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Lagrange's problem without Lagrange multipliers: I. The holonomic case

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Abstract. A new method is presented in this paper to deal with the holonomic type of Lagrange's problem without using any Lagrange multipliers. New characterizations of the constrained extremals are introduced, and the solutions are derived. The new approach has potential advantages over Lagrange's method of multipliers when we numerically determine the optimal solutions.

Key words: Lagrange's problem, calculus of variations, constrained optimization, constrained extremals, Moore-Penrose generalized inverse of a matrix

AMS classification scheme numbers: 49, 70

1. Introduction [1 - 8]

Consider the holonomic type of Lagrange's problem in the calculus of variations. We want to find the extremals of a functional

$$q = \int_{t_0}^{t_1} F(t, x_1, x_2, \ldots, x_n, \dot{x}_1, \dot{x}_2, \ldots, \dot{x}_n)dt \tag{1}$$

subject to the holonomic constraints

$$\phi^i(t, x_1, x_2, \ldots, x_n) = 0, \quad i = 1, 2, \ldots, m, \tag{2}$$

where the end points

$$x_j(t_0) = x_{j0} \quad \text{and} \quad x_j(t_1) = x_{j1}, \quad j = 1, 2, \ldots, n, \tag{3}$$

are fixed.

For over 200 years, the Lagrange method of multipliers has been the dominant approach to handle such a constrained optimization problem. Other methods include dynamic programming and the Pontriyagin maximum principle. In this paper, we present a new set of explicit second-order differential equations for the constrained extremals. The new approach provides potential advantages over the Lagrange's method when we wish to determine numerically the optimal solutions.

The outline of this paper is the following. In section 2, we explore the results of Lagrange's method and introduce three sets of simultaneous equations that the constrained extremals must satisfy. In section 3, we prove that a new set of explicit second-order differential equations is the existent and unique solution to these three sets of equations, and hence it is a characterization of the constrained extremals. In section 4, we extend our discussion to the case that the constraint equations are relaxed to the least square sense. In section 5, we describe the necessary procedures for using the new approach. In section 6, we demonstrate the application of the new approach to a simple constrained optimization problem. Conclusions are in section 7.

2. System of simultaneous equations

As is well known, Lagrange's method of multipliers considers an auxiliary function

$$F^* = F + \sum_{i=1}^{m} \lambda_i \phi^i \tag{4}$$

where λ_i are certain multipliers. The constrained extremals of the functional q are obtained by finding the ordinary extremals for the new unconstrained functional

$$q^* = \int_{t_0}^{t_1} F^*(t, x_1, x_2, \ldots, x_n, \dot{x}_1, \dot{x}_2, \ldots, \dot{x}_n, \lambda_1, \lambda_2, \ldots, \lambda_m) dt. \tag{5}$$

More specifically, these extremals are determined by the Euler equations

$$F^*_{x_j} - \frac{d}{dt} F^*_{\dot{x}_j} = 0, \quad j = 1, 2, \ldots, n, \tag{6}$$

together with the constraint equations

$$\phi^i(t, x_1, x_2, \ldots, x_n) = 0, \quad i = 1, 2, \ldots, m, \ (m \le n) \tag{7}$$

In general, the $m + n$ equations (6) and (7) are enough to determine the $m + n$ unknown functions $x_1, x_2, \ldots, x_n$, and $\lambda_1, \lambda_2, \ldots, \lambda_m$.

Lagrange's method ends here. However, there are still many things that can be done. We first focus our attention on equations (6). Substituting relation (4) into equations (6) gives

$$(F_{x_j} - \frac{d}{dt}F_{\dot{x}_j}) + \sum_{i=1}^{m} \lambda_i \phi^i_{x_j} = 0 \quad j = 1, 2, \ldots, n. \tag{8}$$

Notice that $F_{x_j} - \frac{d}{dt}F_{\dot{x}_j}$, $j = 1, 2, \ldots, n$, are the Euler expressions for the unconstrained functional q. If the constraints $\phi^i(t, x_1, x_2, \ldots, x_n) = 0$ were not present, the Euler equations

$$F_{x_j} - \frac{d}{dt}F_{\dot{x}_j} = 0, \quad j = 1, 2, \ldots, n, \tag{9}$$

would hold. However, this is not the case here. We define the values of the Euler expressions in equations (8) to be $\mathcal{Q}^c_j$, namely,

$$F_{x_j} - \frac{d}{dt}F_{\dot{x}_j} = \mathcal{Q}^c_j, \quad j = 1, 2, \ldots, n. \tag{10}$$

Then, equations (8) are represented by

$$\mathcal{Q}^c_j + \sum_{i=1}^{m} \lambda_i \phi^i_{x_j} = 0, \quad j = 1, 2, \ldots, n. \tag{11}$$

From equations (11), we see that

$$\mathcal{Q}^c_j = -\sum_{i=1}^{m} \lambda_i \phi^i_{x_j}, \quad j = 1, 2, \ldots, n. \tag{12}$$

Let

$$A_{m\times n} = \begin{pmatrix} \phi^1_{x_1} & \phi^1_{x_2} & \cdots & \phi^1_{x_n} \\ \phi^2_{x_1} & \phi^2_{x_2} & \cdots & \phi^2_{x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \phi^m_{x_1} & \phi^m_{x_2} & \cdots & \phi^m_{x_n} \end{pmatrix}, \quad \mathcal{Q}^c = \begin{pmatrix} \mathcal{Q}^c_1 \\ \mathcal{Q}^c_2 \\ \vdots \\ \mathcal{Q}^c_n \end{pmatrix}_{n\times 1},$$

and

$$\lambda_{m\times 1} = \begin{pmatrix} -\lambda_1 \\ -\lambda_2 \\ \vdots \\ -\lambda_m \end{pmatrix}$$

Then, equations (12) in matrix form are equivalent to

$$\mathcal{Q}^c = A^T \lambda. \tag{13}$$

Recalling the fact that $F = F(t, x_1, x_2, \ldots, x_n, \dot{x}_1, \dot{x}_2, \ldots, \dot{x}_n)$, we apply the chain rule to equations (10) and obtain

$$F_{x_j} - (F_{\dot{x}_j t} + F_{\dot{x}_j x_1}\dot{x}_1 + F_{\dot{x}_j x_2}\dot{x}_2 + \cdots + F_{\dot{x}_j x_n}\dot{x}_n + F_{\dot{x}_j \dot{x}_1}\ddot{x}_1 + F_{\dot{x}_j \dot{x}_2}\ddot{x}_2 + \cdots + F_{\dot{x}_j \dot{x}_n}\ddot{x}_n) = \mathfrak{Q}_j^c, \quad j = 1, 2, \ldots, n. \tag{14}$$

Gathering the terms of second-order derivatives in equations (14), we have

$$F_{\dot{x}_j \dot{x}_1}\ddot{x}_1 + F_{\dot{x}_j \dot{x}_2}\ddot{x}_2 + \cdots + F_{\dot{x}_j \dot{x}_n}\ddot{x}_n = (F_{\dot{x}_j t} + F_{\dot{x}_j x_1}\dot{x}_1 + F_{\dot{x}_j x_2}\dot{x}_2 + \cdots + F_{\dot{x}_j x_n}\dot{x}_n) - F_{x_j} + \mathfrak{Q}_j^c, \quad j = 1, 2, \ldots, n. \tag{15}$$

Notice that

$$F_{\dot{x}_j \dot{x}_1}\ddot{x}_1 + F_{\dot{x}_j \dot{x}_2}\ddot{x}_2 + \cdots + F_{\dot{x}_j \dot{x}_n}\ddot{x}_n = (F_{\dot{x}_j t} + F_{\dot{x}_j x_1}\dot{x}_1 + F_{\dot{x}_j x_2}\dot{x}_2 + \cdots + F_{\dot{x}_j x_n}\dot{x}_n) - F_{x_j}, \quad j = 1, 2, \ldots, n, \tag{16}$$

are actually the Euler equations for the unconstrained problem. We assign

$$\mathfrak{Q}_j = (F_{\dot{x}_j t} + F_{\dot{x}_j x_1}\dot{x}_1 + F_{\dot{x}_j x_2}\dot{x}_2 + \cdots + F_{\dot{x}_j x_n}\dot{x}_n) - F_{x_j}, \quad j = 1, 2, \ldots, n. \tag{17}$$

Substituting relations (17) into equations (15) gives

$$F_{\dot{x}_j \dot{x}_1}\ddot{x}_1 + F_{\dot{x}_j \dot{x}_2}\ddot{x}_2 + \cdots + F_{\dot{x}_j \dot{x}_n}\ddot{x}_n = \mathfrak{Q}_j + \mathfrak{Q}_j^c. \quad j = 1, 2, \ldots, n. \tag{18}$$

Let

$$M_{n\times n} = \begin{pmatrix} F_{\dot{x}_1\dot{x}_1} & F_{\dot{x}_1\dot{x}_2} & \cdots & F_{\dot{x}_1\dot{x}_n} \\ F_{\dot{x}_2\dot{x}_1} & F_{\dot{x}_2\dot{x}_2} & \cdots & F_{\dot{x}_2\dot{x}_n} \\ \vdots & \vdots & \vdots & \vdots \\ F_{\dot{x}_n\dot{x}_1} & F_{\dot{x}_n\dot{x}_2} & \cdots & F_{\dot{x}_n\dot{x}_n} \end{pmatrix}, \quad \ddot{X}_{n\times 1} = \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \vdots \\ \ddot{x}_n \end{pmatrix},$$

and

$$\mathfrak{Q}_{n\times 1} = \begin{pmatrix} \mathfrak{Q}_1 \\ \mathfrak{Q}_2 \\ \vdots \\ \mathfrak{Q}_n \end{pmatrix}.$$

Then, equations (18) are represented by

$$M\ddot{X} = \mathfrak{Q} + \mathfrak{Q}^c. \tag{19}$$

Notice that M is an $n \times n$ symmetric matrix, and the Euler equations for the unconstrained problem are given by

$$Ma = \mathfrak{Q}, \tag{20}$$

where a is the vector of second-order derivatives of the unconstrained extremals. If M is positive definite, a is given by

$$a = M^{-1}\mathfrak{Q}. \tag{21}$$

So far, we have seen that equations (6) can be represented by two matrix equations, namely, equations (19) and (13). Next, we will shift our attention to equations (7).

Differentiating the equations (7) with respect to t, we eventually end up with

$$\sum_{j=1}^{n} \phi^i_{x_j}\ddot{x}_j = -\phi^i_{tt} - \sum_{j=1}^{n} \phi^i_{tx_j}\dot{x}_j - \sum_{j=1}^{n} \phi^i_{x_j t}\dot{x}_j - \sum_{j=1}^{n} \dot{x}_j \left(\sum_{k=1}^{n} \phi^i_{x_j x_k}\right), \tag{22}$$

$i = 1, 2, \ldots, m$.

In matrix form, equations (22) are equivalent to

$$A\ddot{X} = b, \tag{23}$$

where A was given earlier and

$$b = \left(-\phi^i_{tt} - \sum_{j=1}^{n} \phi^i_{tx_j}\dot{x}_j - \sum_{j=1}^{n} \phi^i_{x_j t}\dot{x}_j - \sum_{j=1}^{n} \dot{x}_j \left(\sum_{k=1}^{n} \phi^i_{x_j x_k}\right)\right)_{m\times 1}.$$

Equations (7) can be represented by the matrix equation (23). After all, equations (19), (13) and (23) are now the necessary conditions for the constrained extremals.

In summary, we have found three sets of simultaneous equations for the constrained extremals, namely,

(a) $M\ddot{X} = \mathfrak{Q} + \mathfrak{Q}^c$, where $\mathfrak{Q} = Ma$, [equations (19) and (20)]
(b) $A\ddot{X} = b$, [equations (23)]
(c) $\mathfrak{Q}^c = A^T\lambda$, [relations (13)]

In this system, if we denote r as the rank of matrix A, there are n equations in (a), r equations in (b), and $n - r$ equation in (c). Altogether, (a), (b) and (c) provide $2n$ equations, generally enough to determine the $2n$ unknown functions $\ddot{X}_{n\times 1}$ and $\mathfrak{Q}^c_{n\times 1}$.

3. Solutions

Assuming that the constraint equations (b) are consistent and matrix M is positive definite, we assert that

$$\ddot{X} = a + M^{-\frac{1}{2}}(AM^{-\frac{1}{2}})^{+}(b - Aa) \tag{24}$$

and

$$\mathfrak{Q}^c = M^{\frac{1}{2}}(AM^{-\frac{1}{2}})^{+}(b - Aa) \tag{25}$$

are the unique solutions to the simultaneous system (a), (b) and (c). Hence, they are the explicit differential equations for the constrained extremals.

To make the proof simpler, we now do a little transformation on the system (a), (b), and (c). We see that condition (a) is equivalent to

$$M^{\frac{1}{2}}\ddot{X} = M^{-\frac{1}{2}}\mathfrak{Q} + M^{-\frac{1}{2}}\mathfrak{Q}^c, \tag{26}$$

condition (b) is equivalent to

$$AM^{-\frac{1}{2}}M^{\frac{1}{2}}\ddot{X} = b, \tag{27}$$

and condition (c) is equivalent to

$$M^{-\frac{1}{2}}\mathfrak{Q}^c = \left(AM^{-\frac{1}{2}}\right)^T \lambda. \tag{28}$$

Therefore, if we denote $AM^{-\frac{1}{2}} = C_{m\times n}$, $M^{\frac{1}{2}}\ddot{X} = y_{n\times 1}$, $M^{-\frac{1}{2}}\mathfrak{Q} = g_{n\times 1}$, and $M^{-\frac{1}{2}}\mathfrak{Q}^c = h_{n\times 1}$, the system (a), (b) and (c) is equivalent to

$$y = g + h; \tag{a*}$$

$$Cy = b; \tag{b*}$$

$$h = C^T\lambda. \tag{c*}$$

Moreover, the solutions (24) and (25) are equivalent to

$$y = g + C^+(b - Cg) \tag{29}$$

and

$$h = C^+(b - Cg). \tag{30}$$

We first prove the existence. Substituting equation (30) into the right hand side of equation (a*) gives $g + C^+(b - Cg)$, which equals the left hand side when we substitute equation (29) into it. Thus, equation (a*) holds. Substituting equation (29) into the left hand side of equation (b*) gives

$$Cg + CC^+(b - Cg) = Cg + CC^+b - Cg = CC^+b. \tag{31}$$

The consistency of system (b*) requires $CC^+b = b$. Hence, equation (b*) holds. Furthermore, since the range space of C^+ is the same as the range space of C^T, whatever the vector $b - Cg$ is, there exists another vector, say λ, such that

$$C^+(b - Cg) = C^T\lambda. \tag{32}$$

Consequently, equation (30) implies that $h = C^T\lambda$. Therefore, condition (c*) holds.

So far, we have proved the existence of the solutions. Next, we prove the uniqueness.

From equation (a*), we have

$$h = y - g. \tag{33}$$

From equation (b*), we know that

$$y = C^{+}b + (I - C^{+}C)w, \tag{34}$$

where w is an arbitrary vector of dimension $n \times 1$. From equation (c*), and the singular value decomposition of a matrix, we learn that there exists a vector, say μ, such that

$$h = C^{+}\mu. \tag{35}$$

Substituting equation (34) into (33) gives

$$h = C^{+}b + (I - C^{+}C)w - g. \tag{36}$$

From equation (35) and (36), we see that

$$C^{+}b + (I - C^{+}C)w - g = C^{+}\mu. \tag{37}$$

Multiplying both sides of equation (37) by $C^{+}C$ gives

$$C^{+}CC^{+}b + C^{+}C(I - C^{+}C)w - C^{+}Cg = C^{+}CC^{+}\mu, \tag{38}$$

or

$$C^{+}b - C^{+}Cg = C^{+}\mu. \tag{39}$$

Substituting equation (39) into equation (35) gives

$$h = C^{+}b - C^{+}Cg = C^{+}(b - Cg). \tag{40}$$

Substituting equation (40) into equation (a*), we obtain

$$y = g + C^{+}b - C^{+}Cg = g + C^{+}(b - Cg). \tag{41}$$

Therefore, we have proved the uniqueness of the solutions.

4. Extensions [4]

The solutions (24) and (25) even hold when the constraint equations (b) are relaxed to be correct in the least square sense. That is to say, equations (24) and

(25) are also the solutions to the system

$$M\ddot{X} = \mathfrak{Q} + \mathfrak{Q}^c, \quad \text{where} \quad \mathfrak{Q} = Ma; \tag{a}$$

$$\|A\ddot{X} - b\| = \text{minimum}; \tag{b°}$$

$$\mathfrak{Q}^c = A^T\lambda. \tag{c}$$

To see this, we only need to prove that the equations (29) and (30) are the solutions to the system

$$y = g + h; \tag{a*}$$

$$\|Cy - b\| = \text{minimum}; \tag{b♣}$$

$$h = C^T\lambda. \tag{c*}$$

The following is the proof. From condition (c*) and the singular value decomposition of a matrix, we see that there exists a vector, say z, such that

$$h = C^+z, \tag{42}$$

where z is an arbitrary $m \times 1$ vector. Substituting equation (42) into relation (a*) gives

$$y = g + C^+z. \tag{43}$$

Substituting equation (43) into relation (b♣), we have

$$\|C(g + C^+z) - b\|^2 = \text{minimum}. \tag{44}$$

Since

$$\begin{aligned}\|C(g + C^+z) - b\|^2 &= [C(g + C^+z) - b]^T[C(g + C^+z) - b] \\ &= [CC^+z + (Cg - b)]^T[CC^+z + (Cg - b)] \\ &= (CC^+z)^T(CC^+z) + (CC^+z)^T(Cg - b) \\ &\quad + (Cg - b)^T(CC^+z) + (Cg - b)^T(Cg - b),\end{aligned} \tag{45}$$

relation (44) is equivalent to minimizing $f(z)$, where

$$\begin{aligned}f(z) &= (CC^+z)^T(CC^+z) + (CC^+z)^T(Cg - b) \\ &\quad + (Cg - b)^T(CC^+z) + (Cg - b)^T(Cg - b).\end{aligned} \tag{46}$$

Notice that $f(z)$ is a quadratic function of z. Since

$$\begin{aligned}\frac{\partial f}{\partial z} &= 2(CC^+)^T(CC^+)z + 2(CC^+)^T(Cg - b)\\ &= 2CC^+CC^+z + 2CC^+(Cg - b)\\ &= 2CC^+z + 2CC^+(Cg - b),\end{aligned} \tag{47}$$

setting $\frac{\partial f}{\partial z} = 0$ gives

$$CC^+z_{\text{opt.}} + CC^+(Cg - b) = 0, \tag{48}$$

or

$$CC^+z_{\text{opt.}} = CC^+(b - Cg). \tag{49}$$

Multiplying both sides of equation (49) by C^+ yields

$$C^+CC^+z_{\text{opt.}} = C^+CC^+(b - Cg), \tag{50}$$

which is equivalent to

$$C^+z_{\text{opt.}} = C^+(b - Cg). \tag{51}$$

Substituting equation (51) into equations (42) and (43) gives

$$h_{\text{opt.}} = C^+(b - Cg), \tag{52}$$

and

$$y_{\text{opt.}} = g + C^+(b - Cg). \tag{53}$$

Therefore, we have proved that equations (29) and (30) are the optimal solutions to the system (a*), (b♣) and (c*).

Let us now verify that the choices of h and y in equations (52) and (53) really minimize $\|Cy - b\|$, subject to equations (a*) and (c*). Since in section 3, we have shown that equations (52) and (53) do satisfy equations (a*) and (c*), we here evaluate $\|Cy - b\|$ for $y = y_{\text{opt.}} + \varepsilon$, where ε is an allowable increment to the vector $y_{\text{opt.}}$. We hope to show that when $\varepsilon = 0$, the value of $\|Cy - b\|$ has its absolute minimum.

We see that

$$\begin{aligned}&\|C(y_{\text{opt.}} + \varepsilon) - b\| = \|C[g + C^+(b - Cg) + \varepsilon] - b\|\\ &= \|Cg + CC^+b - CC^+Cg + C\varepsilon - b\| = \|Cg + CC^+b - Cg + C\varepsilon - b\|\\ &= \|CC^+b + C\varepsilon - b\| = \|(CC^+ - I)b + C\varepsilon\|\\ &= [(CC^+ - I)b + C\varepsilon]^T[(CC^+ - I)b + C\varepsilon]\end{aligned}$$

$$= [(CC^+ - I)b]^T (CC^+ - I)b + [(CC^+ - I)b]^T C\varepsilon + [C\varepsilon]^T (CC^+ - I)b + [C\varepsilon]^T C\varepsilon. \quad (54)$$

The second term on equation (54) is zero because

$$[(CC^+ - I)b]^T C\varepsilon = b^T (CC^+ - I)^T C\varepsilon = b^T [CC^+ - I] C\varepsilon = b^T [CC^+ C - C]\varepsilon = b^T [C - C]\varepsilon = 0. \quad (55)$$

The third term is also zero because it is the transpose of the second term. The first term does not depend upon ε. The last term is a quadratic form in ε. Thus, when $\varepsilon = 0$, the value of $\|Cy - b\|$ has its absolute minimum. Therefore, condition (b♣) holds.

Overall, we have proved that equations (24) and (25) not only are the existent and unique solutions to the system (a), (b) and (c) when equation (b) is consistent, but also are the optimal solutions to that system when equation (b) is inconsistent yet holds in a least square sense.

5. Procedures

The previous discussion leads to the following formalism.

(i) Construct the Euler equations for the unconstrained system. Determine the matrix M and compute the vector a by formula $a = M^{-1}\mathfrak{Q}$.

(ii) Differentiate the constraint equations twice to get the second-order derivatives of $x_1, x_2, \ldots, x_n$ and determine the matrix A and the vector b.

(iii) Determine $M^{-\frac{1}{2}}$ and $(AM^{-\frac{1}{2}})^+$.

(iv) Determine $\ddot{X}$ by formula (24).

(v) Solve the ordinary differential equations obtained from step (iv) subject to the given boundary conditions.

6. An application

Consider minimizing the integral

$$\int_{t_0}^{t_1} \left[\frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) - y\right] dt \quad (56)$$

subject to the constraint

$$x^2 + y^2 = 1, \quad (57)$$

where the end points $x(t_0) = x_0$, $x(t_1) = x_1$, $y(t_0) = y_0$ and $y(t_1) = y_1$ are given.

To apply the new approach, first construct the Euler equations for the unconstrained problem,

$$\begin{cases} F_x - \frac{d}{dt}F_{\dot{x}} = 0, \\ F_y - \frac{d}{dt}F_{\dot{y}} = 0, \end{cases}$$

where

$$F = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - y. \tag{58}$$

We obtain

$$\begin{cases} \ddot{x} = 0, \\ \ddot{y} = -1. \end{cases} \tag{59}$$

In matrix form, system (59) is equivalent to

$$M\ddot{X} = \mathfrak{Q} \tag{60}$$

where

$$M_{2\times 2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{61}$$

$$\ddot{X}_{2\times 1} = \begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix}, \tag{62}$$

$$\mathfrak{Q}_{2\times 1} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}. \tag{63}$$

The second-order derivatives of the unconstrained extremals are given by

$$a_{2\times 1} = M^{-1}\mathfrak{Q} = \begin{pmatrix} 1^{-1} & 0 \\ 0 & 1^{-1} \end{pmatrix}\begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}. \tag{64}$$

Next, we differentiate the constraint equation (57) twice. We obtain

$$x\ddot{x} + y\ddot{y} = -(\dot{x}^2 + \dot{y}^2). \tag{65}$$

In matrix form, equation (65) is represented by

$$A\ddot{X} = b, \tag{66}$$

where

$$A_{1\times 2} = \begin{pmatrix} x & y \end{pmatrix}, \tag{67}$$

$$b = -(\dot{x}^2 + \dot{y}^2). \tag{68}$$

Equations (73) and the constraint equation (57) constitute a system of equations for getting x, y, and λ. Differentiating equation (57) twice gives equation (65). Substituting equations (73) into (65), we have

$$x(2\lambda x) + y[-1 + (2\lambda y)] = -(\dot{x}^2 + \dot{y}^2). \tag{74}$$

From equation (74), we obtain

$$\lambda = \frac{y - (\dot{x}^2 + \dot{y}^2)}{2(x^2 + y^2)}. \tag{75}$$

Substituting equation (75) into equations (73) gives

$$\begin{cases} \ddot{x} = 0 + \dfrac{y - (\dot{x}^2 + \dot{y}^2)}{(x^2 + y^2)} x, \\ \ddot{y} = -1 + \dfrac{y - (\dot{x}^2 + \dot{y}^2)}{(x^2 + y^2)} y. \end{cases} \tag{76}$$

In matrix form, equations (76) are equivalent to equations (71).

Notice that, equations (71) and (73) both convey the information that the actual second-order derivatives of the constrained extremals are the sum of the second-order derivatives of the unconstrained extremals and an increment due to the constraint. The difference is that equations (71) do not contain the Lagrange multipliers while equations (73) do. In general, the Lagrange's multipliers are difficult to determine. In other words, it is nontrivial to get the explicit equations for second-order derivatives via Lagrange's method of multipliers. The fact that there are no Lagrange multipliers in equations (71) makes it possible to trace the constrained extremals, i.e. the optimal functions, by using numerical methods. This feature, among others, makes the new method unique and valuable.

Moreover, when substituting (61), (62), (63), (64), (67) and (68) into the formula (25), we also obtain

$$\begin{aligned} \mathfrak{Q}^c &= \begin{pmatrix} 1^{\frac{1}{2}} & 0 \\ 0 & 1^{\frac{1}{2}} \end{pmatrix} \left[(x \quad y) \begin{pmatrix} 1^{-\frac{1}{2}} & 0 \\ 0 & 1^{-\frac{1}{2}} \end{pmatrix} \right]^+ \left[-(\dot{x}^2 + \dot{y}^2) - (x \quad y) \begin{pmatrix} 0 \\ -1 \end{pmatrix} \right] \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} (x \quad y)^+ [y - (\dot{x}^2 + \dot{y}^2)] \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{gy - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix} \\ &= \frac{gy - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix} \end{aligned}$$

or

$$\begin{pmatrix} \mathfrak{Q}^c_x \\ \mathfrak{Q}^c_y \end{pmatrix} = \frac{y - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{77}$$

Finally, we substitute (61), (62), (63), (64), (67) and (68) into formula (24) and obtain

$$
\begin{aligned}
\ddot{X} &= a + M^{-\frac{1}{2}}(AM^{-\frac{1}{2}})^{+}(b - Aa) \\
&= \begin{pmatrix} 0 \\ -1 \end{pmatrix} + \begin{pmatrix} 1^{-\frac{1}{2}} & 0 \\ 0 & 1^{-\frac{1}{2}} \end{pmatrix} \left[(x \quad y) \begin{pmatrix} 1^{-\frac{1}{2}} & 0 \\ 0 & 1^{-\frac{1}{2}} \end{pmatrix} \right]^{+} \times \\
&\qquad \left[-(\dot{x}^2 + \dot{y}^2) - (x \quad y) \begin{pmatrix} 0 \\ -1 \end{pmatrix} \right] \\
&= \begin{pmatrix} 0 \\ -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} (x \quad y)^{+} \left[-(\dot{x}^2 + \dot{y}^2) + y \right], \qquad (69)
\end{aligned}
$$

If v is a 1×2 matrix, the generalized inverse of v is given by $v^{+} = v^{T}/v^{T}v$. Therefore,

$$
(x \quad y)^{+} = \frac{1}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix}. \qquad (70)
$$

Substituting equation (70) into equation (69), we have

$$
\begin{aligned}
\ddot{X} &= \begin{pmatrix} 0 \\ -1 \end{pmatrix} + \frac{y - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ -1 \end{pmatrix} + \frac{y - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix},
\end{aligned}
$$

or

$$
\begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} + \frac{y - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix}. \qquad (71)
$$

This is the set of explicit second-order differential equations that the new approach directly provides for this problem.

Let us check the correctness of the equation (71) using Lagrange multipliers. We construct the auxiliary function

$$
F^{*} = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - y + \lambda(x^2 + y^2 - 1). \qquad (72)
$$

The Euler equations for F^{*},

$$
\begin{cases} F^{*}_{x} - \dfrac{d}{dt} F^{*}_{\dot{x}} = 0, \\ F^{*}_{x} - \dfrac{d}{dt} F^{*}_{\dot{y}} = 0, \end{cases}
$$

are given by

$$
\begin{cases} \ddot{x} = 0 + 2\lambda x, \\ \ddot{y} = -1 + 2\lambda y. \end{cases} \qquad (73)
$$

These are the components of the additional "constrained force" that arises by virtue of the constraint (57). That is to say, the new approach can also be used directly to determine the "constrained forces" $\mathfrak{Q}^c$ as well as the increment in the second-order derivatives of the optimal curves, a^c,

$$a^c = M^{-1}\mathfrak{Q}^c = \frac{y - (\dot{x}^2 + \dot{y}^2)}{x^2 + y^2} \begin{pmatrix} x \\ y \end{pmatrix}, \tag{78}$$

due to the constraint forces. Another way to calculate the increment a^c is

$$a^c = \ddot{X} - a = M^{-\frac{1}{2}}(AM^{-\frac{1}{2}})^+(b - Aa). \tag{79}$$

As we have seen from equation (71), the results from equations (78) and (79) are the same.

7. Conclusions

In this paper, we have presented a new approach to Lagrange's problem in the calculus of variations where the constraints are holonomic. Based on the understanding that the second-order derivatives of constrained extremals always have two components – one originates from the unconstrained system itself, the other arises from constraints imposed on the system, we succeed in finding a new characterization for the constrained extremals.

We note that our approach would also be applicable when M is negative definite; hence the assumption that M is positive definite is only for convenience. Indefinite M requires more research.

The new approach provides unique solutions to modeling, predicting and explaining the behavior of complex systems. It has potential advantages over Lagrange's method of multipliers when we numerically determine the optimal solutions to the constrained systems. We believe that it will have applications in various fields.

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