Calculus of Variations (I)

1 Introduction

The generic concept of function of one or several variables is an important and well established Calculus notion. More difficult to grasp is the idea of a *function of functions*, i.e. a function whose argument is another function (or more functions) and whose outcome is a uniquely assigned number. An example will help to clarify such an abstract idea (see Figure 1). Consider the following integral:

$$I \equiv \int_0^1 \left\{ [f(x)]^2 + [f'(x)]^2 \right\} \mathrm{d}x \tag{1}$$

where $f'(x)$ indicates a first derivative. Its numerical value will change according to the function used as $f(x)$. For instance, if we adopt $fx) = -x^2 + 2x$, a straightforward computation yields $I \simeq 1.867$; if $f(x) = x$, then $I \simeq 1.333$, while, if $f(x) = k(e^x - e^{-x})$ with $k = 1/(e - 1/e)$, we have $I \simeq 1.313$. Using a function-like notation of the form $I[f(x)]$, we can express these three values as:

$$I[-x^2 + 2x] \simeq 1.867 \quad , \quad I[x] \simeq 1.333 \quad , \quad I[k(e^x - e^{-x})] \simeq 1.313$$

The argument of I is a function, rather than a number, but I itself is a real number. Objects like this are called *functionals*. They are used in many areas of Theoretical Physics, for instance in the variational approach to Quantum Mechanics or in Density Functional Theory, to mention just a few.

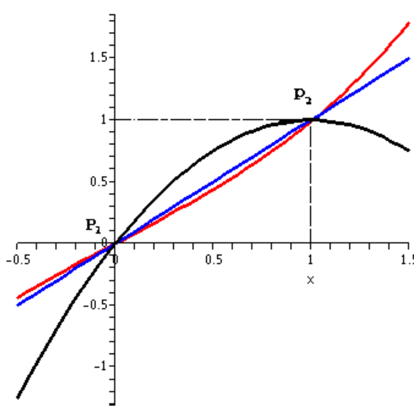

Figure 1: Three different functions, all passing through points $(0, 0)$ and $(1, 1)$. The black line corresponds to $f(x) = -x^2 + 2x$, the blue line to $f(x) = x$, and the red line to $k(e^x - e^{-x})$, with $k = 1/(e - 1/e)$.

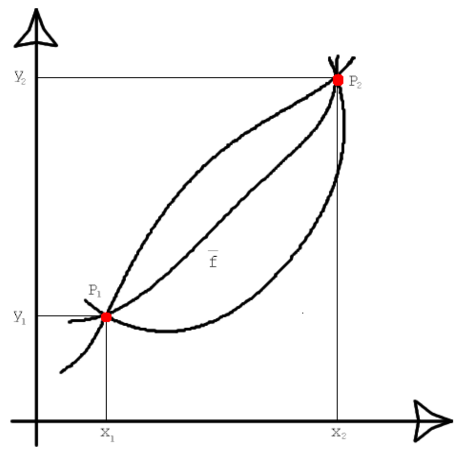

Figure 2: Given a family of functions, all passing through points P_1 and P_2, the central problem in Calculus of Variations is finding a function $\bar{f}(x)$ which makes the functional I a minimum.

We are here interested in using functionals of the following form:

$$I \equiv \int_{x_1}^{x_2} F(x, f(x), f^{'}(x))\mathrm{d}x$$

where F can be any real-valued function. More specifically, we will try to find one or more functions $f(x)$ which make the above integral an extremum. As we will see, the techniques used to deal with the problem go through an analogy with function differentiation in Calculus, but they act on functionals, rather than functions. Therefore such techniques are collectively known by a name different from "Calculus", i.e. *Calculus of variations*, because small variations around a fixed function play a crucial role in the determination of I's extrema.

2 Derivation of the Euler-Lagrange equation

Given the following functional:

$$I \equiv \int_{x_1}^{x_2} F(x, f(x), f^{'}(x))\mathrm{d}x \tag{2}$$

we would like to find one or more functions $f(x)$ which make it an extremum. Desired functions will need to be smooth (i.e. $f(x)$, $f^{'}(x)$ and $f^{''}(x)$ continuous) and they will all have to go through both point $P_1 \equiv (x_1, y_1)$ and $P_2 \equiv (x_2, y_2)$. This implies that $f(x_1) = y_1$ and $f(x_2) = y_2$ for any selected $f(x)$.

It would be nice being able to use a property like $\mathrm{d}I = 0$, as normally done in standard Calculus, to find extrema for expression (2). But we are dealing with a functional, rather than a function, therefore a way to transform I into a one-variable function is needed. Let us fix ideas by requiring that our extremum be a minimum. Although this is not necessarily the case, most of the practical applications we will examine later are, in fact, "minimum" problems. Consider, then, a function $\bar{f}(x)$ for which expression (2) is a minimum. Let us, accordingly, define $\bar{I}$ as $I[\bar{f}(x)]$. Because I has a minimum value at $\bar{f}$, its value will be greater than $\bar{I}$ at every "neighbouring" function, i.e. a function which is arbitrarily close to $\bar{f}(x)$. There are rigorous ways of defining the "closeness" of two functions, but they introduce complications which are here unnecessary. A less rigorous

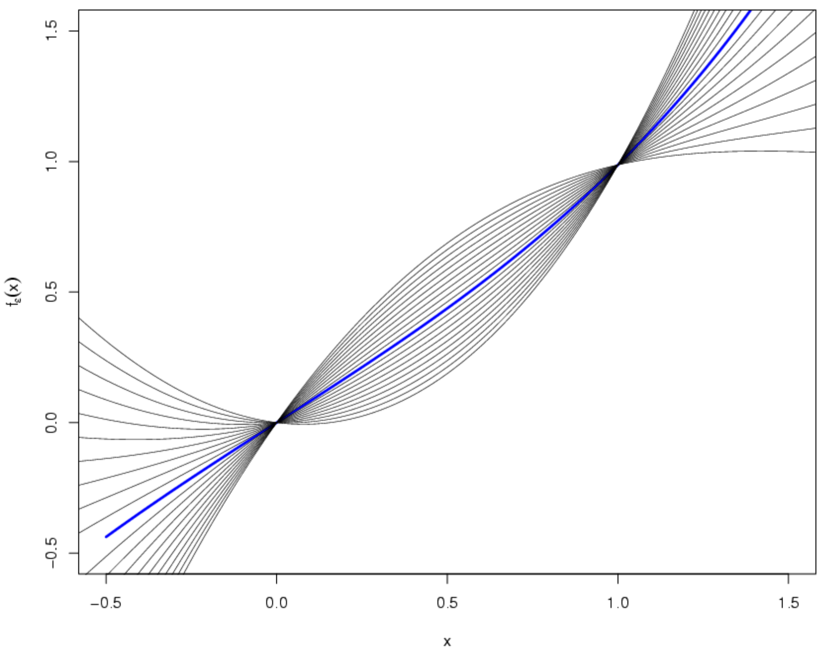

Figure 3: Family of functions close to $\bar{f}(x) = k(e^x - e^{-x})$ (in blue). ϵ varies between -1 and 1.

but easier method to define quantitatively a family of functions which are close enough to $\bar{f}$ is by adopting the following definition:

$$f_\epsilon(x) \equiv \bar{f}(x) + \epsilon\eta(x) \tag{3}$$

where ϵ is a real, arbitrarily small number, and $\eta(x)$ is an arbitrary smooth function obeying the property:

$$\eta(x_1) = \eta(x_2) = 0 \tag{4}$$

This guarantees that $f_\epsilon(x_1) = y_1$ and $f_\epsilon(x_2) = y_2$. Equation (3) defines an infinite number of functions close enough to $\bar{f}$ and all passing through P_1 and P_2, exactly what we were looking for. An example will help to clarify the nature of $f_\epsilon(x)$. The function minimising functional (1) is $\bar{f}(x) = k(e^x - e^{-x})$, with $k = 1/(e - 1/e)$ (this will be proved later as an example). Let us build the following family of functions, $f_\epsilon(x)$, arbitrarily close to $\bar{f}(x)$:

$$f_\epsilon(x) = \bar{f}(x) + \epsilon\eta(x) \equiv k(e^x - e^{-x}) + \epsilon x(x-1) \tag{5}$$

It is readily seen that $\eta(x) \equiv x(x-1)$ satisfies condition (4). Furthermore, from Figure 3, we can visually be convinced that, for sufficiently small values of ϵ, the corresponding functions belonging to the family are sufficiently close to $\bar{f}(x)$. If, at this point, every function included in group (5) is replaced in functional I, a one-to-one correspondence between parameter ϵ and values of integral (1) is created (see Figure 4). It is straightforward to acknowledge that the minimum for expression (1) happens at $\epsilon = 0$.

Through a parametrisation like (3) expression (2) is transformed into a one-variable function, $I(\epsilon)$. To find a minimum for functional $I[f(x)]$ is now equivalent to finding a minimum for function $I(\epsilon)$. This is equivalent to claiming that:

$$\frac{\mathrm{d}I(\epsilon)}{\mathrm{d}\epsilon} = 0 \;\; at \;\; \epsilon = 0 \tag{6}$$

Let us, then, apply equation (6) to expression (2), where $f(x)$ is replaced by $f_\epsilon(x)$ and $f^{'}(x)$ by $f^{'}_\epsilon(x)$:

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\int_{x_1}^{x_2} F(x, f_\epsilon(x), f^{'}_\epsilon(x))\mathrm{d}x = 0$$

By swapping the derivative with the integral, and using the chain rule, we get:

$$\int_{x_1}^{x_2}\left\{\frac{\partial F}{\partial f_\epsilon}\frac{\partial f_\epsilon}{\partial \epsilon} + \frac{\partial F}{\partial f^{'}_\epsilon}\frac{\partial f^{'}_\epsilon}{\partial \epsilon}\right\}\mathrm{d}x$$

or, using expression (3) and splitting the integral in two terms,

$$\int_{x_1}^{x_2}\frac{\partial F}{\partial f_\epsilon}\eta(x)\mathrm{d}x + \int_{x_1}^{x_2}\frac{\partial F}{\partial f^{'}_\epsilon}\eta^{'}(x)\mathrm{d}x = 0 \qquad (7)$$

Let us integrate the second term in (7) by parts:

$$\int_{x_1}^{x_2}\frac{\partial F}{\partial f^{'}_\epsilon}\eta^{'}(x)\mathrm{d}x = \left[\frac{\partial F}{\partial f^{'}_\epsilon}\eta(x)\right]_{x_1}^{x_2} - \int_{x_1}^{x_2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f^{'}_\epsilon}\right)\eta(x)\mathrm{d}x$$

Due to condition (4), the first term in the above expression is zero. We will have, then:

$$\int_{x_1}^{x_2}\frac{\partial F}{\partial f^{'}_\epsilon}\eta^{'}(x)\mathrm{d}x = -\int_{x_1}^{x_2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f^{'}_\epsilon}\right)\eta(x)\mathrm{d}x$$

By replacing this last expression into expression (7) we obtain:

$$\int_{x_1}^{x_2}\left\{\frac{\partial F}{\partial f_\epsilon} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f^{'}_\epsilon}\right\}\eta(x)\mathrm{d}x = 0$$

It has been said before that $\eta(x)$ is an arbitrary function. The only case in which the above integral is zero, no matter what we choose $\eta(x)$ to be, is when the quantity in brackets is zero. Thus, a necessary condition for $\bar{f}(x)$ to be a minimum is that $f_\epsilon(x)$ satisfies the following equation:

$$\frac{\partial F}{\partial f_\epsilon} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f^{'}_\epsilon} = 0$$

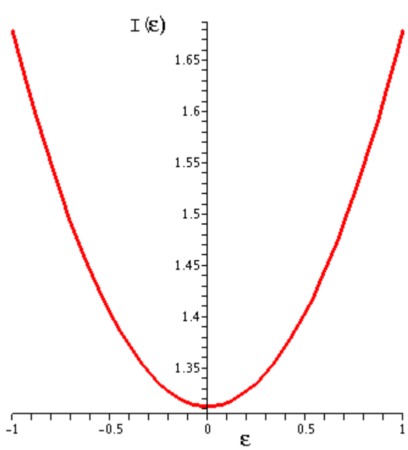

Figure 4: Different values of ϵ provide different values of functional I. The family of functions $f_\epsilon(x)$ is equivalent to a one-variable function $I = I(\epsilon)$. Notice how I has a minimum at $\epsilon = 0$.

At this point we can drop suffix ϵ. A necessary condition for a function f to minimise functional (2) is that it satisfies:

$$\frac{\partial F}{\partial f} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f'} = 0 \tag{8}$$

known as *Euler-Lagrange equation*.

As an example consider integral (1). To build expression (8) we need, first of all, to compute $\partial F/\partial f$ and $\partial F/\partial f'$:

$$\frac{\partial F}{\partial f} = \frac{\partial}{\partial f}\left[f^2 + f'^2\right] = 2f \;\;,\;\; \frac{\partial F}{\partial f'} = \frac{\partial}{\partial f'}\left[f^2 + f'^2\right] = 2f'$$

It is also easy to compute:

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial F}{\partial f'} = \frac{\mathrm{d}}{\mathrm{d}x}[2f'] = 2f''$$

Equation (8) applied to integral (1) gives, then:

$$2f - 2f'' = 0 \Rightarrow f'' = f \Rightarrow f(x) = Ae^x + Be^{-x}$$

A and B can be found using $f(0) = 0$ and $f(1) = 1$. The function minimising integral (1) is thus:

$$f(x) = k(e^x - e^{-x}) \quad , \quad k = \frac{1}{e - 1/e}$$

as previously stated.

3 Geodesics: the shortest path between two points

The shortest curve joining two generic points in a plane is a straight line. We all have a very good experience of this basic fact in our daily walks between two different places. To show this is rigorously true is not that immediate, though. In fact variational calculus turns out to be the perfect tool to deal with this sort of problems. Consider two separate points in a plane, $P_1 \equiv (x_1, y_1)$ and $P_2 \equiv (x_2, y_2)$, and suppose a curve γ, described by equation $y = f(x)$, is the shortest one among all curves joining P_1 and P_2 (see Figure 5). This means that the following quantity:

$$I \equiv \int_{x_1}^{x_2} \mathrm{d}s \tag{9}$$

is a minimum. Quantity $\mathrm{d}s$ in integral (9) is the line element; therefore (9) is a line integral. Let us turn such an integral into a form similar to (2). Using Pythagoras theorem we get, firts of all:

$$\mathrm{d}s = \sqrt{(\mathrm{d}x)^2 + (\mathrm{d}y)^2} = \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2}\mathrm{d}x \equiv \sqrt{1 + [f'(x)]^2}\mathrm{d}x$$

Integral (9) can thus be re-written as:

$$I = \int_{x_1}^{x_2} \sqrt{1 + [f'(x)]^2}\mathrm{d}x \tag{10}$$

Function f which makes integral (10) a minimum comes from the solution of the Euler-Lagrange equation. All we have to do is to compute the partial derivatives of:

$$F(x, f, f') = \sqrt{1 + f'^2}$$

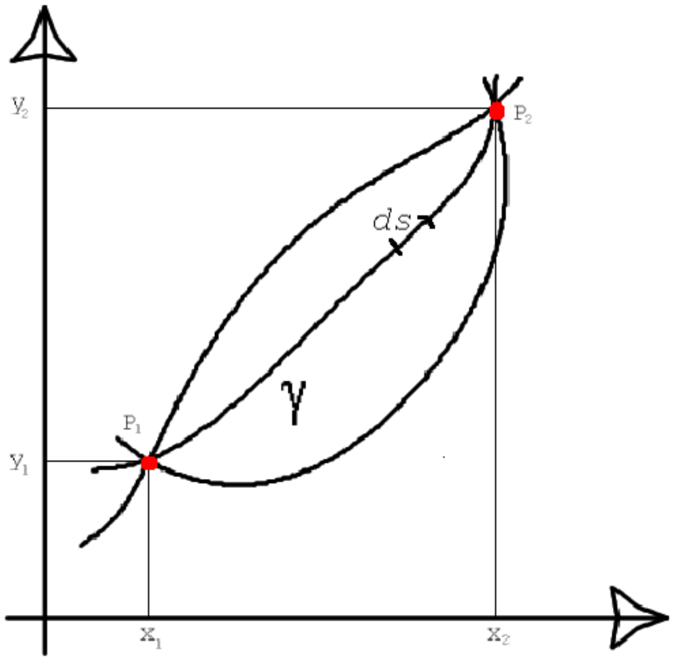

Figure 5: Curve γ represents the shortest-distance between P_1 and P_2. ds is the infinitesimal curve element.

which turn out to be:

$$\frac{\partial F}{\partial f} = 0 \ , \ \frac{\partial F}{\partial f'} = \frac{f'}{\sqrt{1+f'^2}}$$

These, inserted in equation (8), give:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f'}{\sqrt{1+f'^2}}\right) = 0 \ \Rightarrow \ \frac{f'}{\sqrt{1+f'^2}} = c$$

where c is an integration constant. Carrying on with the calculation yields:

$$\frac{f'^2}{1+f'^2} = c^2 \ \Rightarrow \ f' = \pm\frac{c}{\sqrt{1-c^2}}$$

Now, $\pm c/\sqrt{1-c^2}$ is still an integration constant that can be replaced by a global constant A. We simply have, then:

$$f'(x) = A \ \Rightarrow \ f(x) = Ax + B$$

where A and B can be found using conditions $f(x_1) = y_1$ and $f(x_2) = y_2$. Finally we have, then:

$$y = f(x) = \frac{y_1 - y_2}{x_1 - x_2}x + \frac{x_1 y_2 - y_1 x_2}{x_1 - x_2} \tag{11}$$

This is the equation for a straight line joining P_1 and P_2. We have thus just demonstrated that the shortest path between two distant points in a 2D euclidean space is the straight line.

Let us now turn our attention to a different surface, the sphere. As we know, a spherical surface of radius r is better described in spherical coordinates, (θ, φ), where $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$. Once two points, $P_1 \equiv (\theta_1, \varphi_1)$ and $P_2 \equiv (\theta_2, \varphi_2)$, have been chosen, we can try to determine the

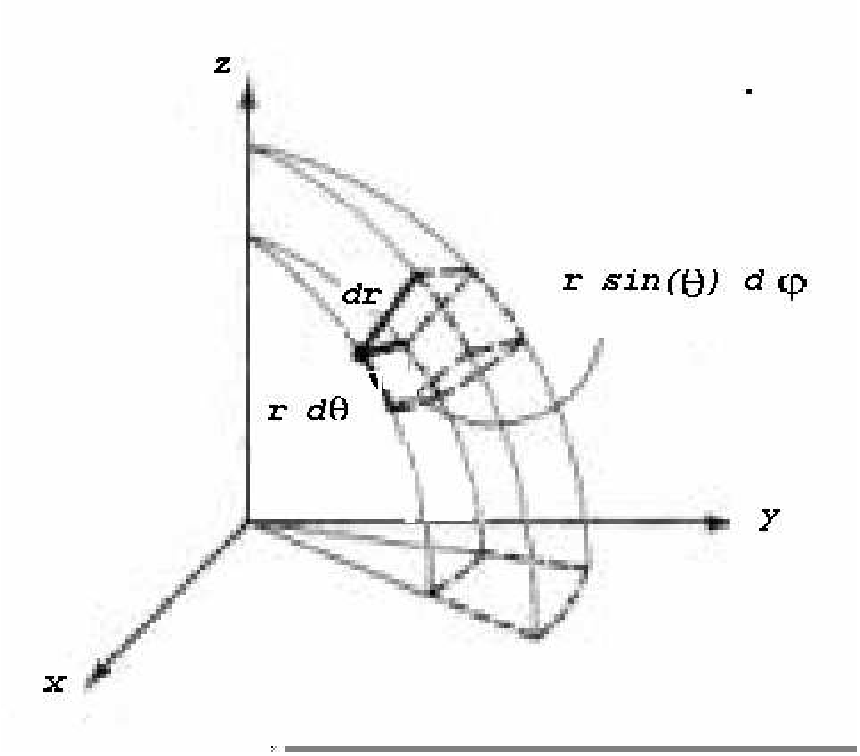

Figure 6: This picture shows a volume element in spherical coordinates. Its sides are dr, rdθ and $r\sin(\theta)$dφ. If we now consider a line element lying on the inner spherical surface, in a diagonal fashion, we can immediately see that its length is found once the two sides, rdθ and $r\sin(\theta)$dφ, of the warped square, are taken into account. This is going to be $\mathrm{d}s = \sqrt{r^2(\mathrm{d}\theta)^2 + r^2\sin^2(\theta)(\mathrm{d}\varphi)^2}$.

shortest path joining these two points. We still have to maximise a line integral like (9), where the integration is carried out along the shortest curve, γ:

$$I = \int_\gamma \mathrm{d}s \tag{12}$$

It is well known that the line element on a spherical surface (see Figure 6) is, in spherical coordinates:

$$\mathrm{d}s = r\sqrt{(\mathrm{d}\theta)^2 + \sin^2(\theta)(\mathrm{d}\varphi)^2} = r\sqrt{1 + \sin^2(\theta)\left(\frac{\mathrm{d}\varphi}{\mathrm{d}\theta}\right)^2}\mathrm{d}\theta$$

We are looking for a function $\varphi = \varphi(\theta)$ which minimises integral (12). This last one can now be re-written as:

$$I = r\int_{\theta_1}^{\theta_2}\sqrt{1 + \sin^2(\theta)\varphi'^2}\mathrm{d}\theta$$

where $\varphi' \equiv \mathrm{d}\varphi/\mathrm{d}\theta$. Starting from last expression it is easy to proceed using Euler-Lagrange equation. In this case $F = F(\theta, \varphi) = r\sqrt{1 + \sin^2(\theta)\varphi'^2}$. The two partial derivatives will be, then:

$$\frac{\partial F}{\partial \varphi} = 0 \ , \ \frac{\partial F}{\partial \varphi'} = \frac{\sin^2(\theta)\varphi'}{\sqrt{1 + \sin^2(\theta)\varphi'^2}}$$

and Euler-Lagrange equation:

$$\frac{\partial F}{\partial \varphi} - \frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\partial F}{\partial \varphi'} = 0$$

yields, in this case,

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\frac{\sin^2(\theta)\varphi'}{\sqrt{1+\sin^2(\theta)\varphi'^2}}\right) = 0 \;\Rightarrow\; \frac{\sin^2(\theta)\varphi'}{\sqrt{1+\sin^2(\theta)\varphi'^2}} = k$$

with k an integration constant. By manipulating this last expression a little bit we obtain:

$$\varphi' = \frac{k}{\sin(\theta)\sqrt{\sin^2(\theta)-k^2}} = \frac{k\csc^2(\theta)}{\sqrt{1-k^2/\sin^2(\theta)}} = \frac{k\csc^2(\theta)}{\sqrt{1-k^2-k^2\cot^2(\theta)}} \tag{13}$$

(the last term was obtained by adding and subtracting k^2 inside the square root). An integration can now be carried out fairly easily, just with the substitution $t = k\cot(\theta)$. The final risult is:

$$\varphi(\theta) = \alpha - \arcsin\left[\beta\cot(\theta)\right] \tag{14}$$

We could determine the two integration constants α and β by simply considering that the curve passes through P_1 and P_2. We will not carry out this step, leaving the constants undetermined, because we are more interested in finding out what kind of curve is the shortest path. Inverting, then, equation (14), and multiplying both members by r we get:

$$r\sin(\alpha-\varphi) = r\beta\cot(\theta)$$

$$\Downarrow$$

$$\beta r\cos(\theta) = r\sin(\theta)\cos(\varphi)\sin(\alpha) - r\sin(\theta)\sin(\varphi)\cos(\alpha)$$

If we now use cartesian coordinates, and remember that:

$$\begin{cases} x &= r\sin(\theta)\cos(\varphi) \\ y &= r\sin(\theta)\sin(\varphi) \\ z &= r\cos(\theta) \end{cases}$$

the previous expression can be re-written as:

$$\beta z = \sin(\alpha)x - \cos(\alpha)y$$

which is the equation of a plane passing through the origin. It cuts the spherical surface of radius r along a curve which is a meridian and goes through P_1 and P_2. The shortest path we were looking for, therefore, is an arc of meridian joining P_1 and P_2.