# Mathematical Optimization – Toán Tối Ưu

### Nguyễn Quản Bá Hồng\*

#### Ngày 4 tháng 11 năm 2024

#### Tóm tắt nội dung

This text is a part of the series Some Topics in Advanced STEM & Beyond: URL: https://nqbh.github.io/advanced\_STEM/.
Latest version:

• Mathematical Optimization – Toán Tối Ưu.

PDF: url: https://github.com/NQBH/advanced\_STEM\_beyond/blob/main/optimization/NQBH\_mathematical\_optimization.pdf.

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### 1 Wikipedia

# 2 Mathematical Optimization

Community - Cộng đồng. MARC QUINCAMPOIX, CÉDRIC VILLANI.

<sup>\*</sup>A Scientist & Creative Artist Wannabe. E-mail: nguyenquanbahong@gmail.com. Bến Tre City, Việt Nam.

#### Resources - Tài nguyên.

- 1. [Vil03]. CÉDRIC VILLANI. Topics in Optimal Transportation.
  - Preface. Optimal mass transportation was born in France in 1781, with a very famous paper by Gaspard Monge, Mémoire sur la théorie des déblais et des remblais. Since, become a classical subject in probability theory, economics, & optimization. Gained extreme popularity, since many researches in different areas of mathematics understood that optimal mass transportation was strongly linked to their subject. A precise birthdate for this revival: 1987 note by Yann Brenier, Décomposition polaire et réarrangement des champs de vecteurs paved the way towards a beautiful interplay between PDEs, fluid mechanics, geometry, probability theory, & function analysis, developed over last 10 years, through contributions of a number of authors, with optimal transportation problems as a common denominator. 2 volumes of Mass transportation problems by Rachev & Rüschenderf depicting many applications of Monge-Kantorovich distance to various problems, together with classical theory of optimal transportation problem in a very abstract setting; survey by Evans, which can also be considered as an introduction to subject, describes several applications of L¹ theory (i.e., when cost function is a distance), extremely clear lecture notes by Ambrosio, centered on L¹ theory from point of view of calculus of variations, lecture notes by Urbas a marvelous reference for regularity theory of Monge-Ampère equation arising in mass transportation.
  - Introduction. Formulation of optimal transportation problem. Assume given a pile of sand, & a hole having to be completely filled up with the sand. Obviously pile & hole must have same volume. Normalize mass of pile = 1. Will model both pile & hole by probability measures  $\mu, \nu$ , defined respectively on some measure spaces X, Y. Whenever A, B: measurable subsets of X, Y, resp.,  $\mu[A]$  gives a measure of how much sand is located inside  $A, \nu[B]$  of how much sand can be piled in B. Moving sand around needs some effort, modeled by a measurable cost function defined on  $X \times Y$ . Informally, c(x, y) tells how much it costs to transport 1 unit of mass from location x to location y. Natural to assume at least: c is measurable & nonnegative. Should not a priori exclude the possibility that c takes infinite values, & so c should be a measurable map from  $X \times Y$  to  $\mathbb{R} \cup \{+\infty\}$ .

**Problem 1** (Central question). How to realize transportation at minimal cost?

Before studying this question, have to make clear what a way of transportation, or a transference plan, is. Will model transference plans by probability measures  $\pi$  on the product space  $X \times Y$ . Informally,  $d\pi(x,y)$  measures amount of mass transferred from location x to location y. Do not a priori exclude the possibility that some mass located at point x may be split into several parts (several possible destination y's). For a transference plan  $\pi \in P(X \times Y)$  to be admissible, of course necessary that all the mass taken from point x coincide with  $d\mu(x)$ , & all the mass transferred to y coincide with  $d\nu(y)$ , i.e.,  $\int_Y d\pi(x,y) = d\mu(x)$ ,  $\int_X d\pi(x,y) = d\nu(y)$ . More rigorously, require  $\pi[A \times Y] = \mu[A]$ ,  $\pi[X \times B] = \nu[B]$  for all measurable subsets  $A \subset X$  &  $B \subset Y$ . Equivalent to stating: for all functions  $\phi$ ,  $\psi$  in a suitable class of test functions,

$$\int_{X \times Y} \phi(x) + \psi(y) \, d\pi(x, y) = \int_{X} \phi(x) \, d\mu(x) + \int_{Y} \psi(y) \, d\nu(y). \tag{1}$$

In general, the natural set of admissible test functions for  $(\phi, \psi)$  is  $L^1(d\mu) \times L^1(d\nu)$ , or equivalently,  $L^{\infty}(d\mu) \times L^{\infty}(d\nu)$ . In most situations of interest, this class can be narrowed to just  $C_b(X) \times C_b(Y)$ , or  $C_0(X) \times C_0(Y)$ . Those probability measures  $\pi$  satisfying  $\pi[A \times Y] = \mu[A]$ ,  $\pi[X \times B] = \nu[B]$  are said to have marginals  $\mu, \nu$ , & will be the admissible transference plans. Denote the set of all such probability measures by  $\Pi(\mu, \nu) := \{\pi \in P(X \times Y); \pi[A \times Y] = \mu[A], \pi[X \times B] = \nu[B] \text{ holds for all measurable } A, B\} \neq \emptyset$  since tensor product  $\mu \otimes \nu \in \Pi(\mu, \nu)$ , corresponding to the most stupid transportation plan that one may imagine: any piece of sand, regardless of its location, is distributed over the entire hole, proportionally to the depth. A clear mathematical def of basic problem:

**Problem 2** (Kantorovich's optimal transportation problem). Minimize  $I[\pi] = \int_{X \times Y} c(x, y) d\pi(x, y)$  for  $\pi \in \Pi(\mu, \nu)$ .

This minimization problem was studied in 40s by Kantorovich awarded a Nobel prize for related work in economics. The optimal transference problem is related to basic questions in economics becomes clear if one thinks of  $\mu$  as a density of production units, & of  $\nu$  as an adensity of consumers. For a given transference plan  $\pi$ , the nonnegative (possibly infinite) quantity  $I[\pi]$  is called the *total transportation cost* associated to  $\pi$ . The *optimal transportation cost* between  $\mu$ ,  $\nu$  is the value  $\mathcal{T}_{c}(\mu,\nu) := \inf_{\pi \in \Pi(\mu,\nu)} I[\pi]$ . The optimal  $\pi$ 's, i.e., those s.t.  $I[\pi] = \mathcal{T}_{c}(\mu,\nu)$ , if they exist, will be called *optimal transference plans*.

Translate Kantorovich problem into its probabilistic equivalent:

**Problem 3** (Probabilistic interpretation). Given 2 probability measures  $\mu, \nu$ , minimize expectation  $I(U, V) = \mathbb{E}[c(U, V)]$  over all pairs (U, V) of random variables U in X, V in Y, s.t.  $law(U) = \mu$ ,  $law(V) = \nu$ .

Basic probabilistic theory. a random variable U in X is a measurable map with values in X, defined on a probability space  $\Omega$  equipped with a probability measure  $\mathbb{P}$ , that the law of U is the probability measure  $\mu$  on X defined by  $\mu[A] := \mathbb{P}[U^{-1}(A)]$ , & the expectation stands for the integral w.r.t.  $\mathbb{P}$ . Transference plans  $\pi \in \Pi(\mu, \nu)$  are all possible laws of the couple (U, V). Such a  $\pi$  is often said to be the *joint law* of random variables U, V; also says that it constitutes a *coupling* of U, V.

Kantorovich's problem is a relaxed version of the original mass transportation problem considered by Monge. Monge's problem is just the same as Kantorovich's, except for 1 thing: additionally required: no mass be split. I.e., to each location

<sup>&</sup>lt;sup>1</sup>the process of moving something from one place, person or use to another.

x is associated a unique destination y. In terms of random variables, this requirement means that we ask for V to be a function of U in  $I(U,V) = \mathbb{E}[c(U,V)]$ . In terms of transference plans, it means that we ask for  $\pi$  in  $I[\pi]$  to have special form  $d\pi(x,y) = d\pi_T(x,y) \equiv d\mu(x)\delta[y = T(x)]$ , where T is a measurable map  $X \to Y$ .

- Chap. 1: Kantorovich Duality.
- Chap. 2: Geometry of Optimal Transportation.
- Chap. 3: Brenier's Polar Factorization Theorem.
- Chap. 4: Monge-Ampère Equation.
- Chap. 5: Displacement Interpolation & Displacement Convexity.
- Chap. 6: Geometric & Gaussian Inequalities.
- Chap. 7: Metric Side of Optimal Transportation.
- Chap. 8: A Differential Point of View on Optimal Transportation.
- Chap. 9: Entropy Production & Transportation Inequalities.
- Chap. 10: Problems.

## 3 Linear Programming – Quy Hoạch Tuyến Tính

**Definition 1** (Linear programming). "Linear programming (LP), also called linear optimization, is a method to achieve the best outcome, e.g., maximum profit or lower cost, in a mathematical model whose requirements  $\mathcal{E}$  objective are represented by linear relationships. Linear programming is a special case of mathematical programming  $\equiv$  mathematical optimization." – Wikipedia/linear programming

More formally, linear programming is a technique for the optimization of a linear linear objective function, subject to linear equality & linear inequality constraints. Its feasible region is a convex polytope, which is a set defined as the intersection of finitely many half spaces, each of which is defined by a linear inequality. Its objective function is a real-valued affine (linear) function defined on this polytope. A linear programming algorithm finds a point in the polytope where this function has the largest (or smallest) value if such a point exists.

Linear programs are problems that can be expressed in standard form as

Find a vector 
$$\mathbf{x}$$
 that maximizes/minimizes  $\mathbf{c}^{\top}\mathbf{x}$  subject to  $A\mathbf{x} \leq \mathbf{b} \ \& \ \mathbf{x} \geq \mathbf{0}$ . (lp)

Here the components of  $\mathbf{x}$  are the variables to be determined,  $\mathbf{b}$ ,  $\mathbf{c}$  are given vectors, & A is a given matrix. The function whose value is to be maximized ( $\mathbf{x} \mapsto \mathbf{c}^{\top} \mathbf{x}$  in this case) is called the objective function. The constraint  $A\mathbf{x} \leq \mathbf{x}$  &  $\mathbf{x} \geq \mathbf{0}$  specify a convex polytope over which the objective function is to be optimized.

Linear programming can be applied to various fields of study, which is widely used in mathematics &, to a lesser extent, in business, economics, & to some engineering problems. There is a close connection between linear programs, eigenequations, John von Neumann's general equilibrium model, & structural equilibrium models (see dual linear program). Industries using linear programming models include transportation, energy, telecommunications, & manufacturing. It has proven useful in modeling diverse types of problems in planning, routing, scheduling, assignment, & design.

Định nghĩa 1 (Quy hoạch tuyến tính). Bài toán quy hoạch tuyến tính là bài toán tìm GTLN/GTNN của hàm mục tiêu trong điều kiện hàm mục tiêu là hàm bậc nhất đối với các biến  $\mathcal E$  mỗi 1 điều kiện ràng buộc là bất phương trình bậc nhất đối với các biến (không kể điều kiện ràng buộc biến thuộc tập số nào, e.g.,  $\mathbb N$ ,  $\mathbb Q$ ,  $\mathbb R$ ,  $\mathbb C$ .

Ta có thể viết bài toán quy hoạch tuyến tính 2 biến x, y về dạng sau:

$$\max T := \alpha x + \beta y \text{ s.t } a_i x + b_i y \le c_i, \ \forall i = 1, 2, \dots, n,$$
 (lp2max)

$$\min T := \alpha x + \beta y \text{ s.t } a_i x + b_i y \le c_i, \ \forall i = 1, 2, \dots, n,$$
 (lp2min)

trong đó các điều kiên ràng buộc đều là các bất phương trình bậc nhất đối với x, y. See also:

- Problem: Inequation & Linear System of Inequations Bài Tập: Bất Phương Trình & Hệ Bất Phương Trình.

  Folder: Elementary STEM & Beyond/Elementary Mathematics/grade 10/linear system inequations/problem: [pdf²][TFX³].
  - ∘ Problem & Solution: Inequation & Linear System of Inequations Bài Tập & Lời Giải: Bất Phương Trình & Hệ Bất Phương Trình.

Folder: Elementary STEM & Beyond/Elementary Mathematics/grade 10/linear system inequations/solution: [pdf<sup>4</sup>][T<sub>F</sub>X<sup>5</sup>].

<sup>&</sup>lt;sup>2</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_10/linear\_system\_inequations/problem/NQBH\_linear\_system\_inequations\_problem.pdf.

<sup>&</sup>lt;sup>3</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_10/linear\_system\_inequations/problem/NQBH\_linear\_system\_inequations\_problem.tex.

<sup>&</sup>lt;sup>4</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_10/linear\_system\_inequations/solution/NQBH\_linear\_system\_inequations\_solution.pdf.

 $<sup>^5 \</sup>mathrm{URL}$ : https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_10/linear\_system\_inequations/solution/NQBH\_linear\_system\_inequations\_solution.tex.

- Problem: Mathematical Optimization Bài Tập: Ứng Dụng Toán Học Để Giải Quyết 1 Số Bài Toán Tối Ưu.
  - $Folder: \ Elementary \ STEM \ \& \ Beyond/Elementary \ Mathematics/grade \ 12/optimization/problem: \ [pdf^6][T_EX^7].$
  - o Problem & Solution: Mathematical Optimization Bài Tập & Lời Giải: Ứng Dụng Toán Học Để Giải Quyết 1 Số Bài Toán Tối Ưu.

Folder: Elementary STEM & Beyond/Elementary Mathematics/grade 12/optimization/solution: [pdf<sup>8</sup>][T<sub>E</sub>X<sup>9</sup>].

### 3.1 How to solve some linear programmings – Cách giải 1 số bài toán quy hoạch tuyến tính

Có thể giải 1 số bài toán quy hoạch tuyến tính dạng (lp2max) hay (lp2min) theo 2 bước:

- 1. Xác định miền nghiệm  $S \subset \mathbb{R}^2$  của hệ bất phương trình  $a_i x + b_i y \leq c_i, \forall i = 1, \dots, n$ .
- 2. Tìm điểm  $(x,y) \in S$  sao cho biểu thức  $T = T(x,y) = \alpha x + \beta y$  có GTLN ở bài toán (lp2max) hoặc có GTNN ở bài toán (lp2min).

Khi miền nghiệm S là đa giác (polygon), biểu thức  $T(x,y) = \alpha x + \beta y$  đạt GTLN/GTNN (gộp chung gọi là *cực trị*) tại  $(x,y) \in \mathbb{R}^2$  là tọa độ 1 trong các đỉnh của đa giác đó. Khi đó, bước 2 có thể được thực hiện như sau:

- (a) Xác định tọa độ các đỉnh của đa giác đó.
- (b) Tính giá trị của biểu thức  $T(x,y) = \alpha x + \beta y$  tại các đỉnh của đa giác đó.
- (c) So sánh các giá trị & kết luận.

[Thá+25, Chuyên đề II, §1, LT1-3, 1., 2., 3., 4., 5., pp. 20-25].

## 4 Control Theory – Lý Thuyết Điều Khiển

"Control theory is a field of control engineering & applied mathematics that deals with the control of dynamical systems in engineered processes & machines. The objective is to develop a model or algorithm governing the application of system inputs to drive the system to a desired state, while minimizing any delay, overshoot, or steady-state error & ensuring a level of control stability; often with the aim to achieve a degree of optimality.

To do this, a *controller* with the requisite corrective behavior is required. This controller monitors the controlled process variable (PV), & compares it with the reference or set point (SP). The difference between actual & desired value of the process variable, called the *error* signal, or SP-PV error, is applied as feedback to generate a control action to bring the controlled process variable to the same value as the set point. Other aspects which are also studied are controllability & observability. Control theory is used in control system engineering to design automation that have revolutionized manufacturing, aircraft, communications, & other industries, & created new fields such as robotics.

Extensive use is usually made of a diagrammatic style known as the block diagram. In it the transfer function, also known as the system function or network function, is a mathematical model of the relation between the input & output based on the differential equations describing the system.

Control theory dates from the 19th century, when the theoretical basis for the operation of governors was 1st described by James Clerk Maxwell. Control theory was further advanced by Edward Routh in 1874, Charles Sturm & in 1895, Adolf Hurwitz, who all contributed to the establishment of control stability criteria; & from 1922 onwards, the development of PID control theory by Nicolas Minorsky. Although a major application of mathematical control theory is in control systems engineering, which deals with the design of process control systems for industry, other applications range far beyond this. As the general theory of feedback systems, control theory is useful wherever feedback occurs – thus control theory also has applications in life sciences, computer engineering, sociology, & operations research." – Wikipedia/control theory

Open-loop & closed-loop (feedback) control. "Fundamentally, there are 2 types of control loop: open-loop control (feed-forward), & closed-loop control (feedback).

In open-loop control, the control action from the controller is independent of the "process output" (or "controlled process variable"). A good example of this is a central heating boiler controlled only by a timer, so that heat is applied for a constant time, regardless of the temperature of the building. The control action is the switching on/off of the boiler, but the controlled variable should be the building temperature, but is not because this is open-loop control of the boiler, which does not give closed-loop control of the temperature.

In closed loop control, the control action from the controller is dependent on the process output. In the case of the boiler analogy this would include a thermostat to monitor the building temperature, & thereby feed back a signal to ensure the controller

 $<sup>^{6} \</sup>mathrm{URL}$ : https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_12/optimization/problem/NQBH\_optimization\_problem.pdf.

<sup>&</sup>lt;sup>7</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_12/optimization/problem/NQBH\_optimization\_problem.tex.

<sup>&</sup>lt;sup>8</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_12/optimization/solution/NQBH\_optimization\_solution.pdf.

<sup>&</sup>lt;sup>9</sup>URL: https://github.com/NQBH/elementary\_STEM\_beyond/blob/main/elementary\_mathematics/grade\_12/optimization/solution/NQBH\_optimization\_solution.tex.

maintains the building at the temperature set on the thermostat. A closed loop controller therefore has a feedback loop which ensures the controller exerts a control action to give a process output the same as the "reference input" or "set point". For this reason, closed loop controllers are also called *feedback controllers*.

The definition of a closed loop control system according to the British Standards Institutin is "a control system possessing monitoring feedback, the deviation signal formed as a result of this feedback being used to control the action of a final control element in such a way as to tend to reduce the deviation to 0."

Likewise; "A Feedback Control System is a system which tends to maintain a prescribed relationship of 1 system variable to another by comparing functions of these variables & using the difference as a means of control."

#### Classical control theory.

# 4.1 Application of $C_0$ -Semigroup in Control Theory – Ứng Dụng của Nửa Nhóm $C_0$ Trong Lý Thuyết Điều Khiển

### 5 $C_0$ Semigroup – Nửa Nhóm $C_0$

#### Resources - Tài nguyên.

1. [AK16]. CUNG THẾ ANH, TRẦN ĐÌNH KẾ. Nửa Nhóm Các Toán Tử Tuyến Tính & Ứng Dụng.

"Ứng dụng của lý thuyết nửa nhóm các toán tử tuyến tính trong lý thuyết điều khiển toán học, bao gồm bài toán điều khiển được, bài toán quan sát, bài toán điều khiển tối ưu, & bài toán ổn định hóa. Nhấn mạnh đến các hệ điều khiển vô hạn chiều, i.e., các hệ điều khiển sinh bởi các PDEs." – [AK16, Chap. IV: Ứng Dụng Trong Lý Thuyết Điều Khiển]

# 6 Feedback Control – Kiểm Soát Phản Hồi/Điều Khiển Hồi Tiếp

#### Resources - Tài nguyên.

1. [Ray07]. J.-P. RAYMOND. Feedback Boundary Stabilization of 3D Incompressible NSEs.

Study local stabilization of 3D NSEs around an unstable stationary solution  $\mathbf{w}$ , by means of a feedback boundary control. 1st determine a feedback law for the linearized system around  $\mathbf{w}$ . Show: this feedback provides a local stabilization of NSEs. To deal with the nonlinear term, the solutions to the closed loop system must be in  $H^{\frac{3}{2}+\varepsilon,\frac{3}{4}+\frac{\varepsilon}{2}}(Q)$  with  $\varepsilon > 0$ . Such a regularity is achieved with a feedback obtained by minimizing a functional involving a norm of the state variable strong enough. The feedback controller cannot be determined by a well posed Riccati equation. Here choose a controller at t=0, is achieved by choosing a time varying control operator in a neighborhood of t=0.

Keywords: Dirichlet control; Navier-Stokes equations; Feedback control; Stabilization; Riccati equation.

An important issue in control theory is the controllability of systems. The local stability of 3D NSEs in a neighborhood of an unstable stationary solution may be deduced from this controllability result. Another important issue is the characterization of stabilizing feedback control laws, pointwise in time.

## 7 Optimal Control – Điều Khiển Tối Ưu

#### Resources - Tài nguyên.

- 1. [LT00]. IRENA LASIECKA, ROBERTO TRIGGIANI. Control Theory for PDEs: Continuous & Approximation Theories II: Abstract Hyperbolic-Like Systems Over a Finite Time Horizon.
- 2. [Lio69]. Jacques-Louis Lions. Quelques méthodes de résolution des problèmes aux limites nonlinéaires Some Methods for Solving Nonlinear Boundary Problems.
- 3. [Lio71]. JACQUES-LOUIS LIONS. Optimal control of systems governed by PDEs.
- 4. [Trö10]. Fredi Tröltzsch. Optimal Control of PDEs.

**Definition 2** (Optimal control theory). "Optimal control theory is a branch of control theory that deals with finding a control for a dynamical system over a period of time s.t. an objective function is optimized. It has numerous applications in science, engineering, & operational research. E.g., the dynamical system might be a spacecraft with controls corresponding to rocket thrusters, & the objective might be to reach the Moon with minimum fuel expenditure. Or the dynamical system could be a nation's economy, with the objective to minimize unemployment; the controls in this case could be fiscal & monetary policy. A dynamical system may also be introduced to embed operations research problems within the framework of optimal control theory."

— Wikipedia/optimal control

"Optimal control is an extension of the calculus of variations, & is a mathematical optimization method for deriving control policies. The method is largely due to the work of Lev Pontryagin & Richard Bellman in the 1950s, after contributions to calculus of variations by Edward J. McShane. Optimal control can be seen as a control strategy in control theory." – Wikipedia/optimal control

General method. Optimal control deals with the problem of finding a control law for a given system s.t. a certain optimality criterion is achieved. A control problem includes a cost functional that is a function of state & control variables. An optimal control is a set of differential equations describing the paths of the control variables that minimize the cost function. The optimal control can be derived using Pontryagin's maximum principle (a necessary condition also known as Pontryagin's minimum principle or simply Pontryagin's principle), or by solving the Hamilton–Jacobi–Bellman equation (a sufficient condition).

**Example 1.** Consider a car traveling in a straight line on a hilly road. Question: How should the driver press the accelerator pedal in order to minimize the total traveling time? The term control law refers specifically to the way in which the driver presses the accelerator & shifts the gears. The system consists of both the car & the road, & the optimality criterion is the minimization of the total traveling time. Control problems usually include ancillary constraints. E.g., the amount of available fuel might be limited, the accelerator pedal cannot be pushed through the floor of the car, speed limits, etc.

A proper cost function will be a mathematical expression giving the traveling time as a function of the speed, geometrical considerations, & initial conditions of the system. Constraints are often interchangeable with the cost function.

Another related optimal control problem may be to find the way to drive the car so as to minimize its fuel consumption, given that it must complete a given course in a time not exceeding some amount. Yet another related control problem may be to minimize the total monetary cost of completing the trip, given assumed monetary prices for time & fuel.

An abstract framework. Minimize the continuous-time cost functional

$$J(t_0, t_f, \mathbf{x}(\cdot), \mathbf{u}(\cdot)) := E(\mathbf{x}(t_0), t_0, \mathbf{x}(t_f), t_f) + \int_{t_0}^{t_f} F(t, \mathbf{x}(t), \mathbf{u}(t)) \, \mathrm{d}t, \tag{2}$$

subject to the 1st-order dynamic constraints (the state equation)

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)),\tag{3}$$

the algebraic path constraints

$$\mathbf{h}(t, \mathbf{x}(t), \mathbf{u}(t)) \le \mathbf{0},\tag{4}$$

& the endpoint conditions

$$\mathbf{e}(t_0, \mathbf{x}(t_0), t_f, \mathbf{x}(t_f)) = \mathbf{0},\tag{5}$$

where  $\mathbf{x}(t)$ : the state,  $\mathbf{u}(t)$  is the control, t: the independent variable (generally speaking, time),  $t_0$ : the initial time, &  $t_f$ : the terminal time. The terms E, F are called the endpoint cost & running cost, respectively. In the calculus of variations, E, F are referred to as the Mayer term & the Lagrangian, respectively. Furthermore, it is noted that the path constraints are in general inequality constraints & thus may not be active (i.e., =0) at the optimal solution. It is also noted that the optimal control problem as stated above may have multiple solutions (i.e., the solution may not be unique). Thus, it is most often the case that any solution  $(t_0^*, t_f^*, \mathbf{x}^*(t), \mathbf{u}^*(t))$  to the optimal control problem is locally minimizing/minimizer.

#### 7.1 Linear Quadratic Control

A special case of the general nonlinear optimal control problem is the linear quadratic (LQ) optimal control problem. The LQ problem is stated as follows. Minimize the quadratic continuous-time cost functional

$$J = \frac{1}{2} \mathbf{x}^{\top}(t_{\mathrm{f}}) S_{\mathrm{f}} \mathbf{x}(t_{\mathrm{f}}) + \frac{1}{2} \int_{t_{0}}^{t_{\mathrm{f}}} \mathbf{x}^{\top}(t) Q(t) \mathbf{x}(t) + \mathbf{u}^{\top}(t) R(t) \mathbf{u}(t) \,\mathrm{d}t, \tag{6}$$

subject to the linear 1st-order dynamic constraints

$$\begin{cases} \dot{\mathbf{x}}(t) = A(t)\mathbf{x}(t) + B(t)\mathbf{u}(t), \\ \mathbf{x}(t_0) = \mathbf{x}_0. \end{cases}$$
 (7)

A particular form of the LQ problem arising in many control system problems is that of the linear quadratic regulator (LQR) where all of the matrices (i.e., A, B, Q, R) are constant, the initial time is arbitrarily set to 0, & the terminal time is taken in the limit  $t_f \to 0$  (this last assumption is what is known as infinite horizon). The LQR problem is stated as follows. Minimize the infinite horizon quadratic continuous-time cost functional

$$J = \frac{1}{2} \int_0^\infty \mathbf{x}^\top(t) Q \mathbf{x}(t) + \mathbf{u}^\top(t) R \mathbf{u}(t) dt,$$
 (8)

subject to the linear time-invariant 1st-order dynamic constraints

$$\begin{cases} \dot{\mathbf{x}}(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \\ \mathbf{x}(t_0) = \mathbf{x}_0. \end{cases}$$
(9)

In the finite-horizon case the matrices are restricted in that Q, R are positive semi-definite & positive definite, respectively. In the infinite-horizon case, however, the matrices Q, R are not only positive-semidefinite & positive-definite, respectively, but are

also constant. These additional restrictions on Q, R in the infinite-horizon case are enforced to ensure that the cost functional remains positive. Furthermore, in order to ensure that the cost function is bounded, the additional restriction is imposed that the pair (A, B) is controllable. Note that the LQ or LQR cost functional can be thought of physically as attempting to minimize the control energy (measured as a quadratic form).

The infinite horizon problem, i.e., LQR, may seem overly restrictive & essentially useless because it assumes that the operator is driving the system to 0-state & hence driving the output of the system to 0. This is indeed correct. However the problem of driving the output to a desired nonzero level can be solved *after* the zero output one is. In fact, can prove that this secondary LQR problem can be solved in a very straightforward manner. It has been shown in classical optimal control theory that the LQ (or LQR) optimal control has the feedback form

$$\mathbf{u}(t) = -K(t)\mathbf{x}(t),\tag{10}$$

where K(t) is a properly dimensioned matrix, given as

$$K(t) = R^{-1}B^{\mathsf{T}}S(t),$$
 (11)

& S(t) is the solution of the differential Riccati equation. The differential Riccati equation is given as

$$\dot{S}(t) = -S(t)A - A^{\top}S(t) + S(t)BR^{-1}B^{\top}S(t) - Q.$$
(12)

For the finite horizon LQ problem, the Riccati equation is integrated backward in time using the terminal boundary condition

$$S(t_{\rm f}) = S_{\rm f}.\tag{13}$$

For the infinite horizon LQR problem, the differential Riccati equation is replaced with the *algebraic* Riccati equation (ARE) given as

$$-SA - A^{\mathsf{T}}S + SBR^{-1}B^{\mathsf{T}}S - Q = \mathbf{0}. \tag{14}$$

Understanding that the ARE arises from infinite horizon problem, the matrices A, B, Q, R are all constant. It is noted that there are in general multiple solutions to the algebraic Riccati equation & the positive definite (or positive semi-definite) solution is the one that is used to compute the feedback again. The LQ (LQR) problem was elegantly solved by Rudolf E. Kálmán.

#### 7.2 Numerical Methods for Optimal Control

"Optimal control problems are generally nonlinear & therefore, generally do not have analytic solutions, e.g., like the linear-quadratic optimal control problem. As a result, it is necessary to employ numerical methods to solve optimal control problems. In the early years of optimal control (c. 1950s–1980s) the favored approach for solving optimal control problems was that of indirect methods. In an indirect method, the calculus of variations is employed to obtain the 1st-order optimality conditions. These conditions result in a 2-point (or, in the case of a complex problem, a multi-point) BVP. This BVP actually has a special structure because it arises from taking the derivative of a Hamiltonian. Thus, the resulting dynamical system is a Hamiltonian system of the form

$$\begin{cases}
\dot{\mathbf{x}} = \partial_{\lambda} H, \\
\dot{\lambda} = -\partial_{\mathbf{x}} H,
\end{cases}$$
(15)

where  $H = F + \lambda^{\top} \mathbf{f} - \mu^{\top} \mathbf{h}$  is the augmented Hamiltonian & in an indirect method, the BVP is solved (using the appropriate boundary or transversality conditions). The beauty of using an indirect method is that the state & adjoint, i.e.,  $\lambda$ , are solved for & the resulting solution is readily verified to be an extremal trajectory. The disadvantage of indirect methods is that the BVP is often extremely difficult to solve (particularly for problems that span large time intervals or problems with interior point constraints). A well-known software program that implements direct methods is BNDSCO.

The approach that has risen to prominence in numerical optimal control since the 1980s is that of so-called *direct methods*. In a direct method, the state or the control, or both, are approximated using an appropriate function approximation (e.g., polynomial approximation or piecewise constant parameterization). Simultaneously, the cost functional is approximated as a *cost function*. Then, the coefficients of the function approximations are treated as optimization variables & the problem is "transcribed" to a nonlinear optimization problem of the form

$$\min F(\mathbf{z}) \tag{16}$$

subject to the algebraic constraints

$$\mathbf{g}(\mathbf{z}) = \mathbf{0}, \ \mathbf{h}(\mathbf{z}) \le \mathbf{0}. \tag{17}$$

Depending upon the type of direct method employed, the size of the nonlinear optimization problem can be quite small (e.g., as in a direct shooting or quasilinearization method), moderate (e.g., pseudospectral optimal control) or may be quite large (e.g., a direct collocation method). In the latter case (i.e., a collocation method), the nonlinear optimization problem may be literally thousands  $a \cdot 10^3$  to tens of thousands  $a \cdot 10^4$  of variables & constraints. Given the size of many NLPs arising from a direct method, it may appear somewhat counter-intuitive that solving the nonlinear optimization problem is easier than solving the BVP. It is, however, the fact that the NLP is easier to solve than the BVP. The reason for the relative ease of computation, particularly of a direct collocation method, is that the NLP is sparse & many well-known software programs exist (e.g., SNOPT) to solve large sparse NLPs. As a result, the range of problems that can be solved via direct methods (particularly direct collocation methods which are very popular these days) is significantly larger than the range of problems that can be solved via indirect methods. In fact,

direct methods have become so popular these days that many people have written elaborate software programs employing these methods. In particular, many such programs include DIRCOL, SOCS, OTIS, GESOP/ASTOS, DITAN., & PyGMO/PyKEP. In recent years, due to the advent of the MATLAB programming language, optimal control software in MATLAB has become more common. Examples of academically developed MATLAB software tools implementing direct methods include RIOTs, DIDO, DIRECT, FALCON.m, & GPOPs, while an example of an industry developed MATLAB tool is PROPT. These software tools have increased significantly the opportunity for people to explore complex optimal control problems both for academic research & industrial problems. Finally, it is noted that general-purpose MATLAB optimization environments such as TOMLAB have made coding complex optimal control problems significantly easier than was previously possible in languages such as C & FORTRAN.

#### 7.3 Discrete-Time Optimal Control

"The examples thus far have shown continuous time systems & control solutions. In fact, as optimal control solutions are now often implemented digitally, contemporary control theory is now primarily concerned with discrete time systems & solutions. The theory of Consistent Approximations provides conditions under which solutions to a series of increasingly accurate discretized optimal control problem converge to the solution of the original, continuous-time problem. Not all discretization methods have this property, even seemingly obvious ones. E.g., using a variable step-size routine to integrate the problem's dynamic equations may generate a gradient which does not converge to 0 (or point in the right direction) as the solution is approached. The direct method RIOTS is based on the Theory of Consistent Approximation.

A common solution strategy in many optimal control problems is to solve for the costate (sometimes called the shadow price)  $\lambda(t)$ . The costate summaries in 1 number the marginal value of expanding or contracting the state variable next turn. The marginal value is not only the gains accruing to it next turn but associated with the duration of the program. It is nice when  $\lambda(t)$  can be solved analytically, but usually, the most one can do is describe it sufficiently well that the intuition can grasp the character of the solution & an equation solver can solve numerically for the values.

Having obtained  $\lambda(t)$ , the turn-t optimal value for the control can usually be solved as a differential equation conditional on knowledge of  $\lambda(t)$ . Again it is infrequent, especially in continuous-time problems, that one obtains the value of the control or the state explicitly. Usually, the strategy is to solve for thresholds & regions that characterize the optimal control & use a numerical solver to isolate the actual choice values in time.

**Example 2.** "Consider the problem of a mine owner who must decide at what rate to extract ore from their mine. They own rights to the ore from date 0 to date T. At date 0 there is  $x_0$  ore in the ground,  $\mathcal{E}$  the time-dependent amount of ore x(t) left in the ground declines at the rate of u(t) that the mine owner extracts it. The mine owner extracts ore at  $\cos \frac{u(t)^2}{x(t)}$  (the cost of extraction increasing with the square of the extraction speed  $\mathcal{E}$  the inverse of the amount of ore left)  $\mathcal{E}$  sells ore at a constant price p. Any ore left in the ground at time T cannot be sold  $\mathcal{E}$  has no value (there is no "scrap value"). The owner chooses the rate of extraction varying with time u(t) to maximize profits over the period of ownership with no time discounting. See discrete-time version vs. Continuous-time version." – Wikipedia/optimal control/finite time

# 7.4 Optimal Control for PDEs – Điều Khiển Tối Ưu Cho Phương Trình Vi Phân Đạo Hàm Riêng

Resources - Tài nguyên.

- 1. [Lio71]. Jacques-Louis Lions. Optimal control of systems governed by PDEs.
- 2. [Trö10]. Fredi Tröltzsch. Optimal Control of PDEs.

#### 7.4.1 Optimal Control for Navier-Stokes Equations – Điều Khiển Tối Ưu Cho Phương Trình Navier-Stokes

#### 8 Stochastic Control

Community - Công đồng. MICHAEL HINTERMÜLLER, CAROLINE GEIERSBACH.

Stochastic control or stochastic optimal control is a subfield of control theory that deals with the existence of uncertainty either in observations or in the noise that drives the evolution of the system. The system designer assumes, in a Bayesian probability-driven fashion, that random noise with known probability distribution affects the evolution & observation of the state variables. Stochastic control aims to design the time path of the controlled variables that performs the desired control task with minimum cost, somehow defined, despite the presence of this noise. The context may be either discrete time or continuous time.

Certainty equivalence. "An extremely well-studied formulation in stochastic control is that of linear quadratic Gaussian control. Here the model is linear, the objective function is the expected value of a quadratic form, & the disturbances are purely additive. A basic result for discrete-time centralized systems with only additive uncertainty is the certainty equivalence property: that the optimal control solution in this case is the same as would be obtained in the absence of the additive disturbances. This property is applicable to all centralized systems with linear equations of evolution, quadratic cost function, & noise entering the model only additively; the quadratic assumption allows for the optimal control laws, which follow the certainty-equivalence property to be linear functions of the observations of the controllers.

Any deviation from the above assumptions – a nonlinear stat equation, a non-quadratic objective function, noise in the multiplicative parameters of the model, or decentralization of control – causes the certainty equivalence property not to hold. E.g., its failure to hold for decentralized control was demonstrated in Witsenhausen's counterexample." – Wikipedia/stochastic controlcertainty equivalence.

**Discrete time.** "In a discrete-time context, the decision-maker observes the state variable, possibly with observational noise, in each time period. The objective may be to optimize the sum of expected values of a nonlinear (possibly quadratic) objective function over all the time periods from the present to the final period of concern, or to optimize the value of the objective function as of the final period only. At each time period new observations are made, & the control variables are to be adjusted optimally. Finding the optimal solution for the present time may involve iterating a matrix Riccati equation backwards in time from the last period to the present period.

In the discrete-time case with uncertainty about the parameter values in the transition matrix (giving the effect of current values of the state variables on their own evolution) &/or the control response matrix of the state equation, but still with a linear state equation & quadratic objective function, a Riccati equation can still be obtained for iterating backward to each period's solution even though certainty equivalence does not apply. The discrete-time case of a non-quadratic loss function but only additive disturbances can also be handled, albeit with more complications.

**Example 3.** A typical specification of the discrete-time stochastic linear quadratic control problem is to minimize

$$\mathbf{E}_1 \sum_{t=1}^{S} y_t^{\top} Q y_t + u_t^{\top} R u_t, \tag{18}$$

where  $E_1$  is the expected value operator conditional on  $y_0$ , S: the time horizon, subject to the state equation  $y_t = A_t y_{t-1} + B_t u_t$ .

Continuous time. "If the model is in continuous time, the controller knows the state of the system at each instant of time. The objective is to maximize either an integral of, e.g., a concave function of a state variable over a horizon from time 0 (the present) to a terminal time T, or a concave function of a state variable at some future date T. As time evolves, new observations are continuously made & the control variables are continuously adjusted in optimal fashion."

Stochastic model predictive control. "In the literature, there are 2 types of MPCs for stochastic systems; Robust model predictive control & Stochastic Model Predictive Control (SMPC). Robust model predictive control is a more conservative method which considers the worst scenario in the optimization procedure. However, this method, similar to other robust controls, deteriorates the overall controller's performance & also is applicable only for systems with bounded uncertainties. The alternative method, SMPC, considers soft constraints which limit the risk of violation by a probabilistic inequality.

**Example 4** (Stochastic model predictive control in finance). "In a continuous time approach in a finance context, the state variable in the stochastic differential equation is usually wealth or net worth, & the controls are the shares placed at each time in the various assets. Given the asset allocation chosen at any time, the determinants of the change in wealth are usually the stochastic returns to assets & the interest rate on the risk-free asset. The field of stochastic control has developed greatly since the 1970s, particularly in its applications to finance. Robert Merton used stochastic control to study optimal portfolios of safe & risky assets. Merton's portfolio problem & that of Black Scholes changed the nature of the finance literature. Influential mathematical textbook treatments were by Fleming & Rishel, & by Fleming & Soner. These techniques were applied by Stein to the financial crisis of 2007–08.

The maximization, say of the expected logarithm of net work at a terminal date T, is subject to stochastic processes on the components of wealth. In this case, in continuous time Itô's equation is the main tool of analysis. In the case where the maximization is an integral of a concave function of utility over an horizon (0,T), dynamic programming is used. There is no certainty equivalence as in the older literature, because the coefficients of the control variables – i.e., the returns received by the chosen shares of assets – are stochastic.

### 9 Shape Optimization – Tối Ưu Hình Dạng

#### Resources - Tài nguyên.

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- 10. [Wal15]. Shawn W. Walker. The Shapes of Things.

**Differential equations on surfaces.** Differential geometry is useful for understanding mathematical models containing geometric PDEs, e.g., surface/manifold version of the standard Laplace equation, which requires the development of the surface gradient & surface Laplacian operators – the usual gradient  $\nabla$  & Laplacian  $\Delta = \nabla \cdot \nabla$  operators defined on a surface (manifold) instead of standard Euclidean space  $\mathbb{R}^n$ . Advantage: provide alternative formulas for geometric quantities, e.g., the summed (mean) curvature, that are much clearer than the usual presentation of texts on differential geometry.

**Differentiating w.r.t. Shape.** The approach to differential geometry is advantageous for developing the framework of *shape differential calculus* – the study of how quantities change w.r.t. changes of independent "shape variable".

"The framework of shape differential calculus provides the tools for developing the equations of mean curvature flow & Willmore flow, which are geometric flows occurring in many applications such as fluid dynamics & biology." – [Wal15, p. 2]

The shape perturbation  $\delta J(\Omega; V)$  is similar to the gradient operator, which is a directional derivative, analogous to  $V \cdot \nabla f$  where V is a given direction, providing information about the local slope, or the sensitivity of a quantity w.r.t. some parameters.

It takes only 2 or 3 numbers to specify a point (x, y) in 2D & a point (x, y, z) in 3D, whereas an "infinite" number of coordinate pairs is needed to specify a domain  $\Omega$ . V is a 2D/3D vector in the scalar function setting; for a shape functional, V is a full-blown function requiring definition at every point in  $\Omega$ . This "infinite dimensionality" is the reason for using the notation  $\delta J(\Omega; V)$  to denote a shape perturbation.  $\delta J(\Omega; V)$  indicates how we should change  $\Omega$  to decrease J, similarly to how  $\nabla f(x, y)$  indicates how the coordinate pair (x, y) should change to decrease f, which opens up the world of shape optimization.

**3 schools of shape optimization.** Cf. engineering shape optimization vs. applied shape optimization [MP10] vs. theoretical shape optimization [SZ92; DZ11].

Shape perturbations allow us to "climb down the hill" in the infinite dimensional setting of shape, which is a powerful tool for producing sophisticated engineering designs in an automatic way.

Extrinsic vs. intrinsic point of views. To make the discussion as clear as possible, we adopt the *extrinsic* point of view: curves & surfaces are assumed to lie in a Euclidean space of higher dimension. The ambient space is 3D Euclidean space. Alternatively, there is the *intrinsic* point of view, i.e., the surface is not assumed to lie in an ambient space, i.e., one is not allowed to reference anything "outside" of the surface when defining it. Moreover, no mathematical structures "outside" of the surface can be utilized. Walker [Wal15] did not adopt the intrinsic view or consider higher dimensional manifolds, general embedding dimensions, etc. for the reasons: [Wal15] is meant as a *practical guide* to differential geometry & shape differentiation that can be used by researchers in other fields.

- [Wal15] is meant to be used as background information for deriving physical models where geometry plays a critical role. Because most physical problems of interest take place in 3D Euclidean space, the extrinsic viewpoint is sufficient.
- Many of the proofs & derivations of differential geometry relations simplify dramatically for 2D surfaces in 3D & require only basic multivariable calculus & linear algebra.
- The concepts of normal vectors & curvature are harder to motivate with the intrinsic viewpoint. What does it meant for a surface to "curve through space" if you cannot talk about the ambient space?
- Walker wants to keep in mind applications of this machinery to geometric PDEs, fluid dynamics, numerical analysis, optimization, etc. An interesting application of this methodology is for the development of numerical methods for mean curvature flow & surface tension driven fluid flow. Ergo (= therefore), the extrinsic viewpoint is often more convenient for computational purposes.
- Walker wants his framework to be useful for analyzing & solving *shape optimization* problems, i.e., optimization problems where geometry/shape is the control variable.

**Prerequisites.** "When reading any mathematical text, the reader must have a certain level of mathematical "maturity" in order to efficiently learn what is in the text.

Example 5 ([Wal15], Sect. 1.2.1, pp. 1–2). Let  $f = f(r,\theta)$  be a smooth function defined on the disk  $B_{R,2}(0,0)$  of radius R in terms of polar coordinates. The integral of f over  $B_{2,R}(0,0)$   $J := \int_{B_{2,R}(0,0)} f \, \mathrm{d}\mathbf{x} = \int_0^{2\pi} \int_0^R f(r,\theta) \, \mathrm{d}r \, \mathrm{d}\theta$  depends on R. Assume f also depends on R, i.e.,  $f = f(r,\theta,R)$  with a physical example: J is the net flow rate of liquid through a pipe with cross-section  $\Omega$ , then f is the flow rate per unit area  $\mathcal E$  could be the solution of a PDE defined on  $\Omega$ , e.g., a Navier-Stokes fluid flowing in a circular pipe. Advantageous to know the sensitivity of J w.r.t. R, e.g., for optimization purposes. Differentiate J w.r.t. R:

$$\frac{d}{dR}J = \int_0^{2\pi} \left( \frac{d}{dR} \int_0^R f(r,\theta;R) r \, \mathrm{d}r \right) \mathrm{d}\theta = \int_0^{2\pi} \int_0^R f'(r,\theta;R) r \, \mathrm{d}r \, \mathrm{d}\theta + \int_0^{2\pi} f(R,\theta;R) \, \mathrm{d}\theta.$$

The dependence of f on R can more generally be viewed as dependence on  $B_{R,2}(0,0)$ , i.e.,  $f(\cdot;R) \equiv f(\cdot;B_{R,2}(0,0))$ . Rewriting d/dRJ using Cartesian coordinates  $\mathbf{x}$ :

$$\frac{d}{dR}J = \int_{B_{R,2}(0,0)} f'(\mathbf{x};\Omega) \,d\mathbf{x} + \int_{S_{R,2}(0,0)} f(\mathbf{x};\Omega) \,dS(\mathbf{x}),\tag{19}$$

where  $d\mathbf{x}$  is the volume measure,  $dS(\mathbf{x})$  is the surface area measure.

**Example 6** (Surface height function of a hill). Let f = f(x, y) be a function describing the surface height of the hill, where (x, y) are the coordinates of our position. Then, by using basic multivariate calculus, finding a direction that will move us downhill is equivalent to computing the gradient (vector) of  $f \in B$  moving in the opposite direction to the gradient. In this sense, we do not need to "see" the whole function. We just need to locally compute the gradient  $\nabla f$ , analogous to feeling the ground beneath.

**Example 7** (Engineering shape optimization: minimizing drag with Navier–Stokes flow of fluid past a rigid body, [Wal15], pp. 3–5). A shape functional representing the drag:

$$J_{d}(\Omega) := -\mathbf{u}_{out} \cdot \int_{\Gamma_{0}} \boldsymbol{\sigma}(\mathbf{u}, p) \mathbf{n} \, d\Gamma = \frac{2}{Re} \int_{\Omega} |\boldsymbol{\varepsilon}(\mathbf{u})|^{2} \, d\mathbf{x} \ge 0, \tag{20}$$

which physically represents the net force that must be applied to  $\Omega_B$  to keep it stationary while being acted upon by the imposed flow field & represents the total amount of viscous dissipation of energy (per unit of time) in the fluid domain  $\Omega$ . Using the machinery of shape perturbations,  $\delta J_d(\Omega;V)$  indicates how  $J_d$  changes when we perturb  $\Omega$  in the direction V. Hence, we can use this information to change  $\Omega$  in small steps so as to slowly deform  $\Omega$  into a shape that has better (lower) drag characteristics. A numerical computation: 2 large vortices appear behind the body, which indicate a large amount of viscous dissipation, i.e., large drag. The optimization process then computes  $\delta J_d(\Omega^0;V)$  for many different choices of V & chooses the one that drives down  $J_d$  the most. This choice of V is used to deform  $\Gamma_B^0$  into a new shape  $\Gamma_B^1$  at iteration 1, with only a small difference between  $\Gamma_B^0$  &  $\Gamma_B^1$ . This process is repeated many times. Note how the vortices are eliminated by the more slender shape.

- Condition (V)\*\*\*
- Family of transformations  $\{T_s: 0 \le s \le \tau\}$ .
- Perturbed domain  $\Omega_s = \Omega_s(V) = T_s(V)(\Omega)$ .
- Assume that the velocity field V satisfies  $V_D$  and, in addition,  $V \in C^0([0,\tau]; C^1_{loc}(\mathbb{R}^d, \mathbb{R}^d))$  and  $\tau > 0$  is small enough such that the Jacobian  $J_s$  is strictly positive:  $J_s(X) := \det DT_s(X) > 0$ ,  $\forall s \in [0,\tau]$ , where  $DT_s(X)$  is the Jacobian matrix of the transformation  $T_s = T_s(V)$  associated with the velocity vector field V.

#### 9.1 Domain Integrals

• Given  $\varphi \in W^{1,1}_{loc}(\mathbb{R}^d)$ , consider for  $s \in [0,\tau]$  the volume integral

$$J(\Omega_s(V)) := \int_{\Omega_s(V)} \varphi \, d\mathbf{x} = \int_{\Omega} \varphi \circ T_s J_s \, d\mathbf{x}. \tag{21}$$

$$dJ(\Omega; V) = \frac{d}{ds} J(\Omega_s(V))|_{s=0} = \int_{\Omega} \nabla \varphi \cdot V(0) + \varphi \operatorname{div} V(0) \, d\mathbf{x} = \int_{\Omega} \operatorname{div}(\varphi V(0)) \, d\mathbf{x}.$$
 (22)

If  $\Omega$  has a Lipschitzian boundary, by Stokes's theorem:

$$dJ(\Omega; V) = \int_{\Gamma} \varphi V(0) \cdot \mathbf{n} \, d\Gamma. \tag{23}$$

**Theorem 1** ([DZ11], Thm. 4.1, pp. 482–483). Let  $\varphi \in W^{1,1}_{loc}(\mathbb{R}^d)$ . Assume that the vector field  $V = \{V(s) : 0 \le s \le \tau\}$  satisfies condition (V).

- (i) For each  $s \in [0, \tau]$  the map  $\varphi \mapsto \varphi \circ T_s : W^{1,1}_{loc}(\mathbb{R}^d) \to W^{1,1}_{loc}(\mathbb{R}^d)$  and its inverse are both locally Lipschitzian and  $\nabla(\varphi \circ T_s) = *DT_s \nabla \varphi \circ T_s$ .
- (ii) If  $V \in C^0([0,\tau]; C^1_{loc}(\mathbb{R}^d, \mathbb{R}^d))$ , then the map  $s \mapsto J_s : [0,\tau] \to C^0_{loc}(\mathbb{R}^d)$  is differentiable and

$$\frac{dJ_s}{ds} = \left[\nabla \cdot V(s)\right] \circ T_s J_s \in C^0_{loc}(\mathbb{R}^d). \tag{24}$$

Hence the map  $s \mapsto J_s$  belongs to  $C^1([0,\tau]; C^0_{loc}(\mathbb{R}^d))$ .

$$\frac{d}{ds}DT_{s}(X) = DV(s, T_{s}(X))DT_{s}(X), \ DT_{0}(X) = I,$$
(25)

$$\frac{d}{ds}\det DT_s(X) = \operatorname{tr} DV(s, T_s(X)) \det DT_s(X) = \nabla \cdot V(s, T_s(X)) \det DT_s(X), \ \det DT_0(X) = 1. \tag{26}$$

**Theorem 2** ([DZ11], Thm. 4.2, pp. 483–484). Assume that there exists  $\tau > 0$  such that the velocity field V(t) satisfies conditions (V) and  $V \in C^0([0,\tau]; C^1_{loc}(\mathbb{R}^d,\mathbb{R}^d))$ . Given a function  $\varphi \in C(0,\tau; W^{1,1}_{loc}(\mathbb{R}^d)) \cap C^1(0,\tau; L^1_{loc}(\mathbb{R}^d))$  and a bounded measurable domain  $\Omega$  with boundary  $\Gamma$ , the semiderivative of the function  $J_V(s) := \int_{\Omega_s(V)} \varphi(s) \, d\mathbf{x}$  at s = 0 is given by

$$dJ_V(0) = \int_{\Omega} \varphi'(0) + \operatorname{div}(\varphi(0)V(0)) \, d\mathbf{x}, \tag{27}$$

where  $\varphi(0)(\mathbf{x}) := \varphi(0, \mathbf{x})$  and  $\varphi'(0)(\mathbf{x}) := \partial_t \varphi(0, \mathbf{x})$ . In addition,  $\Omega$  is an open domain with a Lipschitzian boundary  $\Gamma$ , then

$$dJ_V(0) = \int_{\Omega} \varphi'(0) \, d\mathbf{x} + \int_{\Gamma} \varphi(0)V(0) \cdot \mathbf{n} \, d\mathbf{x}. \tag{28}$$

#### 9.2 Boundary Integrals

#### 9.3 Material derivatives

Let  $\Omega \subset D$  be a bounded domain,

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#### 11 Miscellaneous

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