d(t, \mathbf{x})$ a *desired evolution of the transversal vibrations*²¹. We then obtain the optimal control problem:

$$\min J(y, u) := \frac{1}{2} \int_0^T \int_{\Omega} |y(t, \mathbf{x}) - y_d(t, \mathbf{x})|^2 d\mathbf{x} dt + \frac{\lambda}{2} \int_0^T \int_{\Omega} |u(t, \mathbf{x})|^2 d\mathbf{x} dt,$$

¹⁵**palatable** [a] **1.** (of food or drink) having a pleasant or acceptable taste; **2. palatable (to somebody)** pleasant or acceptable to somebody, OPPOSITE: **unpalatable**.

¹⁶**spit** [n] *in/from mouth* **1.** [uncountable] the liquid produced in your mouth, SYNONYM: **saliva**; **2.** [countable, usually singular] the act of spitting liquid or food out of your mouth; *piece of land* **3.** [countable] a long, thin piece of land that sticks out into the sea, a lake, etc.; *for cooking meat* **4.** [countable] a long, thin, straight piece of metal that you put through meat to hold & turn it while you cook it over a fire.

¹⁷**excite** [v] **1.** to make somebody feel a particular emotion or react in a particular way, SYNONYM: **arouse**; **2. excite somebody** to make somebody feel very pleased, interested or enthusiastic, especially about something that is going to happen; **3. excite somebody/something** to make somebody/something nervous, upset or active & unable to relax; **4. excite something** to produce a state of increased energy or activity in a physical or biological system, SYNONYM: **stimulate**; **5. excite something (physics)** to bring something to a state of higher energy.

¹⁸**oscillation** [n] **1.** [countable, uncountable] **oscillation (of something)** a regular movement between 1 position & another; **2.** [countable] **oscillation (between A & B)** a repeated change between different states, ideas, etc.; **3.** [countable] (*specialist*) regular variation in size, strength or position around a central point or value, especially of an electrical current or electric field.)

¹⁹**transversal** [n] a line that intersects a system of lines.

²⁰**displacement** [n] **1.** [uncountable] the act of displacing somebody/something; the process of being displaced; **2.** [uncountable, singular] **displacement (of something) (physics)** the distance between the final & initial (= 1st) positions of an object which has moved.

²¹**vibration** [n] [countable, uncountable] **1. vibration (of something)** a continuous shaking movement; **2. vibration (of something) (physics)** oscillation in a substance about its equilibrium state.

subject to

$$\begin{cases} y_{tt} - \Delta y = u, & \text{in } Q, \\ y(0) = y_0, & \text{in } \Omega, \\ y_t(0) = y_1, & \text{in } \Omega, \\ y = 0, & \text{on } \Sigma, \end{cases}$$

and $u_a(t, \mathbf{x}) \leq u(t, \mathbf{x}) \leq u_b(t, \mathbf{x})$ in Q . This is a *linear-quadratic hyperbolic control problem with distributed control*. [...] “Interesting control problems for oscillating elastic networks have been treated by Lagnese et al. [LLS94]. An elementary introduction to the controllability of oscillations can be found in [Kra95].

In the linear-quadratic case, the theory of hyperbolic problems has many similarities to the parabolic theory studied in Tröltzsch, 2010. However, the treatment of semilinear hyperbolic problems is much more difficult, since the smoothing properties of the associated solution operators are weaker. As a consequence, many of the techniques presented in Tröltzsch, 2010 fail in the hyperbolic case.” – Tröltzsch, 2010, pp. 6–7

3.1.2 Examples of Nonconvex Problems

“However, linear models do not suffice for many real-world phenomena. Instead, one often needs quasilinear or, much simpler, semilinear equations. Recall that a 2nd-order equation is called *semilinear* if the main parts (i.e., the expressions involving highest-order derivatives) of the differential operators considered in the domain & on the boundary are linear w.r.t. the desired solution. For such equations, the theory of optimal control is well developed.

Optimal control problems with semilinear state equations are, as a rule, nonconvex, even if the cost functional is convex.

“Associated optimal control problems can be obtained by prescribing a cost functional & suitable constraints.” – Tröltzsch, 2010, p. 7

3.1.2.1 Problems involving semilinear elliptic equations

Example 3.3 (Heating with radiation boundary condition). *If the heat radiation of the heated body is taken into account, then we obtain a problem with a nonlinear Stefan–Boltzmann boundary condition. If this case, the control u is given by the temperature of the surrounding medium:*

$$\begin{cases} -\Delta y = 0, & \text{in } \Omega, \\ \partial_{\mathbf{n}} y = \alpha(u^4 - y^4), & \text{on } \Gamma. \end{cases}$$

The nonlinearity y^4 occurs in the boundary condition, while the heat conduction equation itself is linear.

Example 3.4 (Simplified superconductivity).

Example 3.5 (Control of stationary flows).

3.1.2.2 Problems involving semilinear parabolic equations

Quick notes

Primal-dual active set strategies, whose the exposition now leads to the systems of linear equations to be solved.

Chapter 4

Shape Optimization

Chapter 5

Topology Optimization

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