Constrained Optimization: from Lagrangian Mechanics to Optimal Control and PDE Constraints*

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Abstract. The history of constrained optimization spans nearly three centuries. The principal warhorse, Lagrange multipliers, was discovered by Lagrange in the Statics section of his famous book on Mechanics from 1788, by applying the idea of virtual velocities to problems in statics with constraints. The idea of virtual velocities, in turn, goes back to a letter of Johann Bernoulli from 1715 to Varignon, in which he announced a very simple rule for solving hundreds of Varignon's problems in the blink of an eye. Varignon then explains this rule in his book published in 1725. Half a century later, Bernoulli's rule was chosen by Lagrange as the general principle for the foundation of his mechanics, with the multipliers as the main tool for treating mechanical constraints. In the second edition of his mechanics, published in 1811, Lagrange stressed the importance of his multipliers also for constrained optimization. In particular, they provide spectacular simplifications of entire chapters of Euler's treatise on Variational Calculus from 1744. Lagrange multipliers is however a much farther reaching concept; we show how one can discover the important primal and dual equations in optimal control and the famous maximum principle of Pontryagin using only Lagrange multipliers. Pontryagin and his group, however, did not discover the maximum principle this way, since they were coming from a completely different area of mathematics. We finally give the complete formulation of PDE constrained optimization based on duality introduced by Lions, and conclude with an outlook on more recent applications.

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Keywords. Variational Methods, Constrained Optimization, Optimal Control, PDE Constrained Optimization.

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*Our intention is not to write a full historical paper, but to highlight the parts of the historical development we find interesting as mathematicians. For full details on the history of constrained optimization with complete references, see [45] and [46].

Contents

1. Lagrange Multipliers Originating from Mechanics

> "Le *Traité de Dynamique* de M. d'Alembert, ... parut en 1743, ... Cette méthode réduit toutes les loix du mouvement des corps à celles de leur équilibre, & ramene ainsi la Dynamique à la Statique" (Lagrange 1788, Seconde Partie, p. 179)

Lagrange's method of multipliers originates from Lagrange's research in mechanics, more precisely his *Mécanique analytique* [33], first published in 1788, with a second, improved edition [34] in 1811/15. In his long introductions, Lagrange traces the following history for his work:

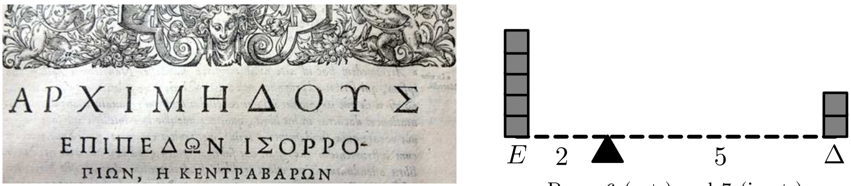
1. Archimedes, Pappus, Varignon: For nearly 2000 years, research in mechanics concerned mainly *Statics*, beginning with the discovery of the law of the *lever* by Archimedes. Then, mainly by researchers as Pappus, Stevin, Roberval and Descartes, theories for the equilibria of ever more complicated "machines" were developed, culminating in the *Nouvelle Mécanique* by Varignon.

2. Galilei, Newton, Leibniz, the Bernoulli brothers, Euler: The next period then concentrated on the *Dynamics* of increasingly complex mechanical systems (mass points, liquids, rigid bodies) with more and more analytical methods (differential equations).

3. Lagrange: Finally, the "principle of d'Alembert" from 1743 reduces problems in dynamics back to problems in statics (see quotation), so that Lagrange's *Mécanique analytique* again started with an extensive "première partie" on statics, comprising nearly 200 pages, as a foundation for the now-called *Lagrangian mechanics* in the second part. The main idea there was the *Principle of Virtual Velocities*, which first appeared in a letter of Joh. Bernoulli from 1715 to Varignon. The extension of this idea to *constrained* mechanical problems then led to the invention of *Lagrange multipliers*.

1.1. Archimedes' Proof for the Lever

The very first great discovery in Statics was made by Archimedes with the law of the lever: *two bodies are in equilibrium if their weights are inversely proportional to their arm lengths* (see Fig. 1 and [1]).



(Opera, printed 1615 in Paris, BGE Ka459) Prop. 6 (rat.) and 7 (irrat.)

FIGURE 1. Archimedes' law for the lever

The proof of Archimedes is very beautiful: He started from the axiom that equal weights at equal distances are in equilibrium (see Fig. 2).

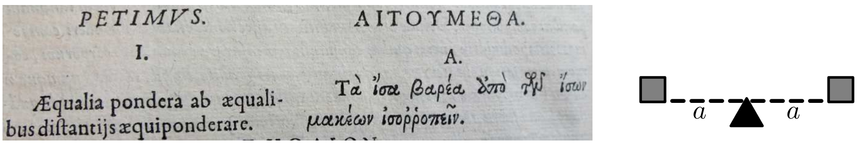


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FIGURE 2. Archimedes' hypothesis

Then, after more axioms, several preliminary propositions and corollaries, he proved his Proposition 6, valid for rational ratios of weights, in two pages of Greek text. His idea was to distribute the weight units left and right in a symmetric way to obtain an overall symmetric configuration (see Fig. 3 for an illustration in the case of a 5 : 2 lever). Fig. 4 shows the corresponding proposition and figure for the ratio 3 : 2, which appear in the 1615 edition of Archimedes' *Opera* (observe that the letters L, E, C, G, D, K of the Latinized version correspond to Archimedes' $\Lambda, E, \Gamma, H, \Delta, K$).

1.2. Virtual Velocities and Joh. Bernoulli's "Regle"

> "... il n'y a pas un seul cas d'equilibre dans toute la mechanique tant des fluides que des solides, qui ne puisse etre expliqué par cette regle ... J'ay

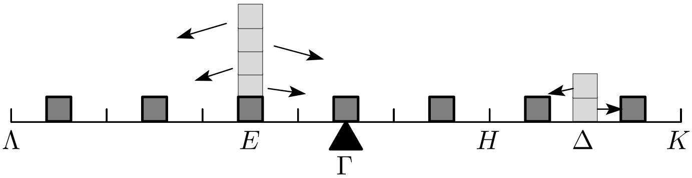
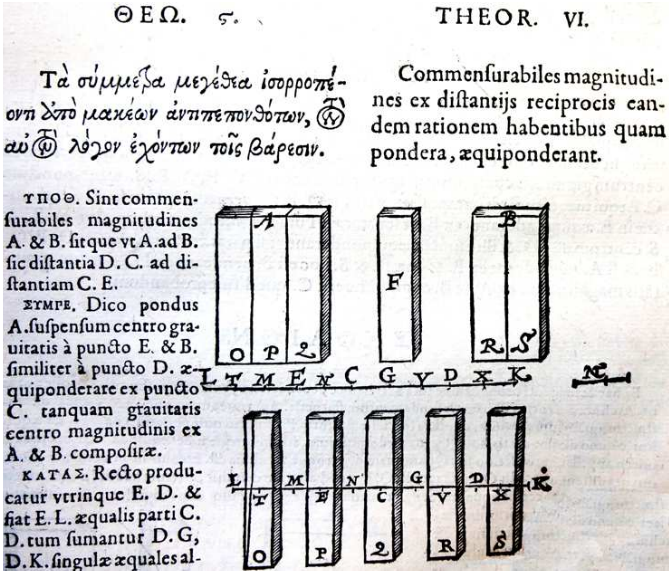


Figure 3. Archimedes' proof of his Prop. 6



ΘΕΩ. ϛ. THEOR. VI.

Τὰ σύμμετρα μεγέθεα ἰσορροπέοντι ἀπὸ μακέων ἀντιπεπονθότων, τὸν αὐτὸν λόγον ἐχόντων τοῖς βάρεσιν.

Commenſurabiles magnitudines ex diſtantijs reciprocis eandem rationem habentibus quam pondera, æquiponderant.

ΥΠΟΘ. Sint commenſurabiles magnitudines A. & B. ſitque vt A. ad B. ſic diſtantia D. C. ad diſtantiam C. E.
ΣΥΜΠΕ. Dico pondus A. ſuſpenſum centro grauitatis à puncto E. & B. ſimiliter à puncto D. æquiponderare ex puncto C. tanquam grauitatis centro magnitudinis ex A. & B. compoſitæ.
ΚΑΤΑΣ. Recto producatur vtrinque E. D. & fiat E. L. æqualis parti C. D. tum ſumantur D. G, D. K. ſingulæ æquales al-

(Opera 1615 (Paris BGE Ka459)

Figure 4. Archimedes' Prop. 6 with figure from the 1615 edition

> donc raison d'appeller le grand et le premier principe de statique sur lequel j'ay fondé ma regle ..." (Joh. Bernoulli in his letter to Varignon, 1715)

> "... je crois pouvoir avancer que tous les principes généraux qu'on pourrait peut-être encore découvrir dans la science de l'équilibre ne seront que le même principe des vitesses virtuelles, envisagé différemment, et dont ils ne différeront que dans l'expression." (Lagrange 1811, Section I, §17)

All the efforts during the centuries after Archimedes in generalizing this result to more and more complicated situations culminated in the work of Pierre Varignon, who elaborated during many decades his *Nouvelle Mécanique* [51], consisting of two heavy volumes published posthumously in 1725 [1], with hundreds of results illustrated on 64 plates of figures (see Fig. 5).

[1]on the frontispiece is written "Dont le projet fut donné en M.DC.LXXXVII".

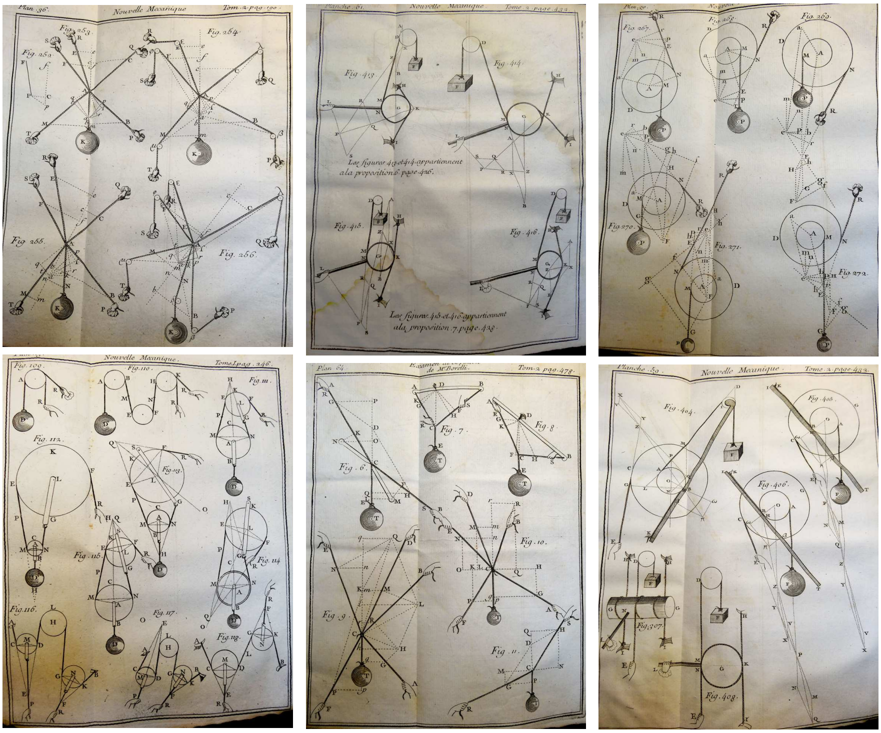


FIGURE 5. Six out of the 64 figure plates from Varignon (1725); (the upper left figure of the upper left plate explains the principle of virtual velocities as in Fig. 1.5 below)

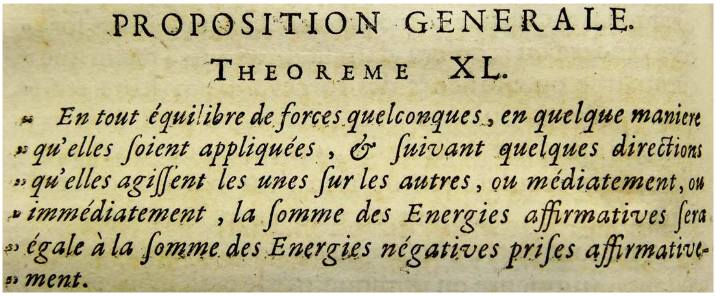
When this work was nearly completed, Joh. Bernoulli explained in a letter to *Mr. le Chev. Renau*, with a copy to Varignon, his “regle” based on the *Virtual Velocities*, which allowed one to replace *all such figures* by *one general equation*. Varignon had some difficulty in admitting that all his work over decades was declared to be an “easy game”[2] and contested the general truth of this rule. Bernoulli then got angry[3] and explained his ideas in more detail, written in a second letter, dated Feb. 26, 1715 [4]. Varignon then included Bernoulli’s “regle” as “Theoreme XL” in “Section IX” (“Corollaire

[2]“Votre *projet d’une nouvelle mechanique* fourmille d’un grand nombre d’exemples, dont quelques uns à en juger par les figures paroissent assez compliqués; mais je vous deffie de m’en proposer un à votre choix, que je ne resolve sur le champ et comme en jouant par ma dite regle.”

[3]“... cependant permettez moy que je vous reproche ici une nonchalance qui vous est arrivé assez souvent en ce que vous portez quelques fois votre jugement un peu à la legere, sans examiner, si ce que vous croyez etre une objection en est veritablement une ; ... c’est donc pour une autre fois que je vous donne cet avertissement à fin que vous soyez à l’avenir sur vos gardes, quand il s’agit de juger...”

[4]Varignon gave in his book the wrong date 1717, which was also copied by Lagrange.

general de la Théorie précedente”) of his book, by saying that, unfortunately, it was too late to rewrite all the rest of the book (see Fig. 6).


PROPOSITION GENERALE.

THEOREME XL.

» *En tout équilibre de forces quelconques, en quelque maniere » qu'elles ſoient appliquées, & ſuivant quelques directions » qu'elles agiſſent les unes ſur les autres, ou médiatement, ou » immédiatement, la ſomme des Energies affirmatives ſera » égale à la ſomme des Energies négatives priſes affirmative- » ment.*

FIGURE 6. Bernoulli's “regle” as published by Varignon (1725, Vol. II, p. 176)

We now describe the derivation of Benoulli's “regle” following the text of Lagrange (Lagrange [33], 1788, Prem. Partie, Section II). However we do not follow the style of Lagrange, who proudly avoided the use of any figures.

We start with a system containing *two* forces P and Q, illustrated here by a lever (see Fig. 7, left) attached at O with arm lengths a and b. We then suppose that the system receives a virtual velocity during an infinitely small interval of time, such that the lever arms receive infinitely small displacements dp and dq proportional to a and b. Archimedes' law then tells us that for equilibrium to occur, the virtual velocities and the forces must be inversely proportional. Thus, if we pay attention to the signs of the displacements, we obtain

$$\frac{P}{Q} = -\frac{dq}{dp} \qquad \text{or} \qquad Pdp + Qdq = 0.$$

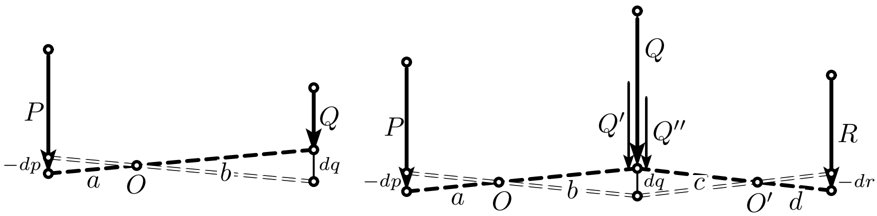


FIGURE 7. The Lever (left); Composed levers (right)

Let us now make the system more complicated by considering *three* forces P, Q and R instead of two (Fig 7, right). We decompose the force Q as sum $Q = Q' + Q''$ in such a way that both subsystems to the left and right are in equilibrium, i.e., such that

$$Pdp + Q'dq = 0 \quad \text{and} \quad Q''dq + Rdr = 0,$$

so we get $Pdp + Qdq + Rdr = 0$ as condition for an equilibrium. By adding more and more forces to the system, we obtain

$$\boxed{Pdp + Qdq + Rdr + \ldots = 0} \tag{1.1}$$

for an equilibrium. This equation, expressed in words and not in formulas, was precisely Joh. Bernoulli's "regle" of Fig. 6. The terms $Pdp, Qdq, \ldots$ were called "Energies" by Bernoulli. Lagrange calls them "moments" of the forces and calls (1.1) "la formule générale de l'équilibre" (see Fig. 8).

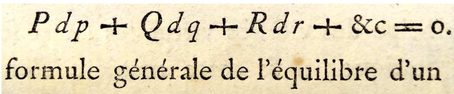

$P\,dp + Q\,dq + R\,dr +$ &c $= 0$.
formule générale de l'équilibre d'un

FIGURE 8. Bernoulli's rule as published by Lagrange 1788

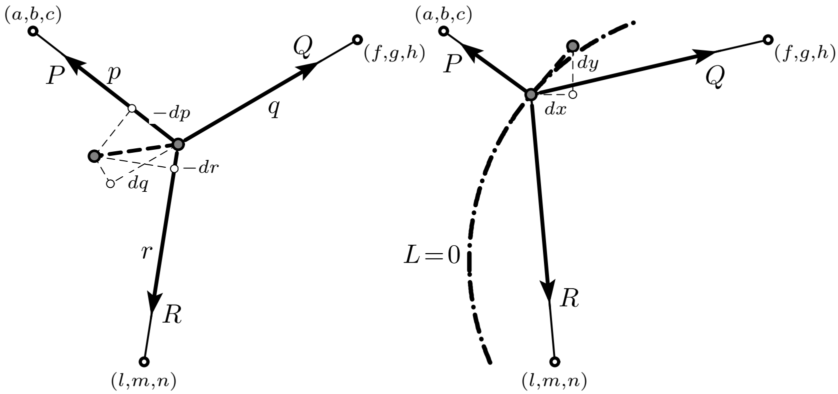


FIGURE 9. A point attached by three forces (left); as constrained problem (right)

Example. The first example Lagrange considers in detail (in Section V) is a mass point attached by several forces P, Q, R to fixed points with Cartesian coordinates $(a, b, c), (f, g, h), (l, m, n)$ (see Fig. 9, left). Inserting

$$p = \sqrt{(x-a)^2 + (y-b)^2 + (z-c)^2}, \; dp = \frac{1}{p} \cdot ((x-a)dx + (y-b)dy + (z-c)dz)\,,$$

and similarly for dq, dr, formula (1.1) becomes

$$Xdx + Ydy + Zdz = 0 \tag{1.2}$$

where $X = P\frac{x-a}{p} + Q\frac{x-f}{q} + R\frac{x-l}{r}$, $Y = P\frac{y-b}{p} + Q\frac{y-g}{q} + R\frac{y-m}{r}$ and $Z = P\frac{z-c}{p} + Q\frac{z-h}{q} + R\frac{z-n}{r}$. Since, at the moment, our mass point is completely free, dx, dy and dz are independent[5], and the condition for equilibrium is

$$X = 0\,, \qquad Y = 0 \qquad \text{and} \qquad Z = 0\,. \tag{1.3}$$

[5] dp, dq, dr are not independent at the equilibrium point.

In the case where the forces P, Q, R are equal (or proportional) to the distances p, q, r, this formula simplifies considerably and the equilibrium position becomes the barycenter of the triangle spanned by the three fixed points (or of a pyramid in the case of four forces, a result which Lagrange attributes to Leibniz).

1.3. The discovery of the multiplier method

Suppose now (see Fig. 9, right) that the mass point is restricted to a surface $L = 0$, so that in (1.2) the displacements dx, dy, dz are *not* independent, but are restricted to the tangent space of $L = 0$, i.e. they must satisfy

$$dL = \frac{\partial L}{\partial x}dx + \frac{\partial L}{\partial y}dy + \frac{\partial L}{\partial z}dz = 0\,. \tag{1.4}$$

This means geometrically that, whenever (1.4) holds, i.e. the vector (dx, dy, dz) is orthogonal to $(\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}, \frac{\partial L}{\partial z})$, we must satisfy (1.2) as well, i.e. the vector (dx, dy, dz) must also be orthogonal to (X, Y, Z). As a consequence, both vectors must be parallel so that there exists a constant λ such that

$$X + \lambda\frac{\partial L}{\partial x} = 0\,, \qquad Y + \lambda\frac{\partial L}{\partial y} = 0 \quad\text{and}\quad Z + \lambda\frac{\partial L}{\partial z} = 0\,. \tag{1.5}$$

However, vectors and scalar products were not yet familiar concepts to Lagrange, so he argued differently ("Il n'est pas difficile de prouver par la théorie de l'élimination des équations linéaires..."): we eliminate one of the unknowns, say dz, by multiplying (1.4) with a suitable constant, which is $\lambda = -Z/\frac{\partial L}{\partial z}$, and add it to (1.2), which gives

$$\left(X + \lambda\frac{\partial L}{\partial x}\right)\cdot dx + \left(X + \lambda\frac{\partial L}{\partial y}\right)\cdot dy = 0\,, \qquad Z + \lambda\frac{\partial L}{\partial z} = 0\,.$$

Here, dx and dy are independent and equations (1.5) must be satisfied, the last one being the formula for λ.

Condition (1.5) just means that we have applied the virtual velocity argument, *without constraints*, to the system

$$Xdx + Ydy + Zdz + \lambda dL = 0\ . \tag{1.6}$$

Lagrange realizes that this "multiplier" λ, whose invention originated from the theory of linear equations, also has a physical meaning: it represents the constant which, when multiplied with the vector $(\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}, \frac{\partial L}{\partial z})$, yields the force that holds the particle onto the surface $L = 0$.

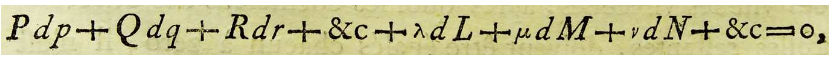

$P\,dp + Q\,dq + R\,dr + \&c + \lambda\, dL + \mu\, dM + \nu\, dN + \&c = 0,$

FIGURE 10. Lagrange's "équation générale" for ALL problems of equilibria

To include an additional constraint $M = 0$, we see from linear algebra that we can simply add another term μdM, and so on. Finally, one can generalize (1.1) to any system with any number of constraints by writing

$$\boxed{Pdp + Qdq + Rdr + \ldots + \lambda dL + \mu dM + \nu dN + \ldots = 0} \tag{1.7}$$

(see Fig. 10). This discovery was called "Méthode très-simple" in Section IV of the first edition from 1788. Twenty-three years later, in [34], Lagrange stressed the importance of this idea by giving it the particular name "Méthode des Multiplicateurs" (see Fig. 11).


§ I.

Méthode des Multiplicateurs.

FIGURE 11. Heading of §1 in Section IV of Lagrange (1811)

2. Problems of Maximum and Minimum

The above problems of *virtual velocities* are closely related to problems of maximizing or minimizing a function. This connection is mentioned briefly in Lagrange (1788), but it was only in the second edition from 1811 that Lagrange stresses this important fact by an entire paragraph (see Fig. 12). If $U(x, y, z)$ is a "potential" function[6] satisfying $\frac{\partial U}{\partial x} = X$, $\frac{\partial U}{\partial y} = Y$ and $\frac{\partial U}{\partial z} = Z$, where X, Y and Z are as in (1.2), then the conditions (1.3) mean nothing else than

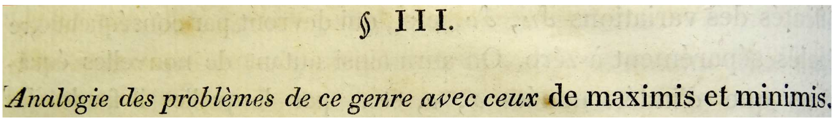
$$U(x, y, z) \longrightarrow \text{min or max.} \tag{2.1}$$

Similarly, in the case where we have to minimize or maximize a function $U(x, y, z)$ under a constraint $L(x, y, z) = 0$, the corresponding equations (1.5) and (1.6) would mean that we have to minimize or maximize

$$U(x, y, z) + \lambda L(x, y, z) \longrightarrow \text{min or max} \tag{2.2}$$

without constraints. This is the *Lagrange multiplier method for constrained optimization.* The geometric meaning of the term $\lambda L(x, y, z)$ is the following: it twists the function $U(x, y, z)$, without changing its values on the surface $L = 0$, such that $U + \lambda L$ becomes flat in all directions at the minimal position.

For additional constraints, we add additional multipliers, and for higher dimensions, we add additional variables.


§ III.

Analogie des problèmes de ce genre avec ceux de maximis et minimis.

FIGURE 12. Heading of §3 in Section IV of Lagrange (1811)

[6]Up to now, we have preserved all letters exactly as they appear in Lagrange, but we have changed this potential, denoted Π by Lagrange, to U, as it is usual now.

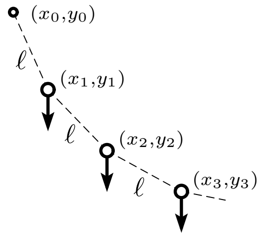
Example: The Catenary. One of the examples Lagrange discusses in detail (Part I, Sect. V) is a chain of particles attached by cords of constant length in an arbitrary force field. If we assume the forces to be constant downwards, we have the situation as in Fig. 13, for which (1.7) becomes

$$dy_1 + dy_2 + ... + \lambda_0 \cdot d((x_0 - x_1)^2 + (y_0 - y_1)^2 - \ell^2) + \lambda_1 \cdot d(...) + ... = 0. \quad (2.3)$$

Differentiating the constraints and collecting the coefficients of, say, dx_2, dy_2, we obtain

$$\begin{aligned} \lambda_2(x_2 - x_3) &= \lambda_1(x_1 - x_2) \\ \lambda_2(y_2 - y_3) &= \lambda_1(y_1 - y_2) - 1 \end{aligned} \quad \Rightarrow \quad \frac{y_2 - y_3}{x_2 - x_3} = \frac{y_1 - y_2}{x_1 - x_2} + \text{const.},$$

which means that the slope is a linear function of the arc length. This fact is in accordance with "... les formules connues de la chainette".



$$\begin{aligned} (x_0 - x_1)^2 + (y_0 - y_1)^2 - \ell^2 &= 0 \\ (x_1 - x_2)^2 + (y_1 - y_2)^2 - \ell^2 &= 0 \\ (x_2 - x_3)^2 + (y_2 - y_3)^2 - \ell^2 &= 0 \\ \dots \end{aligned}$$

FIGURE 13. The Catenary as a constrained mechanical system

The Catenary as optimization problem. If we ask for the chain with $y_1 + y_2 + y_3 + \ldots \longrightarrow \min$ under the same constraints as in Fig. 13, i.e. if we seek the chain with the lowest center of gravity, (2.2) becomes

$$y_1 + y_2 + ... + \lambda_0 \cdot ((x_0 - x_1)^2 + (y_0 - y_1)^2 - \ell^2) + \lambda_1 \cdot (...) + ... \longrightarrow \min. \quad (2.4)$$

This equation, when differentiated, gives precisely the formula (2.3). We thus see that *the catenary is the curve with the lowest center of gravity for a given arc length*, a result Euler ([20] 1744, Chap. V) found in a much more complicated way, as we will see below.

2.1. Variational Problems

Variational problems are optimization problems where not only some values, but an entire function $y(x)$, is unknown, for example

$$J = \int_a^b Z(x, y, p)\, dx \longrightarrow \min \text{ or } \max, \text{ where } p = \frac{dy}{dx} \quad (2.5)$$

and $Z(x, y, p)$ is a given function. We refer to Gander-Wanner ([28] SIREV 2013, formula (1.3), (1.4) and Section 9.1) to see how Euler ([20] 1744, Chap. 2) turned this problem into a differential equation

$$\boxed{N - \frac{d}{dx}P = 0} \qquad \textit{where} \quad N = \frac{\partial Z}{\partial y},\ P = \frac{\partial Z}{\partial p}, \quad (2.6)$$

and, in the case where $Z(y,p)$ is independent of x, how this equation can be simplified to

$$\boxed{Z - p\cdot\frac{\partial Z}{\partial p} = \text{Const.}} \tag{2.7}$$

2.2. Variational Problems with Constraints

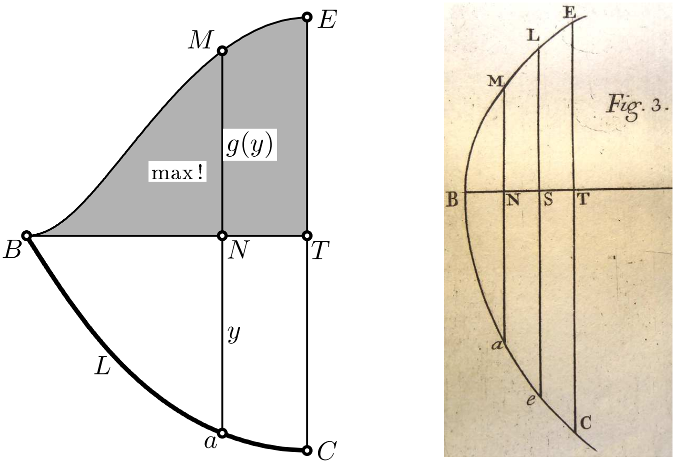


FIGURE 14. The isoperimetric problem of Jakob (left, the drawing is for $g(y)=y^2$); the same picture in Johann's *Opera Omnia* from 1742, vol. 2, p. 270 (right)

The oldest problem of this type, the so-called "isoperimetric problem", was a challenge from Jakob Bernoulli to his brother Johann in 1697: *Given two points B and C (see Fig. 14), find a curve BaC of a given length L such that the area $BMETNB$ is maximal; here, for any distance $aN=y$, the distance $MN=g(y)$ is a given function of y.* In formulas, this means

$$\int_B^T g(y(x))\,dx \longrightarrow \max \quad \text{subject to} \quad \int_B^T \sqrt{1+p^2}\,dx = L\ . \tag{2.8}$$

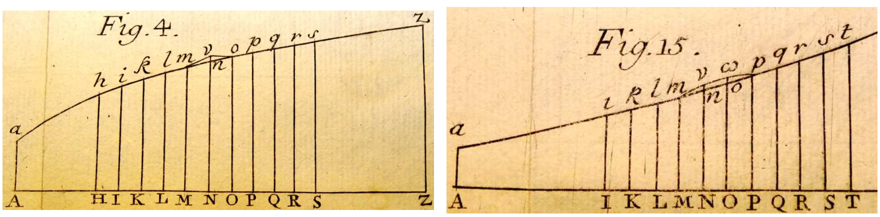


FIGURE 15. Euler's solution of variational problems; unconstrained (left), constrained (right)

Solution. Johann, who had accumulated success after success in the years before, thought that he could solve this seemingly simple problem in "three minutes". The three minutes turned into decades until Johann Bernoulli published an extensive paper in 1718 (Mémoires de l'Acad. Roy. des Sciences de Paris, p. 100). The collection of all the solutions of Jakob and himself fills more than 50 pages in Johann's *Opera Omnia* ([4] vol. 2, p. 214– 269). Finally, Euler ([20] 1744, in Chap. 5 of E65) developed his general theory for such constrained problems. While in Chap. 2, Euler arrived at (2.6) by "virtual" displacements of the function values of the unknown function one-by-one (see Fig. 15, left), he was unable to displace the function values independently for constrained problems of the type (1.4). Instead, he varied the values *two by two* $n \mapsto \nu, o \mapsto \omega$ (see Fig. 15, right) and had to build an entirely new theory (16 pages; §1 through §39 of Chap. 5).

As Lagrange demonstrates proudly in many examples (in Section V), the idea of using multipliers to deal with constraints extends straightforwardly to these new problems. For the historical example (2.8), this turns into (for $B = 0, T = 1$)

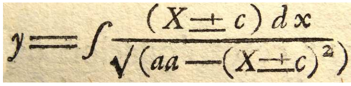
$$J = \int_0^1 \Big(g(y) + \lambda\big(\sqrt{1+p^2} - L\big)\Big)\, dx \longrightarrow \max. \tag{2.9}$$

For this problem, condition (2.7) becomes, after simplification,

$$g(y) + \frac{\lambda}{\sqrt{1+p^2}} = C + \lambda L\,.$$

We set $C + \lambda L = -K$, solve for $p = \frac{dy}{dx}$ and separate the variables. This gives the solution (compared to the one from Johann's *Opera Omnia*, vol. 2, p. 244)

$$\int \frac{g(y)+K}{\sqrt{\lambda^2 - (g(y)+K)^2}}\, dy = x + c\,. \tag{2.10}$$



$y = \int \frac{(X \pm c)\, dx}{\sqrt{(aa - (X \pm c)^2)}}$

This integral only has an elementary solution for $g(y) = y$, i.e. the problem of finding the maximal area surrounded by a curve of prescribed length. As Euler shows in §41 of [20] E65, Caput V, the integral then leads, not surprisingly, to a circular solution (quae est aequatio generalis pro Circulo). The drawing for $g(y) = y^2$ in Fig. 14 (left) has been produced by numerical integrations.

An Example with two constraints. For problems with *two* constraints ("Pluribus Proprietatibus"), Euler developed again an entirely new theory (E65, Chap. VI). With Lagrange, we just have to add a second multiplier. We demonstrate this on Euler's very last example (§24 in Chap. 6): We seek a curve $y(x)$ (the curve $DMAMD$ in Fig. 16, right) of a given length L, as well as a constant a (the distance CQ), such that the area of $NDMAMDNQN$ has a given value M, and the center of gravity of this figure should be as low as possible. Expressed in formulas we have (we choose C as origin and take the curve upside down)

$$\int_{-1}^1 \sqrt{1+p^2}\, dx = L\,, \quad \int_{-1}^1 (y+a)\, dx = M\,, \quad \int_{-1}^1 (y+a)\cdot \frac{y-a}{2}\, dx \longrightarrow \max.$$

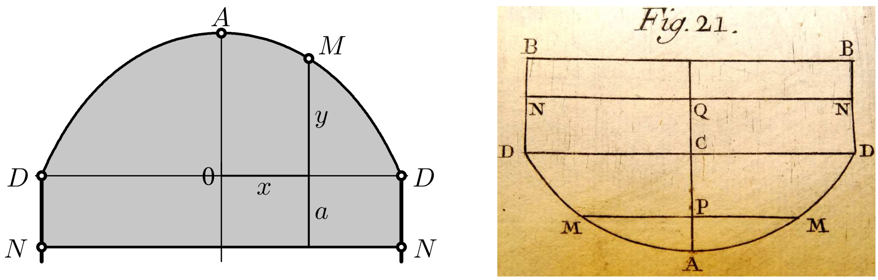


FIGURE 16. Euler's problem from E65 with two constraints

Here, we introduce two multipliers λ and μ and get

$$J = \int_{-1}^{1} \Big((y^2 - a^2) + \lambda\big(\sqrt{1+p^2} - L\big) + \mu\big((y+a) - M\big)\Big)\, dx \longrightarrow \text{min or max.}$$

Since we have two unknowns y and a here, we cannot work with the simplified equation (2.7). Instead, we have to use (2.6) for each of them:

$$\text{for } y: \qquad 2y + \mu - \frac{d}{dx}\big(\lambda \frac{p}{\sqrt{1+p^2}}\big) = 0,$$

$$\text{for } a: \qquad -2a + \mu = 0 \quad \Rightarrow \quad \mu = 2a \ .$$

This, inserted into the first equation, gives

$$\frac{d}{dx}\big(\frac{p}{\sqrt{1+p^2}}\big) = k(y+a) \ .$$

If we think of a water basin, this result expresses the fact that *the curvature of the basin is proportional to the water pressure.*

2.3. Solving Optimal Control Problems with Lagrange multipliers

Before explaining the invention of the maximum principle for control problems in the next section, we first show that the idea of Lagrange multipliers provides an elegant entry point to the treatment of certain classes of such problems. Let us look at a problem of the type

$$\int_a^b k(x,y,u)\, dx \longrightarrow \text{min or max,} \tag{2.11}$$

subject to

$$\frac{dy}{dx} = f(x,y,u), \qquad y(a)=A, \quad y(b)=B.$$

Here we have *two* types of functions to find: the values of $y_i(x)$, which are defined via a system of differential equations, and the so-called *controls* $u_j(x)$, which control the movement of the y's and with the help of which the *cost function* $k(x,y,u)$, when integrated over the interval $[a,b]$, is to be optimized.

Idea: since the differential equations in (2.11) represent an infinite number of constraints as x varies, we introduce Lagrange multipliers $\lambda_i(x)$ as *functions* multiplying the constraints $y_i' - f_i(x,y,u) = 0$. Inserting this into the integral, we thus obtain

$$\int_a^b \{k(x,y,u) + [p^T - f^T(x,y,u)] \cdot \lambda(x)\} \, dx \longrightarrow \text{min or max.} \tag{2.12}$$

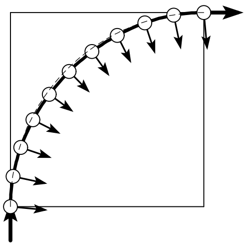
This is now an *unconstrained* variational problem with a "cost function" $Z(x,\lambda,y,p,u)$. Here we have three sets of unknowns, the Lagrange multipliers $\lambda_i(x)$, the differential equation solutions $y_i(x)$ together with their derivatives $p_i(x)$, and the control functions $u_j(x)$. For each of these, we apply Euler's equation (2.6):

$$\begin{aligned}
&\boxed{\tfrac{\partial Z}{\partial \lambda} = 0} &&: \quad y'(x) = f(x,y,u) \\
&\boxed{\tfrac{\partial Z}{\partial y} - \tfrac{d}{dx}\tfrac{\partial Z}{\partial p} = 0} &&: \quad \lambda'(x) = \tfrac{\partial k}{\partial y}(x,y,u) - \tfrac{\partial f}{\partial y}^T(x,y,u) \cdot \lambda(x) \\
&\boxed{\tfrac{\partial Z}{\partial u} = 0} &&: \quad 0 = \tfrac{\partial k}{\partial u}(x,y,u) - \tfrac{\partial f}{\partial u}^T(x,y,u) \cdot \lambda(x)
\end{aligned} \tag{2.13}$$

This is a system of differential algebraic equations (DAEs). The first set of equations are the desired constraints, the second set of equations is the so-called *adjoint system*, whose geometric meaning will be discussed below, and the third set consists of algebraic equations that determine the controls for every value of x.

Example. A body gliding in R^2 without friction should receive a new direction with the help of forces $(u_1(t), u_2(t))$, $0 \le t \le T$ in such a way that this control uses as little energy as possible: $\int_0^T \frac{1}{2}(u_1^2 + u_2^2)\,dt \longrightarrow \text{min}$.

Solution. With y_1, y_2 as the positions of the body and y_3, y_4 as velocities, the equations of motion together with the equations in (2.13) become



$$\begin{aligned}
\dot y_1 &= y_3 & \dot\lambda_1 &= 0 & & \\
\dot y_2 &= y_4 & \dot\lambda_2 &= 0 & u_1 - \lambda_3 &= 0 \\
\dot y_3 &= u_1 & \dot\lambda_3 &= -\lambda_1 & u_2 - \lambda_4 &= 0 \\
\dot y_4 &= u_2 & \dot\lambda_4 &= -\lambda_2 & &
\end{aligned}$$

We see that λ_1, λ_2 are constants, $\lambda_3 = u_1, \lambda_4 = u_2$ are linear, y_3, y_4 quadratic, and thus y_1, y_2 cubic; the solution curves are thus, not surprisingly, cubic splines. The time length T can be freely chosen. In the picture above, T is chosen to be that of a uniform circular movement, but the optimal solution is slightly different.

3. Optimal Control and the Maximum Principle

> An important case in applications is the one in which Ω [containing the controls] is a closed region [...]. In the case that Ω is an open set [...],

> the variational problem formulated here turns out to be a special case of the problem of Lagrange. (Pontryagin 1959 [47])

In the field of optimal control, there were historically two approaches: in the western world, researchers tried to tackle these problems using variational calculus and Lagrange multipliers, as we have already seen for a first example in Subsection 2.3. In Russia, a group of researchers led by Pontryagin tried to solve these problems using direct analysis and geometric arguments, with a particular emphasis on handling the important case of closed and bounded control sets. Their approach led to the invention of the maximum principle in 1956; they only later noticed the relation to Lagrange multipliers, see the quote above. To explain these two approaches historically, we first present the invention of Lagrange from Section 1.3 again, but now using matrix notation in preparation for its use in optimal control problems.

3.1. Invention of Lagrange Multipliers in Matrix Notation

> Lagrange, in his book from 1797: "Théorie des fonctions analytiques, contenant les principes du calcul différentiel, dégagés de toute considération d'infiniment petits, d'évanouissans, de limites ou de fluxions, et réduits à l'analyse algébrique des quantités finies"

Lagrange, who in his youth made his greatest triumphs by free and masterful manipulations of differentials, later in his life condemned them vigorously by replacing "differentials" by "derivatives" and "integrals" by "primitives", see the quote above. Under the influence of Cayley's matrix notation, the above theory subsequently took a different shape, the one we are used to seeing today: we first consider a finite dimensional optimization problem with constraints, and show how the Lagrange multipliers are none other than multipliers like in Gaussian elimination, but without using the notation of differentials that were essential in their invention, as we have seen earlier. This will also reveal a further advantage over the direct solution of the complete optimality system in the presence of constraints, since the system obtained with Lagrange multipliers is much smaller. Suppose we wish to solve the constrained optimization problem

$$f(\boldsymbol{x}) \longrightarrow \min, \quad \boldsymbol{g}(\boldsymbol{x}) = 0, \tag{3.1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is the objective function and $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m$ are the constraints, $m < n$. To eliminate the constraints, we partition the vector $\boldsymbol{x}$ into $\boldsymbol{x} = (\boldsymbol{y}, \boldsymbol{u})$, $\boldsymbol{y} \in \mathbb{R}^m$, $\boldsymbol{u} \in \mathbb{R}^{n-m}$, and invoke the implicit function theorem to obtain $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{u})$ from the constraint $\boldsymbol{g}(\boldsymbol{x}) = 0$. Substituting this into the objective function, we obtain the unconstrained optimization problem

$$f(\boldsymbol{y}(\boldsymbol{u}), \boldsymbol{u}) \longrightarrow \min . \tag{3.2}$$

A necessary condition for a local minimum is therefore

$$\frac{df}{d\boldsymbol{u}} = \frac{\partial f}{\partial \boldsymbol{y}} \cdot \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{u}} + \frac{\partial f}{\partial \boldsymbol{u}} := (Y_u^T \nabla_y f + \nabla_u f)^T = 0, \tag{3.3}$$

where $Y_u : \mathbb{R}^{n-m} \to \mathbb{R}^{m\times(n-m)}$ is the Jacobian of the implicit function $\boldsymbol{y}(\boldsymbol{u})$, and $\nabla_y f = f_y^T$ and $\nabla_u f = f_u^T$ are the gradients (column vectors) of the objective function with respect to the variables $\boldsymbol{y}$ and $\boldsymbol{u}$. The necessary optimality condition (3.3) is a small system involving the $n-m$ unknowns in the vector $\boldsymbol{u}$ only. However, only in very simple situations it is actually possibe to explicitly form the function $\boldsymbol{y}(\boldsymbol{u})$ and differentiate it to obtain Y_u. In general, the Jacobian matrix Y_u is also unknown and depends implicitly on the solution $\boldsymbol{y}$, which must also be calculated. To obtain equations for $\boldsymbol{y}$, one can directly use the constraint $\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}) = 0$, and for the Jacobian, one can write the total derivative with respect to $\boldsymbol{u}$ of $\boldsymbol{g}(\boldsymbol{y}(\boldsymbol{u}),\boldsymbol{u}) = 0$. This leads to the complete optimality system

$$\begin{aligned} Y_u^T\nabla_y f + \nabla_u f &= 0, & (3.4)\\ Y_u^T G_y^T + G_u^T &= 0, & (3.5)\\ \boldsymbol{g} &= 0, & (3.6)\end{aligned}$$

where $G_y : \mathbb{R}^n \to \mathbb{R}^{m\times m}$ is the Jacobian matrix of $\boldsymbol{g}$ with respect to $\boldsymbol{y}$, and $G_u : \mathbb{R}^n \to \mathbb{R}^{m\times(n-m)}$ is the Jacobian matrix of $\boldsymbol{g}$ with respect to $\boldsymbol{u}$. Equation (3.4) contains $n-m$ equations, (3.5) is a matrix equation for the Jacobian matrix Y_u and contains a total of $m(n-m)$ equations, and (3.6) contains m equations from the constraints. This gives a total of $n+m(n-m)$ equations for the n unknowns in $\boldsymbol{y}$ and $\boldsymbol{u}$ combined, and the $m(n-m)$ unknowns in the Jacobian Y_u, a very big system. The key idea of Lagrange in this setting is that one can eliminate many of these equations using Gaussian elimination to arrive at a smaller, but equivalent system. If the Jacobian G_y is invertible, then multiplying the matrix-valued equation (3.5) by the vector-valued multiplier $\boldsymbol{\lambda} := -G_y^{-T}\nabla_y f$ from the right yields

$$Y_u^T G_y\boldsymbol{\lambda} + G_u^T\boldsymbol{\lambda} = -Y_u^T G_y^T G_y^{-T}\nabla_y f + G_u^T\boldsymbol{\lambda} = -Y_u^T\nabla_y f + G_u^T\boldsymbol{\lambda} = 0. \quad (3.7)$$

Adding this equation to (3.4), the cumbersome term with the large Jacobian matrix cancels and we obtain the smaller but equivalent optimality system

$$\begin{aligned} \nabla_u f + G_u^T\boldsymbol{\lambda} &= 0, & (3.8)\\ \nabla_y f + G_y^T\boldsymbol{\lambda} &= 0, & (3.9)\\ \boldsymbol{g} &= 0, & (3.10)\end{aligned}$$

which now contains $(n-m)+m+m = n+m$ equations for the n unknowns $\boldsymbol{y}$ and $\boldsymbol{u}$ combined, plus the m Lagrange multipliers $\boldsymbol{\lambda}$. The system (3.8–3.10) is equivalent to (3.4–3.6), and therefore represents the same necessary condition for a minimum of the original constraint problem (3.1), but it has the advantage of having many fewer unknowns to solve for. The key observation of Lagrange now was that this simpler necessary condition for optimality can be easily obtained from the function

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{y},\boldsymbol{\lambda}) := f(\boldsymbol{y},\boldsymbol{u}) + g(\boldsymbol{y},\boldsymbol{u})^T\boldsymbol{\lambda}, \quad (3.11)$$

by simply taking derivatives with respect to its arguments. The function in (3.11), now known as the Lagrange function or the Lagrangian in honor of its inventor, is obtained by simply adding to the objective function the sum of the constraints, each multiplied by a Lagrange multiplier.

The new formulation, however, introduces an important difficulty when the remaining $\boldsymbol{u}$ variables are not allowed to vary freely, but are constrained to be in a closed set U. This is often the case in optimal control problems, since the controls may not be arbitrarily large. Then the necessary condition (3.3) for a minimum solution of (3.2) is only relevant if the minimum is in the interior of U; when the minimum occurs on the boundary, which often happens in practice, the condition (3.3) need not be satisfied, i.e., the variation of the Lagrangian with respect to $\boldsymbol{u}$ in (3.8) need not vanish. One possibility in that case is to revert to the minimization condition of the Lagrangian with respect to $\boldsymbol{u}$, which leads to the necessary conditions for optimality

$$\begin{aligned} \mathcal{L}(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) &\longrightarrow \min \quad \text{with respect to } \boldsymbol{u} && (3.12)\\ \nabla_y f + G_y^T\boldsymbol{\lambda} &= 0, && (3.13)\\ \boldsymbol{g} &= 0. && (3.14) \end{aligned}$$

Since the constraint $\boldsymbol{g} = 0$ must be satisfied at the optimum, we have $\mathcal{L}(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) = f(\boldsymbol{y},\boldsymbol{u})$ there, so (3.12) is equivalent to saying that

$$f(\boldsymbol{y},\boldsymbol{u}) \longrightarrow \min \quad \text{with respect to } \boldsymbol{u}. \qquad (3.15)$$

In this case, however, the equation (3.13) for the Lagrange multipliers is no longer needed, since they are not used anywhere in the system; if we remove it, we just get back the original problem formulation (3.1), except that one now sees explicitly that the minimization is only possible with respect the remaining "control" variables $\boldsymbol{u}$, since the other variables $\boldsymbol{y}$ are determined by the constraints. Nevertheless, the observation to replace the derivative condition again by the minimization condition points in the direction of results obtained by Pontryagin and his group and leads to the maximum principle for optimal control problems. We will see later that they chose a different function, a Hamiltonian, which has the same stationary points in $\boldsymbol{u}$ as the Lagrangian[7].

A different way of characterizing minima on a closed set of controls U is to ensure that whenever the minimum occurs on the boundary, any variation in $\boldsymbol{u}$ that moves the point away from the boundary into the interior of the closed set must lead to an increase in the objective function, i.e.

$$\begin{aligned} (\nabla_u f + G_u^T\boldsymbol{\lambda})^T\delta\boldsymbol{u} &\geq 0, && (3.16)\\ \nabla_y f + G_y^T\boldsymbol{\lambda} &= 0, && (3.17)\\ \boldsymbol{g} &= 0, && (3.18) \end{aligned}$$

for all admissible variations $\delta\boldsymbol{u}$ such that $\boldsymbol{u} + \delta\boldsymbol{u}$ remains in the closed set of the admissible controls U. This approach became known under the name Karush–Kuhn–Tucker (KKT) conditions, which we will see again in Section 4.2

[7] See also Carathéodory [16] for a general study of equivalent formulations.

3.2. Lagrange Multipliers for Optimal Control Problems

> Using what I had learned at Columbia about flights of airplanes, I set out to formulate this problem as a variational problem. I found that the usual variational formulation did not fit very well. It was too clumsy. And so I reformulated the Problem of Bolza so that it could be applied easily to the time-optimal problem at hand. It turns out that I had formulated what is now known as the general optimal control problem. I wrote it up as a RAND report [31] and it was widely circulated among engineers. (Hestenes, in a letter to Saunders Mac Lane, see [39])

Optimal control problems were becoming important with the invention of moving high-tech mechanical devices, especially in the context of war. A typical example is to guide an airplane along an optimal trajectory to reach a target, and this was precisely the problem considered by Hestenes in his famous RAND report [31], see also the quote above. Hestenes, who had obtained his PhD on the calculus of variations under the direction of Bliss, was a young professor in Chicago during the Second World War and moved to UCLA afterward. He was also doing research for RAND, a nonprofit institution with the goal of improving policy and decision-making through research and analysis, which still exists today (`www.rand.org`). In his report, he formulated the problem of guiding an airplane in an optimal way from an initial position to a final position as an optimization problem with a constraint given by a differential equation. In modern notation, the problem reads

$$\begin{aligned} \int_0^T f(\boldsymbol{y},\boldsymbol{u})dt &\longrightarrow \min, && (3.19)\\ \dot{\boldsymbol{y}} &= \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}), && (3.20)\\ \boldsymbol{y}(0) &= \boldsymbol{y}^0, && (3.21)\\ \boldsymbol{y}(T) &= \boldsymbol{y}_T, && (3.22) \end{aligned}$$

where the vector $\boldsymbol{y}(t)$ contains the position and velocity vectors of the airplane, and the vector $\boldsymbol{u}(t)$ contains the angles of the control vanes of the airplane and the thrust of the engines. Comparing this optimal control problem with the general constrained minimization problem (3.1), Hestenes noticed the striking similarity, so he applied the Lagrange multiplier technique we saw in Subsection 2.3 to obtain a necessary condition for optimality: he introduced the Lagrangian as in (3.11),

$$\mathcal{L}(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) := \int_0^T f(\boldsymbol{y},\boldsymbol{u})dt + \int_0^T (\dot{\boldsymbol{y}} - \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}))^T \boldsymbol{\lambda} dt, \tag{3.23}$$

where all the variables now depend on time, $\boldsymbol{y} = \boldsymbol{y}(t)$, $\boldsymbol{u} = \boldsymbol{u}(t)$, $\boldsymbol{\lambda} = \boldsymbol{\lambda}(t)$ (this is precisely equation (2.12) in the new notation). In order to obtain necessary conditions for optimality, he computed the derivatives with respect to the variables $\boldsymbol{y}$, $\boldsymbol{u}$, and $\boldsymbol{\lambda}$ using variational calculus (as Euler did in E420, see [28]): if $\boldsymbol{y}$ is an optimum, then for an arbitrary variation $\boldsymbol{y} + \varepsilon\boldsymbol{z}$, the derivative of $\mathcal{L}(\boldsymbol{y}+\varepsilon\boldsymbol{z},\boldsymbol{u},\boldsymbol{\lambda})$ with respect to ε must vanish at $\varepsilon = 0$, regardless of what the variation $\boldsymbol{z}$ is. Thus, we obtain as the first necessary condition

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{L}(\boldsymbol{y}+\varepsilon\boldsymbol{z},\boldsymbol{u},\boldsymbol{\lambda})|_{\varepsilon=0} &= \int_0^T \nabla_y f^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{z}dt + \int_0^T (\dot{\boldsymbol{z}} - G_y(\boldsymbol{y},\boldsymbol{u})\boldsymbol{z})^T \boldsymbol{\lambda}dt \\ &= \int_0^T (\nabla_y f(\boldsymbol{y},\boldsymbol{u}) - \dot{\boldsymbol{\lambda}} - G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda})^T\boldsymbol{z}dt + \boldsymbol{\lambda}^T\boldsymbol{z}|_0^T = 0,\end{aligned}$$

where we used integration by parts to factor out the arbitrary variation $\boldsymbol{z}$, and the fact that

$$(G_y\boldsymbol{z})^T\boldsymbol{\lambda} = \boldsymbol{z}^T G_y^T\boldsymbol{\lambda} = (\boldsymbol{z}^T G_y^T\boldsymbol{\lambda})^T = \boldsymbol{\lambda}^T G_y\boldsymbol{z} = (G_y^T\boldsymbol{\lambda})^T\boldsymbol{z}.$$

Now the variation $\boldsymbol{z}(t)$ must be zero for $t = 0$ and $t = T$, since the values of $\boldsymbol{y}$ are fixed there, see (3.21) and (3.22); thus, we have $\boldsymbol{z}(0) = \boldsymbol{z}(T) = 0$, so the boundary terms $\boldsymbol{\lambda}^T\boldsymbol{z}|_0^T$ in (3.24) must vanish as well. However, apart from the initial and final conditions, the variation $\boldsymbol{z}(t)$ is otherwise arbitrary, and hence from (3.24), the term multiplying $\boldsymbol{z}(t)$ under the integral must be zero. This leads to a differential equation for $\boldsymbol{\lambda}$, namely

$$\dot{\boldsymbol{\lambda}} = -G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} + \nabla_y f(\boldsymbol{y},\boldsymbol{u}), \tag{3.24}$$

without initial or final condition, since $\boldsymbol{y}$ was fixed at both ends. Similarly, since $\boldsymbol{u}$ is optimal, we can add an arbitrary variation $\boldsymbol{u}+\varepsilon\boldsymbol{v}$ and require the derivative of $\mathcal{L}(\boldsymbol{y},\boldsymbol{u}+\varepsilon\boldsymbol{v},\boldsymbol{\lambda})$ with respect to ε to vanish at $\varepsilon = 0$ for all variations $\boldsymbol{v}$. This yields the next necessary condition

$$\begin{aligned}\frac{d}{d\varepsilon}\mathcal{L}(\boldsymbol{y},\boldsymbol{u}+\varepsilon\boldsymbol{v},\boldsymbol{\lambda})|_{\varepsilon=0} &= \int_0^T \nabla_u f^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{v}dt + \int_0^T (-G_u(\boldsymbol{y},\boldsymbol{u})\boldsymbol{v})^T \boldsymbol{\lambda}dt \\ &= \int_0^T (\nabla_u f(\boldsymbol{y},\boldsymbol{u}) - G_u^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda})^T\boldsymbol{v}dt = 0.\end{aligned}$$

Since the variation $\boldsymbol{u}(t)$ is arbitrary, from (3.25), the term multiplying $\boldsymbol{v}(t)$ under the integral must be zero, which leads to an equation for $\boldsymbol{u}$, namely

$$G_u^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} = \nabla_u f(\boldsymbol{y},\boldsymbol{u}). \tag{3.25}$$

Finally, adding an arbitrary variation $\boldsymbol{\lambda}+\varepsilon\boldsymbol{\mu}$, the derivative of $\mathcal{L}(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}+\varepsilon\boldsymbol{\mu})$ with respect to ε must vanish at $\varepsilon = 0$ for all variations $\boldsymbol{\mu}$, and we obtain as the last necessary condition

$$\frac{d}{d\varepsilon}\mathcal{L}(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}+\varepsilon\boldsymbol{\mu})|_{\varepsilon=0} = \int_0^T (\dot{\boldsymbol{y}} - \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}))^T \boldsymbol{\mu}dt = 0, \tag{3.26}$$

and we simply get back the equations of motion. Hence, for an optimal control problem, we get from the Lagrange multiplier rule a system of necessary conditions for optimality that is very similar to the classical conditions (3.8–3.10), and identical to (2.13):

$$\begin{aligned}\nabla_u f(\boldsymbol{y},\boldsymbol{u}) - G_u^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} &= 0, & (3.27)\\ \nabla_y f(\boldsymbol{y},\boldsymbol{u}) - G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} &= \dot{\boldsymbol{\lambda}}, & (3.28)\\ \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}) &= \dot{\boldsymbol{y}}, & (3.29)\end{aligned}$$

the only difference is that the sign is flipped on the G terms, because this is how we introduced the constraints, and that a term with a time derivative appears on the right, because the constraint is an ordinary differential equation. This system contains precisely enough equations for the number of unknowns: there are as many algebraic equations in (3.27) as unknowns in $\boldsymbol{u}(t)$ for $t \in [0,T]$, and (3.28)–(3.29) is a coupled first-order system of ordinary differential equations in $\boldsymbol{y}(t)$ (optimal trajectory) and $\boldsymbol{\lambda}(t)$ (multipliers) with precisely two boundary conditions at $t = 0$ and $t = T$ (both on the unknown $\boldsymbol{y}$ in our case). Hestenes was therefore able to solve this coupled system numerically to obtain candidates for the optimal trajectory.

The optimality system (3.27–3.29) reveals a very interesting mathematical structure[8]. Defining the Hamiltonian function

$$H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) := -f(\boldsymbol{y},\boldsymbol{u}) + \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u})^T\boldsymbol{\lambda}, \tag{3.30}$$

we see that the boundary value problem (3.28), (3.29) is in fact given by

$$\begin{array}{rclcl} \dot{\boldsymbol{y}} & = & \nabla_\lambda H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) & = & \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}), \\ \dot{\boldsymbol{\lambda}} & = & -\nabla_y H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) & = & -G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} + \nabla_y f(\boldsymbol{y},\boldsymbol{u}), \end{array} \tag{3.31}$$

where $\nabla_y H = H_y^T$ and $\nabla_\lambda H = H_\lambda^T$. Therefore, we have a Hamiltonian system, which has the property that

$$\frac{d}{dt}H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) = H_y\dot{\boldsymbol{y}} + H_u\dot{\boldsymbol{u}} + H_\lambda\dot{\boldsymbol{\lambda}} = H_y\nabla_\lambda H + H_u\dot{\boldsymbol{u}} + H_\lambda(-\nabla_y H) = 0 \tag{3.32}$$

along optimal trajectories, since $H_u^T = \nabla_u H = -\nabla_u f(\boldsymbol{y},\boldsymbol{u}) + G_u^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\lambda} = 0$ whenever the optimality condition (3.27) holds. Thus, the Hamiltonian is conserved in this case. The fact that the derivative of the Hamiltonian (3.30) with respect to the controls $\boldsymbol{u}$ coincides with the corresponding derivatives of the Lagrangian in (3.23),

$$\nabla_u H = -\nabla_u f + G_u^T\boldsymbol{\lambda} = -\nabla_u \mathcal{L}, \tag{3.33}$$

implies that an identical necessary condition for an interior minimum in the controls $\boldsymbol{u}$ can be obtained from both the Lagrangian and the Hamiltonian. Instead of minimizing the Lagrangian (3.23) with respect to the controls $\boldsymbol{u}$, which means minimizing the objective function on an optimal trajectory satisfying $\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}) = 0$

$$\int_0^T f(\boldsymbol{y},\boldsymbol{u})dt \longrightarrow \min \quad \text{with respect to } \boldsymbol{u}(t), \tag{3.34}$$

one could also maximize the Hamiltonian (3.30)

$$H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) \longrightarrow \max \quad \text{with respect to } \boldsymbol{u}(t), \tag{3.35}$$

pointwise for each $t \in [0,T]$. Minimizing the Lagrangian (3.34) just leads back to the original problem formulation (3.19–3.22), since $\boldsymbol{\lambda}$ disappears from the

[8] This was already discovered by Carathéodory [16], see also subsection 3.7

H(t,q,p,A) ≤ H(t,q,p,a)

must hold for every admissible element (t,q,A).

Thus, H has a maximum value with respect to a_h along a minimizing curve C_0.

FIGURE 17. Hestenes' discovery that the Hamiltonian must be maximized along a minimizing solution in the RAND report from 1950.

optimality system (3.27–3.29) when (3.27) is replaced by (3.34). However, maximizing the Hamiltonian (3.35) leads to a new problem formulation

$$H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}) \longrightarrow \max \quad \text{with respect to } \boldsymbol{u}(t), \tag{3.36}$$

$$\dot{\boldsymbol{y}} = \nabla_\lambda H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}), \tag{3.37}$$

$$\dot{\boldsymbol{\lambda}} = -\nabla_y H(\boldsymbol{y},\boldsymbol{u},\boldsymbol{\lambda}), \tag{3.38}$$

since $\boldsymbol{\lambda}$ does not disappear from this new optimality system (3.36-3.38). This was already noticed by Hestenes in his famous RAND report from 1950, see Figure 17. At the time, due to the lack of computing power, Hestenes was unable to solve the optimality system numerically. However, it was only a matter of time before digital computers became available, and Hestenes already anticipated this development in his manual to engineers, see Plail [46].

There is however a very important issue we did not address so far in the above attempt for optimizing the controls: the controls $\boldsymbol{u}$ of the airplane may not take on arbitrary values, but are instead confined to a closed and bounded set, since the thrust of the engine cannot be arbitrarily large, and the control vanes of the airplane cannot turn arbitrarily far. The optimality system (3.27–3.29) is therefore only a necessary condition if the solution lies in the interior of the domain of controls; the formulation in its present form cannot identify potential optima on the boundary of the range of the controls because (3.27), which comes from requiring the derivative with respect to the controls $\boldsymbol{u}$ to be zero, need not hold on the boundary. We see however that the new optimality system (3.36–3.38), written with the Hamiltonian, does not have this problem and deals with the optimal trajectories correctly, even when the control $\boldsymbol{u}$ lies on the boundary, since the minimization is not characterized by a derivative. Next, we will see how this insight was found historically, and led to the famous maximum principle of Pontryagin.

3.3. Early non-classical optimal control problems

An interesting problem, very much related to the fact that the controls in many real applications must be bounded, was studied by Feldbaum in Russia in [22]: he considered the problem of guiding an object from one position to another with a control that can only take two states, a so-called "bang-bang

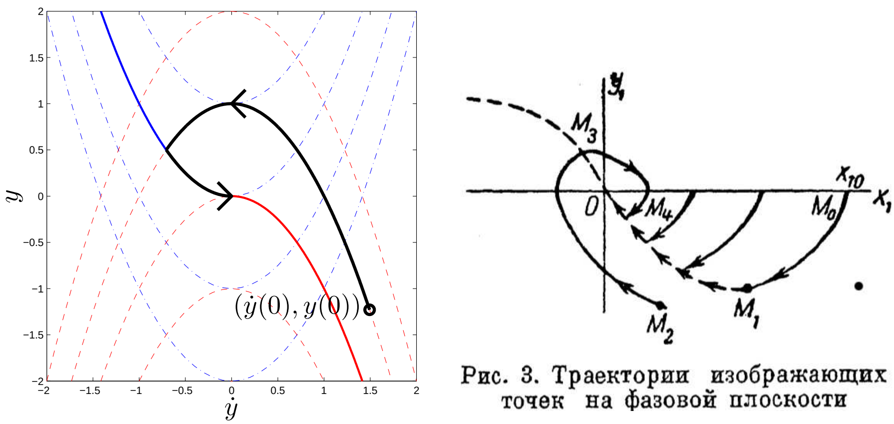


FIGURE 18. Solutions of the bang-bang system of Feldbaum from 1949 on the left, and an original drawing of Feldbaum from 1949 leading to his understanding of the bang-bang solution

system" of second order. This was modeled by the equation of motion

$$\ddot{y} = \pm M, \tag{3.39}$$

and the goal was to determine, for a given control strength constant M, when to choose the positive and when to choose the negative sign in order to go as quickly as possible from an initial position $y(0)$ at initial speed $\dot{y}(0)$ back to the origin at rest, i.e. $y(T) = \dot{y}(T) = 0$. Here, the controls are a discrete set, and depending on the sign chosen, we get the general solution branches by integration,

$$\begin{aligned} \dot{y}^{\pm} &= \pm Mt + C_1^{\pm}, \\ y^{\pm} &= \pm\frac{1}{2M}(\pm Mt + C_1^{\pm})^2 + C_2^{\pm} = \pm\frac{1}{2M}(\dot{y}^{\pm})^2 + C_2^{\pm}. \end{aligned}$$

Because $y^{\pm}$ is a quadratic function of $\dot{y}^{\pm}$, these solution branches are best drawn in phase space, where $y^{\pm}$ is a parabola as a function of $\dot{y}^{\pm}$ centered at $\dot{y}^{\pm} = 0$, as illustrated in Figure 18 on the left.

On the red dashed curves, the control $-M$ is active, and we are moving from the right to the left. On the blue dashed-dotted curves, the control M is active, and we are moving from left to right. There are only two curves, shown as solid lines, that pass through the target $y(T) = \dot{y}(T) = 0$, namely $y^{\pm} = \pm\frac{1}{2M}(\dot{y}^{\pm})$, and from any point along these curves, the fastest is just to stay on these curves with the corresponding control. Now from any point in the phase space to the right of this solid curve, one can use the control $-M$ to arrive as quickly as possible on the blue solid curve, where the control has to be switched to M to arrive at the origin. An example of such a trajectory is shown in Figure 18 in black. Similarly, from any point in the phase space to the left of the solid curve, one can use the control M to arrive as quickly as possible on the red solid curve, where the control has to be switched to $-M$ to arrive at the origin. In a follow-up paper [23] published four years later, Feldbaum made the key step of allowing not only the discrete set of controls $\{-M, M\}$, but the entire continuum of all controls in the closed interval $[-M, M]$, and the problem (3.39) became

$$\ddot{y} = \pm u, \quad |u| \leq M. \tag{3.40}$$

It was at this moment that the notational convention of using u for the control was born. Feldbaum gave a precise mathematical formulation of the minimum time problem for (3.40), and proved that for every initial point in the phase space, there exists a unique time-optimal control $u(t)$ which is still the bang-bang solution found for the control problem with only two discrete controls (3.39): on the optimal trajectory, the control is never used from within the interior of the interval $[-M, M]$! This was the first solution of what Boltyanski calls in his review [9] a non-classical variational problem. Bushaw made a similar discovery in his PhD thesis [13], see also [14]. Feldbaum then generalized this result in two follow-up papers [24, 25] to higher order problems of the form

$$y^{(n)} = -\sum_{j=0}^{n-1} a_j y^{(j)} + u, \quad |u| \leq M,$$

and proved what he called the n-interval theorem, namely that the optimal control is still piecewise constant with values $\pm M$, and that there are no more than n distinct intervals where the control u is constant. Feldbaum was therefore undoubtedly one of the pioneers in the field of optimal control where the domain of the controls is a closed set.

Around the same time, Lerner, also in Russia, considered putting a constraint on the phase coordinates, restricting them to be in a closed set [35, 36]. He considered the same problem as Feldbaum (3.40), but now also with the additional constraint $a_1 \leq y \leq a_2$. Figure 19 shows the solution in that case from his publication [36]. Note that the trajectory constraint is sometimes active, and sometimes not, whereas the control is always on the boundary, i.e., its constraint is always active.

3.4. Invention of the Maximum Principle

> This fact appears in many cases as a general principle, which we call the *maximum principle* (translated from Boltyanski, Gamkrelidze and Pontryagin 1956 [10], see Figure 22 for the original)

It was in this context that Pontryagin started to work with his students Boltyanski and Gamkrelidze on optimal control.[9] Pontryagin was known worldwide at the time for his work on homotopic topology, even though he had become blind after an accident involving an explosion at the age of twelve. However, around the 1950s, his results in homotopic topology started to be

[9]For more details on the historical context for this development, see Plail [46] and also [45].

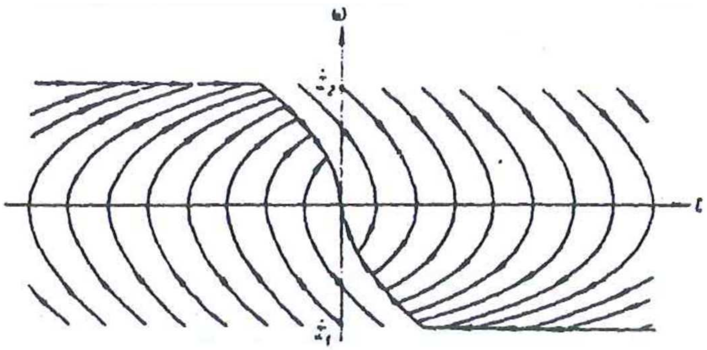


Рис. 3. Совокупность кратчайших процессов в системе, ограниченной по скорости и ускорению.

FIGURE 19. Lerner's solution to problem (3.39) with an additional inequality constraint on the trajectory

surpassed by the achievements of the French school around Leray, Serre and Cartan [9], and Pontryagin decided to leave this area of research and focus on the very different area of optimal control. This was in part due to his friendship with A. Andronov, with whom Pontryagin had worked on rough systems, but also because the university administration and the communist party organization encouraged more applied research. Together with his students, Pontryagin started an active research seminar to which engineers were also invited, and where the talks always had to have an applied side. Feldbaum also spoke several times at this seminar about his research on optimal control problems. In 1955, Pontryagin's group met Colonel Dobrohotov from the military academy of the Russian air force, and this contact led them to the important problem of guiding a flying object in minimal time in air combat. Even though the problems were not formulated as such, Pontryagin and his group realized immediately that the framework of optimal control was mathematically the correct one.

In their first publication in 1956, see [10], Pontryagin, Boltyanski and Gamkrelidze present the ideas which led them to formulate the maximum principle. There is only one reference in this paper, to Feldbaum's paper from 1955 [24], and the authors refer to the references given there. The problem they consider is to control in a time optimal way the system governed by the equations

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u}), \quad \boldsymbol{y}(0) = \boldsymbol{y}^0, \quad \boldsymbol{y}(T) = \boldsymbol{y}_T, \tag{3.41}$$

which describe the trajectory $\boldsymbol{y} : \mathbb{R} \to \mathbb{R}^m$ of the object for a given set of control functions $\boldsymbol{u} : \mathbb{R} \to \mathbb{R}^{n-m}$. The precise problem formulation is to find among all admissible controls $\boldsymbol{u}(t)$ the one that leads to the shortest travel time, i.e. $T = T(\boldsymbol{u})$ should be minimized. The authors say right at the beginning that the controls often have to satisfy further constraints, for example

$|u_j| \le 1$. They therefore introduce an open set Ω where the controls live, and also its closure $\bar{\Omega}$, and carefully distinguish these two cases for the control. They start with the control in the open set Ω, where one could easily derive optimality conditions using Lagrange multipliers. However, since the group of Pontryagin had their roots in a different field from variational calculus, they derive the optimality conditions with their bare hands: they assume existence of an optimal control $\boldsymbol{u}$, and derive a necessary optimality condition by considering a variation of the control $\boldsymbol{u}(t) + \delta\boldsymbol{u}(t)$ and the associated variation in the trajectory $\boldsymbol{y}(t) + \delta\boldsymbol{y}(t)$. Inserting these variations into the equations of motion (3.41), we obtain

$$\frac{d\boldsymbol{y}}{dt} + \frac{d\delta\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y} + \delta\boldsymbol{y}, \boldsymbol{u} + \delta\boldsymbol{u}) = \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u}) + G_y\delta\boldsymbol{y} + G_u\delta\boldsymbol{u},$$

and therefore the variation in the trajectory satisfies the linear inhomogeneous system of ordinary differential equations

$$\frac{d\delta\boldsymbol{y}}{dt} = G_y\delta\boldsymbol{y} + G_u\delta\boldsymbol{u}, \tag{3.42}$$

where $G_u\delta\boldsymbol{u}$ plays the role of the forcing term. Now the initial condition for the motion is fixed, and therefore the initial variation $\delta\boldsymbol{y}(0)$ must vanish. Using the technique of variation of constants, we can solve the system (3.42) as follows: if we denote by the matrix $Y(t)$ the solution of the linear homogeneous system

$$\dot{Y} = G_y Y, \quad Y(0) = I \quad (I \text{ the identity}),$$

the general solution of the homogeneous part of (3.42) is given by $Y\boldsymbol{c}$ for an arbitrary constant vector $\boldsymbol{c}$. Now varying the constant by setting $\boldsymbol{z} := Y\boldsymbol{c}(t)$, we get

$$\dot{\boldsymbol{z}} = \dot{Y}\boldsymbol{c} + Y\dot{\boldsymbol{c}} = G_y\boldsymbol{z} + Y\dot{\boldsymbol{c}}.$$

By letting $\boldsymbol{z} = \delta\boldsymbol{y}$ and comparing with (3.42), we get $Y\dot{c} = G_u\delta\boldsymbol{u}$, and hence $\boldsymbol{c} = \boldsymbol{c}_0 + \int_0^t Y^{-1}(\tau)G_u\delta\boldsymbol{u}(\tau)d\tau$. The solution of (3.42) is thus given by $\delta\boldsymbol{y} = Y\boldsymbol{c}$, and with the zero initial condition, we obtain

$$\delta\boldsymbol{y}(t) = Y(t)\int_0^t Y^{-1}(\tau)G_u\delta\boldsymbol{u}(\tau)d\tau. \tag{3.43}$$

Now the end point is fixed as well, $\boldsymbol{y}(T) = \boldsymbol{y}_T$, but the time at which the solution trajectory passes through this endpoint is not. Pontryagin argues as shown in Figure 20, which translated to English says (we use in the translation the symbols and equation numbers used in our presentation, instead of the original ones):

> Because of the linearity of system (3.42), the points $\boldsymbol{y}(T) + \delta\boldsymbol{y}(T)$ which correspond to any sufficiently small perturbation $\delta\boldsymbol{u}$ fill the whole range of some linear mapping P', which passes through $\boldsymbol{y}(T)$. From the optimality of the trajectory $\boldsymbol{y}(t)$, it is easy to see that the dimension of the range of P' does not exceed $m-1$, and P', in general, does not touch the trajectory $\boldsymbol{y}(t)$. Let $P(T)$ be some $m-1$ dimensional surface which contains P' and does not touch

В силу линейности системы (2) точки $x(t_1) + \delta_1 x(t_1)$, соответствующие всевозможным, достаточно малым по модулю, возмущениям $\delta_1 u(t)$, заполняют область некоторого линейного многообразия P', проходящего через точку $x(t_1)$. Из оптимальности траектории $x(t)$ легко вытекает, что размерность многообразия P' не превосходит $n-1$ и P', вообще говоря, не касается траектории $x(t)$. Пусть $P(t_1)$ — некоторая $(n-1)$-мерная плоскость, содержащая P' и не касающаяся траектории $x(t)$. Ковариантные координаты $(n-1)$-мерной плоскости $P(t_1)$ обозначим через $a_1,\dots,a_n$; тогда $a_\alpha \delta_1 x^\alpha(t_1) = 0$.

FIGURE 20. Geometric idea of Pontryagin, leading to the adjoint equation without knowing about Lagrange multipliers (see text for a translation)

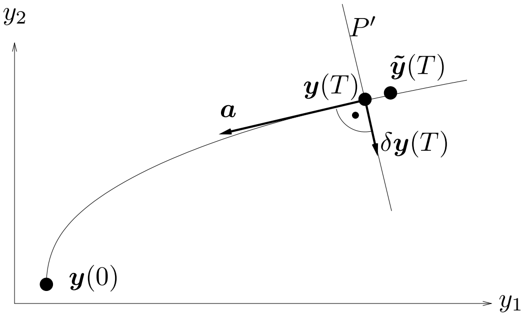


FIGURE 21. Explanation of Pontryagin's geometric idea.

the trajectory $\boldsymbol{y}(t)$. Let the covariant coordinates of this $m-1$ dimensional surface $P(T)$ be $a_1, a_2, \dots, a_m$. Then $\boldsymbol{a}^T \delta\boldsymbol{y}(T) = 0$.

It seems that this insight was obtained by Pontryagin very rapidly over two or three sleepless nights, see [46, 27][10]. To understand his argument, Figure 21 is useful: If the trajectory $\boldsymbol{y}(t)$ is optimal, no variation $\delta\boldsymbol{u}(t)$ is allowed to produce a trajectory $\tilde{\boldsymbol{y}}(t)$ with $\tilde{\boldsymbol{y}}(T)$ beyond $\boldsymbol{y}(T)$, since otherwise this trajectory could have arrived at $\boldsymbol{y}(T)$ at a time $t < T$. Therefore, variations are only allowed to be orthogonal to the optimal trajectory[11], in a manifold P' of dimension at most $m-1$, where $m = 2$ in the two dimensional example in

[10]Personal communication of Plail with Boltyanski, and explanation by Gamkrelidze in his paper about the discovery of the maximum principle:

> **The first and the most important step toward the final solution was made by L. S. right after the formulation of the problem, during three days, or better to say, during three consecutive sleepless nights.**

[11]In fact, since the endpoint is fixed as well, no variations are allowed at the endpoint either, but then Pontryagin could not have obtained the solution (3.43) of the then overdetermined system of ordinary differential equations (3.42), and thus he decided to first only fix the starting point [27, page 442]. This flaw was only later fixed by Boltyanski, see the end of this subsection.

Figure 21. There must therefore exist a vector $\boldsymbol{a}$ orthogonal to this manifold, $\boldsymbol{a}^T\delta\boldsymbol{y}(T)=0$. Since we know the solutions for the variations from (3.43), we can compute

$$\boldsymbol{a}^T\delta\boldsymbol{y}(T)=\boldsymbol{a}^TY(T)\int_0^T Y^{-1}(\tau)G_u\delta u(\tau)d\tau=\int_0^T \boldsymbol{\psi}^T(\tau)G_u\delta u(\tau)d\tau=0, \tag{3.44}$$

where we defined the vector $\boldsymbol{\psi}(t):=Y^{-T}(t)Y^T(T)\boldsymbol{a}$. This vector is solution to a differential equation: taking a time derivative of the identity $Y^{-1}Y=I$, we get

$$(\dot{Y^{-1}})Y+Y^{-1}\dot{Y}=0 \implies (\dot{Y^{-1}})=-Y^{-1}G_y \implies (\dot{Y^{-T}})=-G_y^TY^{-T},$$

and hence $\boldsymbol{\psi}$ is the solution of the differential equation

$$\dot{\boldsymbol{\psi}}=-G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\psi}, \tag{3.45}$$

with final condition $\boldsymbol{\psi}(T)=Y^T(T)\boldsymbol{a}$. Since the variation $\delta\boldsymbol{u}$ is arbitrary in (3.44), the term under the integral sign must vanish, and Pontryagin and his students obtained the classical necessary conditions for an interior maximum

$$\begin{aligned}\boldsymbol{\psi}^TG_u(\boldsymbol{y},\boldsymbol{u}) &= 0, &(3.46)\\ \dot{\boldsymbol{\psi}} &= -G_y^T(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\psi}, &(3.47)\\ \dot{\boldsymbol{y}} &= \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}), \quad \boldsymbol{y}(0)=\boldsymbol{y}^0, \quad \boldsymbol{y}(T)=\boldsymbol{y}_T, &(3.48)\end{aligned}$$

which is just a special case of (3.27–3.29)[12], with $\boldsymbol{\psi}$ playing the role of the Lagrange multiplier $\boldsymbol{\lambda}$, and with an objective function f that depends neither on $\boldsymbol{y}$ nor on $\boldsymbol{u}$. Pontryagin, however, did not know of the relation between this and the Lagrangian at the time of publication; according to Boltyanski [9], they only learned about this several months later when reading the Russian translation of Bliss' monograph [5] from 1946.

Next, the authors note that the functions $\boldsymbol{\psi}$ can be multiplied by a convenient constant in order to obtain $\boldsymbol{\psi}^T\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u})|_{t=0}>0$ without causing any changes to the necessary conditions for optimality (3.46–3.48), since this quantity is conserved along optimal trajectories, see (3.32). This then implies $\boldsymbol{\psi}^T\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u})>0$ for all t. Now if the control $\boldsymbol{u}$ is only allowed to vary in the closed set $\bar{\Omega}$, the authors explain that the first condition (3.46) needs to be replaced by

$$\boldsymbol{\psi}^TG_u(\boldsymbol{y},\boldsymbol{u})\boldsymbol{\delta u}\le 0 \tag{3.49}$$

for all admissible variations $\boldsymbol{u}+\boldsymbol{\delta u}$ that remain in $\bar{\Omega}$. With this modification, the optimal control may now also be on the boundary. This remark could have led them directly to the KKT system (3.16).

[12] To solve the time optimal control problem correctly using Lagrange multipliers, we need to introduce the time variable as a state variable, $y_0(t):=t$, which implies $\dot{y}_0=1$, $y_0(0)=0$. The correct Lagrangian then becomes $\mathcal{L}(\boldsymbol{y},\boldsymbol{\lambda},\boldsymbol{u})=y_0(T)+\int_0^T\boldsymbol{\lambda}^T(\dot{\boldsymbol{y}}-\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}))dt$, where all vectors are now one element longer. Computing the variational derivative with respect to $\boldsymbol{y}$, we obtain now in addition to the earlier equations $\dot{\lambda}_0=0$ and $z_0(T)+\lambda_0(T)z_0(T)=0$ for arbitrary variation z_0, which implies $\lambda_0(T)=-1$ and hence $\lambda_0(t)=-1$ to complete the time optimality system with $y_0(t):=t$.

Этот факт является частным случаем следующего общего принципа, который мы называем п р и н ц и п о м м а к с и м у м а (принцип этот доказан нами пока лишь в ряде частных случаев):

Пусть функция $H(x, \psi, u) = \psi_\alpha f^\alpha(x, u)$ *при любых фиксированных* x, ψ *имеет максимум по* u, *когда вектор* u *меняется в замкнутой области* $\bar{\Omega}$; *обозначим этот максимум через* $M(x, \psi)$. *Если* $2n$-*мерный вектор* (x, ψ) *является решением гамильтоновой системы*

$$\left.\begin{aligned} \dot{x}^i &= f^i(x, u) = \frac{\partial H}{\partial \psi_i}, \\ \dot{\psi}_i &= -\frac{\partial f^\alpha}{\partial x^i}\psi_\alpha = -\frac{\partial H}{\partial x^i}, \end{aligned}\right\} \quad i = 1, \ldots, n, \tag{8}$$

где кусочно-непрерывный вектор $u(t)$ *в каждый момент времени удовлетворяет условию* $H(x(t), \psi(t), u(t)) = M(x(t), \psi(t)) > 0$, *то* $u(t)$ *является оптимальным управлением, а* $x(t)$ — *соответствующей оптимальной (в малом) траекторией системы* (1).

FIGURE 22. The historical moment when the maximum principle was invented

The second result in [10] is a sufficient condition for optimality, obtained according to [9] by Gamkrelidze, and again only for points in the interior of the control domain. The result is based on second variations of the function $\boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u})$, whose first derivative with respect to $\boldsymbol{u}$ was in the necessary condition for optimality in (3.46). With the change in sign such that $\boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u}) > 0$, Gamkrelidze showed that if, in addition to (3.46–3.48), the Hessian of $\boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u})$ with respect to $\boldsymbol{u}$ is negative definite at $t = 0$, then the control $\boldsymbol{u}(t)$ and associated trajectory $\boldsymbol{y}(t)$ are optimal in a neighborhood of $t = 0$. This sufficient condition was not a new result either, as it is a particular case of the sufficient condition of Legendre type [5, Chapter IX], which the authors did not know at that time. They then however note that if the Hessian is indefinite, then there is no optimal control in the interior of Ω, so any optimal control inside the closed set $\bar{\Omega}$ of admissible controls must occur on the boundary.

The authors then conclude, based on the necessary conditions (3.46–3.48) and the fact that the Hessian of $\boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u})$ with respect to $\boldsymbol{u}$ must be negative definite for optimality, that the Hamiltonian $H(\boldsymbol{y}, \boldsymbol{u}, \boldsymbol{\psi}) := \boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u})$ must attain a local maximum in $\boldsymbol{u}(t)$ for fixed $\boldsymbol{y}(t)$ and $\boldsymbol{\psi}(t)$ satisfying (3.46–3.48): under the condition that the variations $\boldsymbol{\delta u}$ are admissible and small enough, the inequality

$$\boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u}) \geq \boldsymbol{\psi}^T \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u} + \boldsymbol{\delta u}) \tag{3.50}$$

must hold for all time whenever (3.46–3.48) are satisfied and the Hessian is negative definite.

This was the historical moment of the invention of the maximum principle. The Hamiltonian could also be used to define the important differential equations involved, see Figure 22 for the original paragraph in Russian, which translates as (we use again the notation from our text in the translation):

> This fact appears in many cases as a general principle, which we call the *maximum principle* (we have only proved this principle so far for several special cases): Let $H(\boldsymbol{y},\boldsymbol{u}) = \boldsymbol{\psi}^T\boldsymbol{g}(\boldsymbol{y},\boldsymbol{u})$ have, for arbitrary but fixed $\boldsymbol{y}$, $\boldsymbol{\psi}$ a maximum as $\boldsymbol{u}$ varies within the closed set $\bar{\Omega}$. We denote this maximum by $M(\boldsymbol{y},\boldsymbol{\psi})$. If the $2m$-dimensional vector $(\boldsymbol{y},\boldsymbol{\psi})$ is a solution of the Hamiltonian system
>
> $$\dot{\boldsymbol{y}} = \boldsymbol{g}(\boldsymbol{y},\boldsymbol{u}) = \nabla_{\boldsymbol{\psi}} H,$$
> $$\dot{\boldsymbol{\psi}} = -G_y^T\boldsymbol{\psi} = -\nabla_{\boldsymbol{y}} H,$$
>
> and a piecewise continuous vector $\boldsymbol{u}(t)$ satisfies for each point in time
>
> $$H(\boldsymbol{y}(t),\boldsymbol{\psi}(t),\boldsymbol{u}(t)) = M(\boldsymbol{y}(t),\boldsymbol{\psi}(t)) > 0,$$
>
> then $\boldsymbol{u}(t)$ is the optimal control and $\boldsymbol{y}(t)$ the corresponding (locally) optimal trajectory of system (3.41).

This first publication only gave a criterion for the solution of the time optimal control problem, and it was formulated as a sufficient condition. Pontryagin also hoped that the criterion would give the global optimal control, and put the word "locally" in parentheses [9], see also Figure 22. The maximum principle allowed the authors to immediately solve the Bushaw-Feldbaum problem we have seen earlier,

$$\ddot{y} = u, \quad |u| \leq 1,$$

as follows: we first transform the system to first order

$$\dot{y}_1 = y_2, \quad \dot{y}_2 = u,$$

and the Hamiltonian becomes

$$H = \psi_1 y_2 + \psi_2 u.$$

For the auxiliary functions, we obtain the differential equations

$$\dot{\psi}_1 = 0, \quad \dot{\psi}_2 = -\psi_1.$$

These equations can be easily integrated to give $\psi_1(t) = C_1$ and $\psi_2(t) = C_2 - C_1 t$, where C_1 and C_2 are constants. To maximize H under the condition that $|u| \leq 1$, the control must satisfy

$$u(t) = \operatorname{sign}(\psi_2(t)) = \operatorname{sign}(C_2 - C_1 t),$$

and is therefore piecewise constant and can change at most once, since $\psi_2(t)$ is a linear function of t. We thus obtain precisely the bang-bang solution found by Feldbaum for this problem, but in a very simple way with the maximum principle. The maximum principle also worked very well for many similar problems that could not be solved earlier, which explains the high hopes Pontryagin had for it.

After this first publication, the work was divided by Pontryagin as follows: Gamkrelidze was asked to generalize the results obtained during the calculation of examples, and he quickly found the work by Bellman, Glicksberg and Gross [2], who had established a necessary and sufficient condition for the linear case

$$\dot{\boldsymbol{y}} = A\boldsymbol{y} + B\boldsymbol{u}, \quad |u_j| \leq 1,$$

and the time optimal control to get to $\boldsymbol{y} = 0$. For constant matrices A and B, where the eigenvalues of A have negative real parts, the optimal control is $\boldsymbol{u}^T(t) = \text{sign}(\boldsymbol{b}^T Y(t))$, where $Y(t) = X^{-1}(t)B$ and X solves the matrix equation $\dot{X} = AX$. Here $\boldsymbol{b}$ is an appropriately chosen vector, and the result holds under a general position condition, see [2]. Gamkrelidze managed to show that this necessary and sufficient condition coincides with the maximum principle, and hence for linear problems, the maximum principle is indeed a necessary and sufficient condition for optimality.

Boltyanski was supposed to work out in detail the results in the first paper [10], and Pontryagin was supposed to find a general justification of the maximum principle. Boltyanski started working on the first result in [10] and tried to formulate it differently from the classical analysis textbook style in which the argument was given, and searched for a geometrical proof. After a more careful study of the second, sufficient condition in [10], Boltyanski finally arrived, "in a brilliant half hour" [9], at the conclusion that the maximum principle was only a necessary condition. He immediately called Pontryagin in his apartment and told him that the maximum principle was only a necessary condition, but a global one. Pontryagin was angry when he received the call because it had woken him up from his afternoon nap, but he called back five minutes later to say that if Boltyanski had really found a proof, this would be of great interest, so it had to be checked carefully. Gamkrelidze did the careful checking, and the argument was correct, so Boltyanski asked Pontryagin if he could publish the results [9]:

> "It was proposed to publish it, as a joint paper of four authors. I refused point-blank. Then it was proposed (i) to name that theorem *Pontryagin's maximum principle*, and (ii) to add at the end of my paper a paragraph dictated by Pontryagin that pointed out his role in creation of the principle. Pontryagin was the head of the laboratory in the Steklov Mathematical Institute, and at that time could insist on his interests. I had to agree. After that, my paper was presented to Doklady AN SSSR [8].

Boltyanski indeed named the maximum principle after Pontryagin in the single authored paper [8]:

> Высказанный Л. С. Понтрягиным в качестве гипотезы принцип максимума
>
> The maximum principle suggested by Pontryagin as a hypothesis...

and we also show in Figure 23 the final paragraph dictated by Pontryagin to Boltyanski from the end of the same paper. The literal translation of this paragraph is:

Публикуемые здесь результаты получены мною при работе в руководимом Л. С. Понтрягиным семинаре по теории колебаний и автоматического регулирования. Л. С. Понтрягин указал мне на одно упрощение в доказательстве принципа максимума, благодаря чему мое доказательство стало пригодным для произвольного топологического пространства U (первоначальный вариант доказательства содержал лишнюю, нигде фактически не использовавшуюся конструкцию, которая заставляла ограничиваться случаем, когда U есть замкнутая область векторного пространства с кусочно-гладкой границей и выпуклыми внутренними углами в точках перелома).

FIGURE 23. The last paragraph Boltyanski had to add in his single authored paper, dictated by Pontryagin (see translation in the text)

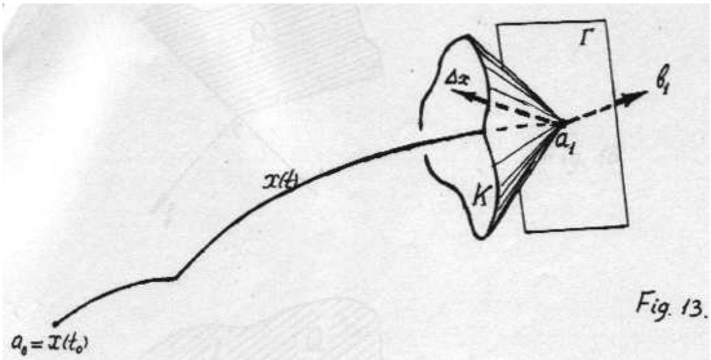


FIGURE 24. Original drawing by Boltyanski removing the initial flaw of variations at the endpoint in the proof of the maximum principle

> I got the results which are published in this paper working in the Pontryagin seminar on the theory of oscillations and automatic regulation. Pontryagin pointed out to me one simplification in the proof of the maximum principle, and because of that my proof became applicable to arbitrary topological spaces U (the first variant of the proof contained an unnecessary, actually nowhere used, construction that forced the restriction on the case, when U is a closed domain in a vector space with piecewise-smooth boundary and convex inner corners in breaking points).

As we have seen already in footnote 11, the initial argument of Pontryagin, which allowed the end point to vary in a lower dimensional manifold, was not quite correct. To remove this flaw, Boltyanski resorted in [8] to the tool of needle variations, which already appeared in McShane in 1939 [40]; however, Boltyanski insists that he was unaware of McShane's work at the time and came up with the technique independently [7]. We show in Figure 24 the hand drawing of Boltyanski from [9]. One can clearly see that a cone appears, instead of the variations orthogonal to the trajectory, and the role of the manifold is now played by Γ at the tip of the cone. The complete original proof also relies on techniques from topology, the field of origin of the group. It is quite long and technical; details can be found in the historical book by the four authors from 1962 [48], which was quickly translated into many languages and made Pontryagin and the Russian school of optimal control famous with their maximum principle. However, from Boltyanski's point of view, it was he who formulated and proved the maximum principle correctly. Pontryagin's insistence on publishing the result as a joint paper led to a period of deep bitterness for Boltyanski, during which he could not even do mathematics any more, as he tells in [9].

3.5. General formulation of the Maximum Principle

> The times t_0 and t_1, in this statement of the problem, are not fixed. We only require that the object should be in state x_0 at the initial time, and at state x_1 at the final time, and that the functional should achieve a minimum. (Pontryagin, Boltyanski, Gamkrelidze and Mishchenko 1962 [48])

Pontryagin and his students then generalized the problem of minimizing travel time to one of minimizing an arbitrary function [11]. The model for the technical object is again the system of ordinary differential equations

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y}, \boldsymbol{u}), \quad \boldsymbol{y}(t_0) = \boldsymbol{y}^0 \tag{3.51}$$

for the trajectory $\boldsymbol{y} : \mathbb{R} \to \mathbb{R}^m$ of the object, depending on the control functions $\boldsymbol{u} : \mathbb{R} \to \mathbb{R}^{n-m}$. These controls are supposed to be chosen such that when the object arrives at time t_1 at a given location $\boldsymbol{y}(t_1) = \boldsymbol{y}^1$, the general functional

$$J := \int_{t_0}^{t_1} g_0(\boldsymbol{y}(t), \boldsymbol{u}(t))dt \tag{3.52}$$

is minimized. Here the scalar function $g_0 : \mathbb{R}^m \times \mathbb{R}^{n-m} \to \mathbb{R}$ was on purpose denoted by the index zero, since a first step was then to define an additional ordinary differential equation

$$\frac{dy_0}{dt} = g_0(\boldsymbol{y}, \boldsymbol{u}), \quad y_0(t_0) = 0.$$

Appending this equation to the system of ordinary differential equations for the technical object as the zeroth coordinate, $\tilde{\boldsymbol{y}} := (y_0, y_1, \ldots, y_m)$, and similarly $\tilde{\boldsymbol{g}} := (g_0, g_1, \ldots, g_m)$, the new system of ordinary differential equations

$$\frac{d\tilde{\boldsymbol{y}}}{dt} = \tilde{\boldsymbol{g}}(\tilde{\boldsymbol{y}}, \boldsymbol{u}), \quad \tilde{\boldsymbol{y}}(t_0) = (0, \boldsymbol{y}^0) \tag{3.53}$$

encodes, in addition to the trajectory, also the current value of the objective function in its zeroth component:

$$y_0(t) = \int_{t_0}^{t} g_0(\boldsymbol{y}(t), \boldsymbol{u}(t))dt.$$

The authors now give a geometric interpretation of the optimal control problem in this higher dimensional space: given an initial point $\boldsymbol{y}^0$ and a target $\boldsymbol{y}^1$

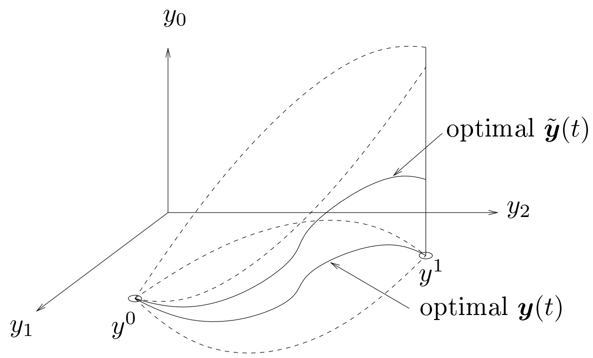


FIGURE 25. Interpretation of the optimal control problem in the higher dimensional space including the objective function coordinate y_0

in $\mathbb{R}^m$, as shown in Figure 25, among all the trajectories solution of (3.53) and ending at $\boldsymbol{y}^1$ (dashed line examples in Figure 25), find the one that crosses the vertical line in the y_0 direction above with the lowest coordinate value $y_0(t_1)$ possible (see solid line in Figure 25). Next, they explain several properties of this optimal control problem: first, the problem is time invariant, since the right hand side of the state equation and the objective function do not depend on time. One can therefore do translations in time without changing the problem, see Figure 26 from their book [48]. Because of this, one can also consider several points in phase space, and search for controls separately to move from one to the next sequentially, and then concatenate the controls in order to get a single control to go from the first to the last point in phase space. Doing this, one just has to sum the local objective function values to obtain the global value of the objective function. Concatenating the controls this way, however, is not possible in the space of continuous controls in general, and therefore one must expect the optimal control to be piecewise continuous only, as illustrated in Figure 27 from [48]. Finally, in preparation of their proof, they argue that the optimal trajectory must also be locally optimal: if it were not optimal on a sub-interval, then one could simply replace

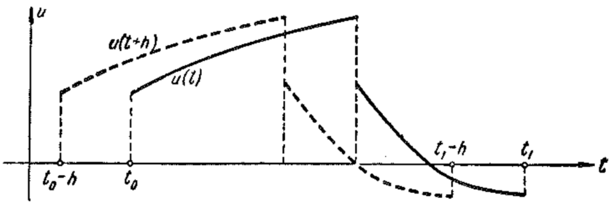


FIGURE 26. Graph to illustrate time translation invariance from [48]

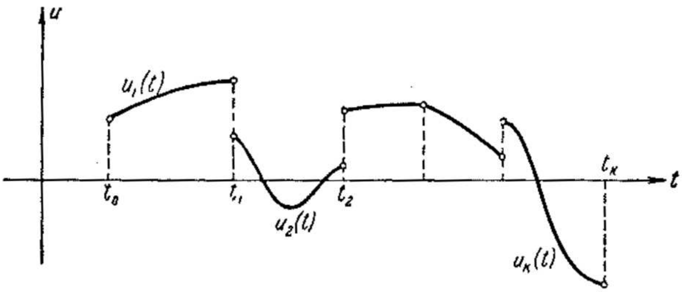


FIGURE 27. Graph to illustrate that the optimal controls are piecewise continuous, from [48]

the control there by a better one, and since the objective functions are just summed, the global objective function would decrease, see Figure 28 from [48] for an illustration of this.

For the formal statement of the maximum principle, the authors introduce as before the adjoint system (but now without explanation)

$$\frac{d\tilde{\psi}_i}{dt} = -\sum_{j=0}^{m} \frac{\partial g_j(\boldsymbol{y},\boldsymbol{u})}{\partial y_i}\tilde{\psi}_j, \quad i = 0, 1, \ldots, m \tag{3.54}$$

and the Hamiltonian

$$H(\tilde{\boldsymbol{\psi}}, \tilde{\boldsymbol{y}}, \boldsymbol{u}) := \tilde{\boldsymbol{\psi}}^T \tilde{\boldsymbol{g}}(\boldsymbol{y}, \boldsymbol{u}), \tag{3.55}$$

but now the maximum principle is no longer stated as a sufficient condition: a necessary condition for the control $\boldsymbol{u}$ and associated trajectory $\boldsymbol{y}$ to be optimal is that there exist $\boldsymbol{\psi}$ such that the Hamiltonian system

$$\frac{dy_i}{dt} = \frac{\partial H}{\partial \tilde{\psi}_i}, \quad i = 0, 1, \ldots, m \tag{3.56}$$

$$\frac{d\tilde{\psi}_i}{dt} = -\frac{\partial H}{\partial y_i}, \quad i = 0, 1, \ldots, m \tag{3.57}$$

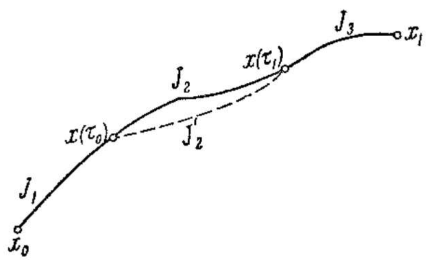


FIGURE 28. Graph to illustrate that the solution must be locally optimal, from [48]

holds and that for each admissible control $\boldsymbol{v}$ the inequality

$$H(\tilde{\boldsymbol{\psi}}, \tilde{\boldsymbol{y}}, \boldsymbol{v}) \leq H(\tilde{\boldsymbol{\psi}}, \tilde{\boldsymbol{y}}, \boldsymbol{u}) \tag{3.58}$$

be satisfied, i.e. the optimal control $\boldsymbol{u}$ is the value of $\boldsymbol{v}$ maximizing the Hamiltonian.

Suppose now that the optimum is in the interior of the domain. Then the inequality (3.58) implies that we are at a stationary point, i.e. the derivative with respect to $\boldsymbol{u}$ must vanish,

$$\tilde{\boldsymbol{\psi}}^T \tilde{G}_u(\boldsymbol{y}, \boldsymbol{u}) = 0 \quad \Longleftrightarrow \quad \psi_0 \nabla_u g_0(\boldsymbol{y}, \boldsymbol{u}) + G_u^T(\boldsymbol{y}, \boldsymbol{u})\boldsymbol{\psi} = 0.$$

Since the Hamiltonian does not depend on y_0, ψ_0 is just a constant, $\psi_0 = -1$ and we find naturally the condition (3.27) from the Lagrange multiplier approach[13]. So the maximum principle stating that the Hamiltonian has to be maximized is equivalent to stating explicitly that the Lagrangian has to be minimized, and not just at a stationary point, and the reason why it is a maximum for the Hamiltonian and a minimum for the Lagrangian comes just from the sign change in the definition of the Hamiltonian (3.30).

3.6. Example of an ODE Control Problem

We illustrate the use of Pontryagin's maximum principle on the following example. Suppose we have a system with a state variable $y = y(t) \in \mathbb{R}$ and a control variable $u = u(t) \in \mathbb{R}$ governed by

$$\dot{y} = u, \qquad y(0) = 0,$$

subject to the box constraints $|u(t)| \leq 1$ for all t. We would like to find the control $u(t)$ such that $y(1) = \frac{1}{2}$ and which minimizes the cost

$$J(y, u) = \frac{1}{2} \int_0^1 y^2 \, dt.$$

Without the constraint on the control, the optimality system (3.27–3.29) leads to $\dot{y} = u$, $\dot{\psi} = y$, $0 = 1 \cdot \psi$ and thus $\psi = 0$, $y = 0$ and $u = 0$. Since we must however have $y(1) = \frac{1}{2}$, one can force the solution in the last moment with a very large control to this value, and make the integral $\int y^2 dt$ arbitrarily small. With the constraint on the control, the best one can do is use $u = 1$, and we need to use this control over the second half of the interval to get $\dot{y} = 1$, in order to reach $y(1) = \frac{1}{2}$, which is the optimal solution, see Figure 29.

Lets now see how Pontryagin's maximum principle guides us to this solution: it says that if $u(t)$ is the optimal control, then for every $t \in (0, 1)$, we have

$$H(y(t), u(t), \psi(t)) = \max_{|\xi| \leq 1} H(y(t), \xi, \psi(t)),$$

[13] see also Footnote 12

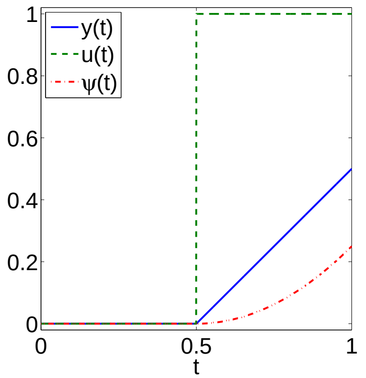


FIGURE 29. Solution of the simple optimal control problem.

where $y(t)$ and $\psi(t)$ are the state and adjoint state of the optimal trajectory at time t, and H is the Hamiltonian

$$H(y, u, \psi) = \psi u - \frac{1}{2}y^2.$$

Thus, by inspection, we have

$$u(t) = \begin{cases} 1, & \text{if } \psi(t) > 0, \\ -1 & \text{if } \psi(t) < 0. \end{cases}$$

If $\psi(t) = 0$, then we get no information from the maximum principle. We now deduce the optimal control and trajectory based on these properties.

1. We know that $y(1) = \frac{1}{2}$, so by the adjoint equation $\dot{\psi} = y$, we see that ψ has a positive slope in a neighborhood of $t = 1$, so it cannot vanish identically there. So if we assume that $\psi(1) \leq 0$, then $\psi(t) < 0$ in some interval $t \in (t_1, 1)$ with $t_1 = 1 - \delta$, $\delta > 0$, so $u(t) = -1$ there. This yields
$$y(t) = y(1) - \int_t^1 \dot{y}(\tau)d\tau = y(1) + 1 - t = \frac{3}{2} - t. \tag{3.59}$$
Thus, $y(t) \geq \frac{1}{2}$ for all $t \in (t_1, 1)$, so $\psi(t)$ is a strictly increasing function with $\psi(1) \leq 0$, implying that $\psi(t) < 0$ for all $t \in (t_1, 1)$. In particular, $\psi(t_1) < 0$, so continuing this argument now over the interval $(t_1 - \delta, t_1)$, etc. shows that (3.59) in fact holds for the whole interval $(0, 1)$. This implies $y(0) = \frac{3}{2}$, which contradicts the initial condition $y(0) = 0$. Hence $\psi(1)$ cannot be negative (or zero).
2. Suppose now that $\psi(1) = \psi_1 > 0$. Then there exists a neighborhood around $t = 1$ in which $\psi(t) > 0$. Let $t^* \in [0, 1)$ be the smallest t such that $\psi(t) > 0$ whenever $t > t^*$. Then by the continuity of ψ, we have $\psi(t^*) = 0$. Moreover, $u = 1$ on $(t^*, 1)$, which implies
$$y(t) = y(1) - \int_t^1 u(\tau)d\tau = y(1) - 1 + t = t - \frac{1}{2} \tag{3.60}$$

whenever $t \in (t^*, 1]$.

3. We show that $y(t^*) = 0$ by excluding both $y(t^*) > 0$ and $y(t^*) < 0$. If $y(t^*) > 0$, then $\psi(t^* - \delta) < 0$ for $\delta > 0$ small enough, so $u = -1$ on the interval $(t^* - \delta, t^*)$. This means $y(t^* - \delta) > y(t^*) > 0$; continuing this argument backwards in time, we obtain $y(0) > y(t^*) > 0$, a contradiction. On the other hand, if we assume that $y(t^*) < 0$, then $\dot{\psi}(t^*) < 0$ and $\psi(t^*) = 0$ together implies that $\psi(t^* + \delta) < 0$ for $\delta > 0$ small enough, which contradicts the definition of t^*. Thus, $y(t^*) = 0$. Since (3.60) is satisfied for all $t \in (t^*, 1]$, we deduce that $t^* = \frac{1}{2}$.
4. The optimal trajectory and control are now determined for the interval $[\frac{1}{2}, 1]$. Since $\int_{1/2}^{1} y^2 \, dt$ is now fixed, we are left with the minimization problem

$$\int_0^{1/2} y^2 \, dt \to \min \qquad \text{s.t. } y(0) = y(\tfrac{1}{2}) = 0,$$

where $\dot{y} = u$ and $|u(t)| \leq 1$. The optimal solution is obviously

$$y(t) \equiv 0, \qquad u(t) \equiv 0 \qquad \forall t \in (0, \tfrac{1}{2}).$$

Note that the adjoint state must also vanish, since u would not be allowed to take on values different from ± 1 otherwise.

We thus obtain the same solution from Figure 29. Note that unlike problems with a pure bang-bang solution, our optimal control contains both an interior part ($u = 0$ on $t \in (0, \frac{1}{2})$) and a boundary part ($u = 1$ on $t \in (\frac{1}{2}, 1)$). We also see that in this case, the maximum principle is useful in the sense that it guides us towards the optimal solution bit by bit, but it does not provide an algorithm for computing the optimal control directly.

3.7. Caratheodory

> Auf den folgenden Seiten soll auf das allgemeine Problem der Variationsrechnung in einem $(n+1)$-dimensionalen Raum mit p gewöhnlichen Differentialgleichungen als Nebenbedingungen die Methode der geodätischen Äquidistanten angewandt werden[14] (Carathéodory 1926 [16])

Constantin Carthéodory had already worked in his PhD thesis on discontinuous solutions in the calculus of variations [15], and became one of the eminent researchers in this field. In a paper published in 1926, see also the quote above, he set out to solve precisely the same type of problem we have seen before, but thirty years earlier. He studied the minimization problem

$$I := \int_{t_1}^{t_2} L(t, \boldsymbol{x}, \dot{\boldsymbol{x}}) dt \quad \longrightarrow \quad \min$$

under the constraints given by implicit differential equations

$$\boldsymbol{G}(t, \boldsymbol{x}, \dot{\boldsymbol{x}}) = 0, \tag{3.61}$$

[14] On the following pages we will solve the general problem of variational calculus in an $(n+1)$ dimensional space with p ordinary differential equations as constraints, using the method of geodesic equal distances

$$H(t, x_i, y_i) = -M(t, x_j, \varphi_j, \chi_{k'}) + \sum_j y_j \varphi_j,$$
$$\dot{x}_i = H_{y_i}, \quad \dot{y}_i = -H_{x_i}$$

FIGURE 30. Formulation of necessary conditions using the Hamiltonian for optimal control problems already found in the work by Carathéodory from 1926

where $L : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, and $\boldsymbol{G} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^p$. Using geodesic arguments, he was led to define the scalar quantity

$$M(t, \boldsymbol{x}, \dot{\boldsymbol{x}}, \boldsymbol{\mu}) := L(t, \boldsymbol{x}, \dot{\boldsymbol{x}}) + \boldsymbol{\mu}^T \boldsymbol{G}(t, \boldsymbol{x}, \dot{\boldsymbol{x}}),$$

for some parameter functions $\boldsymbol{\mu}$. He then applied the Legendre transform to M, which led him to the Hamiltonian

$$H(t, \boldsymbol{x}, \boldsymbol{y}) := -M(t, \boldsymbol{x}, \boldsymbol{\varphi}, \boldsymbol{\chi}) + \boldsymbol{y}^T \boldsymbol{\varphi}.$$

Here, $\boldsymbol{\varphi}$ represents the right hand side when the implicit differential equation (3.61) is solved to obtain an explicit form $\dot{x}_i = \varphi_i(t, \boldsymbol{x})$, and $\boldsymbol{\chi} = \boldsymbol{\mu}$, which gives

$$H(t, \boldsymbol{x}, \boldsymbol{y}) = -L(t, \boldsymbol{x}, \boldsymbol{\varphi}) - \boldsymbol{\chi}^T \boldsymbol{G}(t, \boldsymbol{x}, \boldsymbol{\varphi}) + \boldsymbol{y}^T \boldsymbol{\varphi}.$$

Now along a solution satisfying the constraint, we have $\boldsymbol{G}(t, \boldsymbol{x}, \boldsymbol{\varphi}) = 0$, and Carathéodory obtains as the main result[15], as we have seen earlier, that the solution candidates must satisfy the differential equations

$$\dot{\boldsymbol{x}} = \nabla_y H, \quad \dot{\boldsymbol{y}} = -\nabla_x H, \tag{3.62}$$

which he says play such a prominent role in mechanics, see also the original formulas in Figure 30. In contrast to Pontryagin later, he does however only consider local optima in open sets. For more explanations on the derivation of the Hamiltonian formulation of Carathéodory, see [44], and also the very interesting description of the history of the maximum principle and optimal control in [46], see also [45, 43].

4. PDE Constrained Optimization

We have seen in the previous section how the desire to optimize the trajectory of a system governed by ODEs gave birth to the field of optimal control. In many applications, however, the system is not governed by ODEs, but by partial differential equations (PDEs), and the desire to optimize certain outputs leads to PDE constrained optimization problems. This field is nowadays an active research area, as attested by the many conferences and papers in

[15]Das Hauptresultat besteht darin, dass unsere Gefällkurven mit den Cauchyschen Charakteristiken zusammenfallen und Lösungen der kanonischen Differentialgleichungen (3.62) sind, die in der Mechanik eine so bedeutende Rolle spielen

recent years. Here we mention only three sample applications; other applications abound and new ones arise every day, so it is impossible to mention them all.

- Oil reservoir management: the flow of fluids in an oil field satisfies a system nonlinear PDEs that models the conservation of chemical species transported by different fluid phases. Here, the only interaction with the subsurface oil field is through wells, either by injecting fluid (water or gas) into the ground or by controlling how much fluid (typically a mixture of oil, water and gas) can come out of it. Thus, the goal could be, for instance, to optimize the oil output over the lifetime of the reservoir by optimizing over the control variables, such as the injection rate of water or gas at an injection well, or the fluid pressure or production rate at the production wells. Here the control variables can be functions of time, just like in the ODE case.
- Shape and topology optimization: consider the design of an airfoil. Depending on the purpose of the airfoil, one can maximize the lift, minimize the drag, or minimize the vortices created by the airfoil when air flows around it. Thus, the objective function depends on the solution of the PDE governing the flow of air around the airfoil, e.g., a Laplace-type potential flow equation, or the full Navier–Stokes equation. Here, the control variable is the "shape" of the airfoil, i.e., the function that defines the boundary of the domain, and the PDE constraint is the Laplace or Navier–Stokes equation.
- Inverse problems: consider an underground rock formation, of which we would like to understand its internal composition (types of rock, existence of layers and faults, etc.) One way of obtaining information without drilling is to send seismic or electromagnetic waves into the ground and install detectors on the surface to measure the reflected waves. If the rock parameters were known ahead of time, then the reflected waves can by calculated by solving a PDE (elasticity or wave equation). However, since our goal is precisely to estimate these parameters, we must solve an *optimization problem* by choosing the parameters that *minimize the discrepancy* between the predicted and measured waves, subject to the constraint that the waves satisfy a PDE.

4.1. Early Work

The discovery of Pontryagin's maximum principle and its ability to explain bang-bang type solutions generated great interest in the optimal control community. In particular, starting from the 1960s, there was a push to generalize both results to systems described by PDE rather than ODE constraints. The earliest reference appears to be a series of papers by Egorov [18]–[19] starting in 1962, which contains a detailed study of the minimal time problem for the parabolic control problem of the type

$$\begin{aligned} \frac{\partial y}{\partial t} + Ay + b(u)y = f + u \quad &\text{on } \Omega \times (0,T), \\ y = 0 \quad &\text{on } \partial\Omega \times (0,T), \end{aligned} \tag{4.1}$$

with initial condition $y(t_0; u) = y_0$ and target $y(t_1; u) = y_T$, but the arguments therein are rather opaque[16].

Stateside, a proof of the bang-bang property when $b = 0$ and u is restricted to the set

$$U_{ad} = \{u : |u(t)| \leq 1 \text{ a.e.}\}$$

was given in 1964 by Fattorini [21], who wrote his Ph.D. thesis on the topic under the supervision of P. D. Lax. The proof proceeds in two steps. First, Fattorini writes $y(\tau; u)$ in terms of the Green's function

$$y(\tau; u) = G(\tau)y_0 + \int_0^\tau G(\tau - \sigma)u(\sigma)\, d\sigma.$$

Using this representation, he shows that if $|u(t)| \leq 1-\epsilon$ for some $\epsilon > 0$ *almost everywhere* in the interval $(0, \tau)$, then one can produce another control $v(t)$ such that $|v(t)| \leq 1$ and $y(s; v) = y_T$ with $s < \tau$, so that τ is not the optimal time. He then shows that even in the case where $|u(t)| \leq 1 - \epsilon$ only on a *subset* $e \subset (0, \tau)$ of positive measure, u cannot optimal. To show this, let e be the subset in which $|u(t)| \leq 1 - \epsilon$. Then using semi-group theory, Fattorini shows that there exists a control $\bar{g}(t)$ with bounded values and *support in* e such that $y(\tau; \bar{g}) = y(\tau; u) = y_T$. By taking a weighted average of u and $\bar{g}$, one obtains a new control $v = (1-\theta)u + \theta\bar{g}$ that satisfies $|v(t)| \leq 1-\hat{\epsilon}$ everywhere for some $\hat{\epsilon} > 0$, but without changing the target y_T, since $y(\tau, v) = (1-\theta)y(\tau; u) + \theta y(\tau; \bar{g}) = y_T$. Thus, by the previous argument, τ is not the shortest time necessary to arrive at y_T, so u is not time-optimal. This proof does not use any variant of the Pontryagin's maximum principle, so none was formulated in the paper.

Proofs of the bang-bang property for other systems, notably boundary control problems, appeared subsequently, see for instance Friedman [26]. However, it was a research monograph of Jacques-Louis Lions that launched the systematic study of optimal control under PDE constraints and shaped the field as we know it today.

4.2. Lions

> A new adventure began for Lions in the early 1960s, when he met (in spirit) another of his intellectual mentors, John von Neumann. By then, using computers built from his early designs, von Neumann was developing numerical methods for the solution of PDEs from fluid mechanics and meteorology. At a time when the French mathematical school was almost exclusively engaged in the development of the Bourbaki program, Lions — virtually alone in France — dreamed of an important future

[16] According to J.-L. Lions: "Le travail de Yu. V. Egorov contient une étude détaillée de ce problème, mais nous n'avons pas pu comprendre tous les points des démonstrations de cet auteur, les résultats étant très probablement tous corrects."

> for mathematics in these new directions; he threw himself into this new work, while still continuing to produce high-level theoretical work on PDEs. (R. M. Temam, Obituary of Jacques-Louis Lions (SIAM News, July 10, 2001)

Jacques-Louis Lions (1928–2001) was one of the most influential figures of his time in applied mathematics in France and throughout the world. Under the influence of his PhD supervisor, the Fields medalist L. Schwartz, Lions' early work was of a theoretical nature, emphasizing the use of distributions and appropriate function spaces in the study and solution of PDEs. During his time as scientific director at IRIA[17], he discovered "systems theory", which subsequently became a new component of his research in the form of control theory. Given his expertise in PDEs and variational formulations, it is no surprise that his theory of PDE constrained optimization is heavily based on function (especially Sobolev) spaces and variational arguments.

Lions' first contribution in PDE constrained optimization was a research monograph entitled "Contrôle optimal de systèmes gouvernés par des équations aux dérivées partielles" [37]. It was published in 1968 and became the standard reference of the subject. In this volume, Lions developed his theory systematically by first considering the control of elliptic problems, and then moving on to time-dependent problems of the parabolic and hyperbolic types. The stated goals of the volume, which appear in the introduction, are as follows:

1. to obtain necessary (and maybe also sufficient) conditions for local extrema of the PDE constrained optimization problems;
2. to study the structure and properties of equations expressing such conditions;
3. to obtain constructive algorithms that can be used to calculate the optimal controls numerically.

This last point was particularly groundbreaking at a time when PDE research was mostly theoretical, see the quote above. It is especially fitting that variational formulations and Hilbert spaces play a fundamental role in the monograph, giving its results a natural algorithmic realization in the form of finite element methods, cf. [28].

To illustrate his approach, let us consider the problem of minimizing the cost functional

$$J(u) = \|Cy(u) - z_d\|_H^2 + (Nu, u)_U.$$

Here, the desired state z_d belongs to a Hilbert space H, where as the state variable $y = y(u)$ belongs to a possibly different Hilbert space V. The state variable $y(u)$ depends on the control variable u via the PDE

$$Ay = f + Bu, \tag{4.2}$$

[17]Institut de Recherche en Informatique et Automatique, the precursor of the modern INRIA.

where $A : V \to V'$ is generally taken to be a differential operator. The minimization is done over all controls u lying in the admissible set U_{ad}, a closed convex subset of a Hilbert space U. The quadratic form $(Nu, u)_U$, with N self-adjoint and semi-positive definite, penalizes large control variables u. From the definition of $J(u)$, we see that for all $v \in U_{ad}$, we have

$$\begin{aligned} J(v) &= (Cy(v) - z_d, Cy(v) - z_d)_H + (Nv, v)_U \\ &= \|Cy(u) - z_d\|_H^2 + 2(Cy(u) - z_d, C(y(v) - y(u)))_H + \|C(y(v) - y(u))\|_H^2 \\ &\quad + (Nu, u)_U + 2(Nu, v - u)_U + (N(v - u), v - u)_U \\ &= J(u) + 2(Cy(u) - z_d, C(y(v) - y(u)))_H + 2(Nu, v - u)_U \\ &\quad + \|C(y(v) - y(u))\|_H + (N(v - u), v - u)_U. \end{aligned}$$

Now since u is the minimizer, we must have $J(v) - J(u) \geq 0$, so that

$$\begin{aligned} &2(Cy(u) - z_d, C(y(v) - y(u)))_H + 2(Nu, v - u)_U \\ &\qquad\qquad + \|C(y(v) - y(u))\|_H^2 + (N(v - u), v - u)_U \geq 0, \end{aligned}$$

which must hold for all $v \in U_{ad}$. So if $\|v - u\| = O(\epsilon)$ and we let ϵ tend to zero, the two quadratic terms become negligible, so we obtain after division by 2 the optimality condition

$$(Cy(u) - z_d, C(y(v) - y(u)))_H + (Nu, v - u)_U \geq 0 \qquad \forall v \in U_{ad}, \tag{4.3}$$

which is analogous to (3.16) in the KKT conditions. The inequality (4.3) can be rewritten as

$$(C^*\Lambda(Cy(u) - z_d), y(v) - y(u))_V + (Nu, v - u)_U \geq 0 \qquad \forall v \in U_{ad}, \tag{4.4}$$

where $\Lambda : H \to H'$ is the canonical isomorphism from H to its dual space H'. Lions then defines the *adjoint state* $p(v) \in V$ implicitly via

$$A^* p(v) = C^*\Lambda(Cy(v) - z_d), \tag{4.5}$$

where $A^* : V \to V'$ is the adjoint of A. Then substituting (4.5) into (4.4) yields

$$\begin{aligned} (C^*\Lambda(Cy(u) - z_d), y(v) - y(u))_V + (Nu, v - u)_U \\ &= (A^*p(u), y(v) - y(u))_V + (Nu, v - u)_U \\ &= (p(u), A(y(v) - y(u))_V + (Nu, v - u)_U \\ &= (p(u), B(v - u))_V + (Nu, v - u)_U \\ &= (\Lambda_U^{-1}B^*p(u) + Nu, v - u)_U \geq 0 \qquad \forall v \in U_{ad}, \end{aligned} \tag{4.6}$$

where $B^* : V \to U'$ is the adjoint of B, $\Lambda_U : U \to U'$ is the canonical isomorphism from U to U', and we have used the fact that

$$A(y(v) - y(u)) = f + Bv - (f + Bu) = B(v - u).$$

In other words, the definition of $p(v)$ in (4.5) can be seen as an intelligent guess that allows one to eliminate the state $y(u)$ from the optimality condition (4.4), similar to the way we chose the Lagrange multiplier $\boldsymbol{\lambda}$ in Section 3.1

to eliminate the state $\boldsymbol{y}$ in the finite-dimensional case. Inequality (4.6) can be reformulated as

$$(\Lambda_U^{-1}B^*p(u)+Nu,u)_U=\inf_{v\in U_{ad}}(\Lambda_U^{-1}B^*p(u)+Nu,v)_U,$$

which then looks like an elliptic analogue of Pontryagin's maximum principle.[18]

The advantage of the abstract Hilbert space approach is that the results are immediately applicable to many different types of control problems. For instance, consider a problem in which the control function is Neumann data on part of the boundary $\Gamma_0\subset\Gamma=\partial\Omega$, and we want the Dirichlet trace on another part of the boundary $\Gamma_1\subset\partial\Omega$, $\Gamma_0\cap\Gamma_1=\emptyset$ to be as close as possible to some desired trace z_d. Then the analogue of (4.6) in the boundary control case states that the optimal control $u\in U_{ad}\subset L^2(\Gamma)$ must satisfy

$$\int_\Gamma p(u)(v-u)\,d\Gamma\geq 0\qquad\forall v\in U_{ad}.\tag{4.7}$$

If the set of admissible controls is defined by pointwise box constraints, e.g., if

$$U_{ad}=\{v:\mathrm{Supp}(v)\subset\Gamma_0\text{ and }|v(x)|\leq 1\text{ a.e. on }\Gamma_0\},$$

then a standard argument allows one to convert the variational inequality (4.7) into a pointwise one of the form

$$p(x;u)(\xi-u(x))\geq 0\qquad\forall\xi\in[-1,1].\tag{4.8}$$

Under some smoothness assumptions on the domain boundary Γ and the coefficients of the elliptic PDE, Lions shows that the optimal control $u\in U_{ad}$ satisfies either $p(x;u)\equiv 0$, in which case $y(u)|_{\Gamma_1}=z_d$, or $p(x;u)\neq 0$ almost everywhere. Then (4.8) implies

$$\begin{aligned}p(x;u)>0&\implies u(x)=-1,\\ p(x;u)<0&\implies u(x)=1.\end{aligned}$$

Thus, we have a bang-bang property in the elliptic case, a result which, to Lions' knowledge, had not been published at the time.

4.3. Derivation by Lagrange Multipliers

It was never explicitly mentioned what motivated Lions to define the adjoint state p via (4.5). One possibility is that he was influenced by the work of Pontryagin; another reason could simply be that he wanted to eliminate the state variables $y(u)$ and $y(v)$ algebraically, just as we did in Section 3.1. Here, we show that the same variable p can be obtained using a formal Lagrange multiplier argument. Let the Lagrangian be defined by

$$\mathcal{L}(y,u,p)=\frac{1}{2}\|Cy-z_d\|_H^2+\frac{1}{2}(Nu,u)_U-(Ay-f-Bu,p)_V,$$

[18]"La formulation (1.31) peut être considérée comme un analogue du « principe du maximum de Pontryagin », pour lequel nous référons [...] à Pontryagin-Boltyanski-Gamkrelidze-Mischenko" [37].

where $p \in V$ now acts as the Lagrange multiplier. Next, we take the variational derivative with respect to y, i.e., we calculate

$$\frac{d}{d\epsilon}\,\mathcal{L}(y+\epsilon z, u, p)\big|_{\epsilon=0} = (Cz, Cy - z_d)_H - (Az, p)_V \overset{!}{=} 0$$

for all $z \in V$. We thus have

$$(Cz, Cy - z_d)_H - (Az, p)_V = (z, C^*\Lambda(Cy - z_d))_V - (z, A^*p)_V = 0,$$

which implies $A^*p = C^*\Lambda(Cy - z_d)$. So the adjoint state is nothing but the Lagrange multiplier for the constrained problem! We check that this formulation gives the same optimality condition for u: we want u to be a minimizer of $\mathcal{L}(y, u, p)$, i.e., for all $v \in U_{ad}$, we have

$$\begin{aligned} 0 \le \mathcal{L}(y, v, p) - \mathcal{L}(y, u, p) &= (B(v-u), p)_V + (Nu, v-u)_U + \frac{1}{2}(N(v-u), v-u)_U \\ &= (v-u, \Lambda_U^{-1}B^*p + Nu)_U + \frac{1}{2}(N(v-u), v-u)_U. \end{aligned}$$

In particular, for $v = u + \epsilon w \in U_{ad}$, we have

$$\epsilon(w, Nu + \Lambda_U^{-1}B^*p)_U + \frac{\epsilon^2}{2}(Nw, w)_U \ge 0,$$

so by letting $\epsilon \to 0$, we obtain the same condition as (4.6). One can only speculate whether Lions had this derivation in mind[19].

4.4. Later developments

Lions' monograph only signaled the beginning of the rapid development of PDE constrained optimization as a modern field of research. Fueled by practical needs in industry and advances in other branches of applied mathematics, the field saw major progress in terms of both theory and algorithms — this is in addition to the number of application areas to which PDE constrained optimization is applied. The following list is by no means exhaustive; the goal is to show a sample of achievements in the intervening decades.

Theory. Much of the theory in Lions' monograph, including the existence and regularity of optimal controls and the maximum principle, has been extended to more general problems. For instance, Pontryagin's maximum principle for linear parabolic problems has been generalized to semilinear parabolic problems by von Wolfersdorf [52, 53]. It is also possible to include state constraints, i.e., constraints on the state variables y rather than on the control u. For a comprehensive modern introduction to the subject, see the recent book by Tröltzsch [50].

Another major theoretical development, related to the existence of optimal controls, is the theory of controllability, where the goal is to determine whether it is possible to find a control function that steers an object from any initial state y_0 to a given target state y_T. An important result, which appeared in [38] in 1988, was proved by Lions himself: he introduced what is known as

[19] According to J. Blum, it was R. Glowinski, one of the former students of Lions, who showed Lions once on the board that the adjoint state can simply be interpreted as a Lagrange multiplier. This was confirmed by R. Glowinski (personal communication)

the Hilbert Uniqueness Method. The method takes a linear time-reversible PDE (such as the wave equation), an initial state y_0 and a target state y_T, and constructs a control u (belonging to some specially chosen Hilbert space H) that steers y_0 to y_T, provided that the system is observable and the time horizon is long enough. For a more recent survey, see the articles by Zuazua [54, 55].

Algorithms. There has also been significant development on the algorithmic front: here, the goal is to discretize the infinite-dimensional PDE constrained problem, e.g. using finite element methods, in order to obtain a finite dimensional approximation, which can then be solved numerically. In principle, one can discretize the KKT formulation (3.16)–(3.18) and then use standard optimization routines, such as line search, trust region and interior point methods to solve the finite dimensional problem; however, one must be careful to discretize the forward and adjoint problems consistently to retain optimality in the discrete setting, see [12]. Using such routines allows one to take advantage of advances in sparse matrix factorizations and preconditioners that have been developed for general saddle-point problems, see for instance [3].

Shooting methods, or more precisely multiple shooting methods, were originally developed for solving two-point boundary value problems [41, 32, 42]. While the finite element method has become the method of choice for most boundary value problems (especially of the elliptic type), multiple shooting remained a viable approach for optimal control problems, since they are able to integrate systems that are highly unstable and very sensitive to changes in initial/final conditions, see the PhD thesis by Bock [6]. More recently, multiple shooting has been applied successfully to problems with PDE constraints, see for example [49], [29], [30], and the recent work by Rannacher et al. [17].

With the rapid increase in computing power in the form of multi-core processors and parallel clusters, there is increasing interest in parallel algorithms for solving PDE constrained optimization and optimal control problems. Methods such as domain decomposition and multigrid, which have been developed and analyzed extensively for discretized PDE problems, are particularly suited for this purpose. For the use of domain decomposition in parabolic optimal control problems, see Heinkenschloss [29] and references therein.

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