In [1]:
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%matplotlib notebook
%pylab
```

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Using matplotlib backend: nbAgg
Populating the interactive namespace from numpy and matplotlib
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Calculus of Variations

The problem of minimizing *functionals* over a space of functions arises often in many applied mathematics problems. A typical example is that of finding the shortest path between two points.

Define a functional $\mathbf{J}[y]$ as

$$\mathbf{J}[y(x)] = \int_0^1 F(x, y(x), y'(x)) \; dx$$

where $F(x, y, z)$ is some function in three variables. The functional $\mathbf{J}$ maps functions y (defined here on $[0, 1]$) in a suitable class of *admissiable functions* to a scalar value.

$$\mathbf{J} : y \to \mathcal{R}, \qquad y \in \text{ piecewise } C^1[0, 1]$$

Because $\mathbf{J}[y]$ is a scalar value, we can look for conditions on y which will minimize this functional.

Let $\eta(x)$ be a function on $[0, 1]$ satisfying $\eta(0) = \eta(1) = 0$. Then, we have that $\mathbf{J}[y_0(x)]$ is a minimum only if

$$\frac{\partial \mathbf{J}}{\partial \alpha}[y_0(x) + \alpha\eta(x)]\bigg|_{\alpha=0} = 0$$

or if

$$\delta \mathbf{J} \equiv \int_0^1 \left(\frac{\partial F}{\partial y}\eta(x) + \frac{\partial F}{\partial y'}\eta'(x) \right) \; dx = 0$$

Integrating by parts, we get

$$\delta \mathbf{J} = \int_0^1 \left[\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'} \right) \right] \eta(x) \; dx = 0$$

or

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0$$

This is this *Euler-Lagrange* equation for the functional $\mathbf{J}$.

Example : Shortest path

What is the shortest path between points $(0, a)$ and $(1, b)$? Assume that we have a path $y(x)$ for which $y(0) = a$ and $y(1) = b$. Then the distance from the point 0 to any point $(x, y(x))$ is given by the arc-length formula

$$s(x) = \int_0^x \sqrt{1 + y'(t)^2}\; dt$$

The distance along the entire path between the two points is then just

$$s(1) = \int_0^1 \sqrt{1 + y'(t)^2}\; dt$$

But now, we assume that we don't know the path, and instead write the integral on the left as a *functional* of a function $y(x)$

$$\mathbf{J}[y] = \int_0^1 \sqrt{1 + y'(t)^2}\; dt$$

The goal now is to find the function $y(x)$ which minimizes the functional $\mathbf{J}$, or that $\delta\mathbf{J} = 0[y]$. We can use the Euler-Lagrange formulation with the function

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

to get

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = \frac{d}{dx}\left(\frac{y'(x)}{\sqrt{1 + y'(x)^2}}\right) = 0$$

With a bit of algebra, it can be shown that $y'(x)$ is a constant, from which we get the straight line $y(x) = a(1 - x) + b$.

Example : Brachistrochrone Curve

Find the path with the shortest travel time from a point $A = (0, 0)$ to a point $B = (1, b)$. This is the classic "Brachistrochrone problem", first posed by John Bernoulli in 1696, and is often cited as the inspiration for the field of Calculus of Variations.

As in the above problem, we assume that our curve is described by a path $y(t)$, although this time, we will orient the y-axis so that $y(t)$ is positive in the *downward* direction. The value of $y(t)$ is the drop in the distance from the starting point A.

The potential energy drop from the point A to a point $(t, y(t))$ on the curve should equal the kinetic energy at that point.

$$\frac{1}{2}mv(t)^2 = gmy(t)$$

or

$$v(t) = \sqrt{2gy(t)}$$

The distance travel at time *t* is given by the arc-length formula

$$s(t) = \int_0^t \sqrt{1 + y'(\tau)^2}\, d\tau$$

from which we get that

$$v(t) = \frac{ds}{dt} = \sqrt{1 + y'(t)^2}$$

Since we are interested in the shortest *travel time* (and not the shortest distance), we invert this relation to get

$$\frac{dt}{ds} = \frac{1}{v(t(s))}$$

The total travel time can then be written as the functional

$$\mathbf{T}[y] = \int_0^a dt = \int_0^a \frac{1}{v(t(s))} ds = \int_0^a \frac{\sqrt{1 + y'(t)^2}}{\sqrt{2gy(t)}}\, dt$$

From this, we see that the appropriate function $F(t, y(t), y'(t))$ is

$$F(t, y(t), y'(t)) = \frac{\sqrt{1 + y'(t)^2}}{\sqrt{2gy(t)}}$$

(after some algebra ...), the optimal curve turns out to be the cycloid curve, given by

$$(x(t), y(t)) = \left(t - \frac{1}{2}\sin(2t), \frac{1}{2} - \frac{1}{2}\cos(2t)\right)$$

Example : Solving the Euler-Lagrange problem subject to a constraint

Suppose you want to find the curve passing through points $(0, 0)$ and $(1, 0)$, with length $\bar{L}$, that encloses the largest area.

The area under the curve $y(x)$ is given by

$$A[y] = \int_0^1 y(x)dx$$

while the constraint on the length of the curve is given by

$$L[y] = \int_0^1 \sqrt{1 + y'(x)^2}\, dx - \bar{L} = 0$$

The functional we want to maximize then, is given by

$$\mathbf{J}[y] = A[y] + \lambda L[y] = \int_0^1 \left(y(x) + \lambda\sqrt{1 + y'(x)^2}\right)\, dx - \bar{L}$$

where λ is a *Lagrange multiplier*. Writing this as

The Euler-Lagrange equation this problem is given by

$$\frac{\partial F(x, y(x), y'(x))}{\partial y} - \frac{d}{dx}\left(\frac{\partial F(x, y(x), y'(x))}{\partial y'}\right) = 1 - \lambda \frac{y'(x)}{\sqrt{1 + y'(x)^2}} = 0$$

The solution, expressed in terms of arc-length s, is given by

$$\begin{aligned} x(s) &= \lambda\left(\sin\left(\frac{s - \bar{L}/2}{\lambda}\right) + \sin\left(\frac{\bar{L}}{2\lambda}\right)\right) \\ y(s) &= \lambda\left(\cos\left(\frac{s - \bar{L}/2}{\lambda}\right) - \cos\left(\frac{\bar{L}}{2\lambda}\right)\right) \end{aligned}$$

Question: How does this constrain λ?

Functions of more than one variable

An interesting application of the Euler-Lagrange equations is to the area of "data-assimilation". The idea is that we have a model of a system - typically a PDE, and we want to "fit" our model to observed data by adjusting input functions such as the initial conditions, boundary conditions, a forcing function, and so on. The goal, then will be be to minimize the error between our model and the observed data by perturbing these input functions

The model equations will be functions of both space and time, and so we need to extend our definition of the Euler=Lagrange equations to handle functions of more than variable. The functional $\mathbf{J}$ in this case can be written as

$$\mathbf{J}[\mathbf{y}] = \int_D F\left(x_1, x_2, x_3, \ldots, x_k, y, \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \frac{\partial y}{\partial x_3}, \ldots, \frac{\partial y}{\partial x_k}\right) dx_1\; dx_2\;, \ldots, dx_k$$

where $D = R^{k-1} \times [0, T]$ for example.

Requiring the first variable to vanish, we get

$$\delta\mathbf{J}[\mathbf{y}] = \int_D \left(\frac{\partial F}{\partial y}\eta(\mathbf{x}) + \sum_{i=1}^{k} \frac{\partial F}{\partial z_i}\frac{\partial \eta}{\partial x_i}\right) dx_1\; dx_2\;, \ldots, dx_k = 0$$

To evaluate the second term, we

$$\int_D \sum_{i=1}^{k} \frac{\partial}{\partial x_i}\left(\eta(\mathbf{x})\frac{\partial F}{\partial x_i}\right) dV = \int_D \sum_{i=1}^{k}\left(\eta(\mathbf{x})\frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial z_i}\right) + \frac{\partial F}{\partial z_i}\frac{\partial \eta}{\partial x_i}\right) dV = \int_{\partial D} \eta(\mathbf{x})\left(\frac{\partial F}{\partial z_i}\cdot \mathbf{n}\right) ds$$

If we assume that η is zero on the boundary, then we get

$$\int_D \frac{\partial F}{\partial z_i}\frac{\partial \eta}{\partial x_i} dV = -\int_D \eta(\mathbf{x}) \sum_{i=1}^{k} \frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial z_i}\right) dV$$

so that

$$\delta\mathbf{J}[\mathbf{y}] = \int_D \left(\frac{\partial F}{\partial y} - \sum_{i=1}^{k}\frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial z_i}\right)\right) \eta(\mathbf{x})\; dx_1\; dx_2\;, \ldots, dx_k = 0$$

As in the single variable case, we assume that above is true for any η, and so we get the Euler-Lagrange equations for the multi-variable case.

$$\frac{\partial F}{\partial y} - \sum_{i=1}^{k}\frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial z_i}\right), \qquad z_i = \frac{\partial y}{\partial x_i}$$

Including boundary terms

In the above, we assumed that $\eta(x,t)$ is zero on the boundary. If we do not make this assumption, the above becomes

$$\int_D \frac{\partial F}{\partial z_i}\frac{\partial \eta}{\partial x_i} dV = -\int_D \eta(\mathbf{x}) \sum_{i=1}^{k} \frac{\partial}{\partial x_i}\left(\frac{\partial F}{\partial z_i}\right) dV + \int_{\partial D} \eta(\mathbf{x}) \left(\frac{\partial F}{\partial z_i} \cdot \mathbf{n}\right) ds$$

In this case, we can require that

$$\frac{\partial F}{\partial z_i} \cdot \mathbf{n} = 0$$

Example : Scalar advection

Suppose we have a very simple model of a tracer field (e.g. smoke, pollution, moisture) in the atmosphere. In this 1d model, the background "wind" is a constant velocity $

$$q_t + uq_x = 0, \qquad x \in [0, L]$$

where $q(x,t)$ is a concentration of a tracer in the fluid and u is a constant velocity. We will assume that at time $t = 0$, $q = I(x)$ for some initial conditions $I(x)$. At the boundaries of $[0, L]$, we will impose periodic boundary conditions.

In addition to the model, we also have M observed measurements of the tracer concentration (e.g. in PPM) at space adn time (x_m, t_m), $m = 1, 2, 3, \ldots, M$. Our goal is to try to fit our model to the data.

Fitting the model to data

It is very unlikely that our model will just fit the data right out of the box. But moreover, our model is just that - a model. And as such, we have likely missed important effects. For example, we have not included any source of tracer. The solution to this advection equation is given by

$$q(x,t) = q(x - ut, 0)$$

For the constant coefficient case, this solution is just a translation of the initial conditions at velocity u.
We are unlikely to know the initial conditions (we cannot measure the tracer field everywhere at time $t = 0$) and so already, we have a significant modeling error. Moreover, we have not included any sources of tracer (a burning wildfire, for example) in our domain.

Our goal, therefore is to make adjustments to the model that allow us to fit the observed data. One simple adjustment we might think of making is adding a source term so that our model becomes

$$q_t + uq_x = f(x,t)$$

Minimization problem

The source term $f(x,t)$ should be chosen in such a way as to minimize the distance between the model and the observed data points. To minimize this error, we formulate the following functional to be minimized

$$\mathbf{J}[u] = W\int_0^T\int_0^L f(x,t)^2\;dx\,dt + w\sum_{m=1}^M (u(x_m,t_m) - d_m)^2$$

The second term involving our observed data acts a bit like a constraint, but without a Lagrange multiplier. Instead, we multiply both terms by weights W and w so we can relax the requirement that the model interpolate the data points exactly. The weighting factors allow us to prescribe just how much we trust the model verses the data.

We can write the second term as an integral by using the Dirac delta function.

$$\mathbf{J}[u] = W\int_0^T\int_0^L f(x,t)^2\;dx\,dt + w\int_0^T\int_0^L\sum_{m=1}^M (u(x,t) - d_m)^2\delta(x-x_m)\,\delta(t-t_m)\;dx\,dt$$

Replacing $f(x,t)$ with the model leads to

$$\begin{aligned}\mathbf{J}[u] &= W\int_0^T\int_0^L (u_t + cu_x)^2\;dx\,dt + w\int_0^T\int_0^L\sum_{m=1}^M (u(x,t) - d_m)^2\delta(x-x_m)\,\delta(t-t_m)\;dx\,dt \\ &= \int_0^T\int_0^L F(x,t,u,u_x,u_t)\;dx\,dt\end{aligned}$$

where

$$F(x,t,u,u_x,u_t) = W(u_t + cu_x)^2 + w\sum_{m=1}^M (u(x,t) - d_m)^2\delta(x-x_m)\,\delta(t-t_m)$$

The Euler-Lagrange equations for this system can then be written as follows.

$$\begin{aligned}\frac{\partial F}{\partial u} &= 2w\sum_{m=1}^M (u(x,t) - d_m)\delta(x-x_m)\,\delta(t-t_m) \\ \frac{\partial F}{\partial u_x} &= 2W(u_t + cu_x)(c) \\ \frac{\partial F}{\partial u_t} &= 2W(u_t + cu_x)\end{aligned}$$

Setting $\lambda(x,t) = W(u_t + cu_x)$, we can combine the above into the Euler-Lagrange equations to get

$$w\sum_{m=1}^M (u(x,t) - d_m)\delta(x-x_m)\,\delta(t-t_m) - \lambda_t - c\lambda_x = 0$$

subject to conditions on $\lambda(x,t)$ at $x=0$, $x=L$, and $t=0$ and $t=T$.

Euler-Lagrange system for our model problem

Recall that when deriving the Euler-Lagrange equations, we made the assumption that our perturbation $\eta(x)$ satisfied homogeneous boundary conditions. This assumption allowed us to drop boundary terms in the integration by parts step that led to the Euler-Lagrange equations.

The full Euler-Lagrange system for our model problem includes the boundary terms below.

$$\frac{\partial \mathbf{J}}{\partial \alpha} = \int_0^T \int_0^L \left(\frac{\partial F}{\partial u} - \frac{\partial}{\partial x}\frac{\partial F}{\partial u_x} - \frac{\partial}{\partial t}\frac{\partial F}{\partial u_t} \right) \eta(x)\ dx + \left[\int_0^L \frac{\partial F}{\partial u_t} \eta(x,t)\, dx \right]_{t=0}^{t=T} + \left[\int_0^T \frac{\partial F}{\partial u_x} \eta(x,t)\, dt \right]_{x=(}^{x=l}$$

Rather than enforce $\eta(x,t) = 0$ along the space-time boundary, we instead impose homogeneous boundary conditions on $\partial F/\partial u_x$ and $\partial F/\partial u_x$ on any boundaries for which $\eta(x,t) \neq 0$. In the above, for example, we might impose

$$\begin{aligned}
\frac{\partial F(x,0)}{\partial u_x} &= 2c\lambda(x,0) = 0 \\
\frac{\partial F(x,T)}{\partial u_x} &= 2c\lambda(x,T) = 0 \\
\frac{\partial F(0,L)}{\partial u_t} &= 2\lambda(0,t) = 0 \\
\frac{\partial F(L,t)}{\partial u_t} &= 2\lambda(L,t) = 0
\end{aligned}$$

or

$$\lambda(0,t) = \lambda(L,t) = \lambda(x,0) = \lambda(x,T) = 0$$

Questions:

- Do we impose all four of these boundary conditions for the model problem?
- If we assume $\eta(x,t) = 0$ along one of the boundaries, does that mean that we don't impose a condition on $\lambda(x,t) = 0$ on that boundary?
- If we want to allow a boundary condition or initial condition to vary, does that mean that we are not assuming $\eta(x,t) = 0$ on that boundary?

A boundary value problem

The full system to be solved then takes the form of a boundary value problem, given by

$$
\begin{aligned}
-\lambda_t - c\lambda_x &= -w\sum_{m=1}^{M}(u(x,t) - d_m)\delta(x - x_m)\,\delta(t - t_m) \\
\lambda(0,t) &= 0 \\
\lambda(L,t) &= 0 \\
\lambda(x,0) &= 0 \\
\lambda(x,T) &= 0
\end{aligned}
$$

This system is awkward, with conditions imposed at both boundaries and at both the initial and final time. This formulation is problematic for at least two reasons.

- The model equations allow for input from the right boundary (assuming $c > 0$) but only "outflow" at the left boundary. The value at the right boundary is determined by information flow from the left, and causality prevents us from imposing a value there.
- It isn't obvious how the above system leads to an equation for the optimal solution $u(x,t)$ to our minimization problem.

Forward and backward problem

To get around the problems with the above formulation, we reformulate boundary value problem as a coupled "forward problem" and a "backward" problem. This dual system will consist of two sets of problems.

We start with the **backward problem** for $\lambda(x,t)$, given by

$$\begin{aligned} -\lambda_t - c\lambda_x &= -w\sum_{m=1}^{M}(u(x,t)-d_m)\delta(x-x_m)\,\delta(t-t_m) \\ \lambda(L,t) &= 0 \\ \lambda(x,T) &= 0 \end{aligned}$$

The solution to the backwards problem is solved "backwards" in time, starting at $t = T$. And because of the negative sign on the speed c, we are permitted to impose "inflow" boundary conditions at $x = L$, the right edge of our domain.

We derive a **forward problem** from the original definition of λ, given by

$$\lambda(x,t) = W(u_t + cu_x)$$

From this, the forward problem is then

$$\begin{aligned} u_t + cu_x &= W^{-1}\lambda(x,t) \\ u(x,0) &= I(x)) \\ u(0,t) &= B(t) \end{aligned}$$

The forward problem is now driven by the solution to the backward problem.

For this system, the forward and backward problems are both constant coefficient advection-type equations. The reason for this is that our model equation, expressed in terms of the operator $L[u] = u_t + cu_x$ is self-adjoint, and for this reason the two systems above have essentially the same form.

More generally, the backwards equation is referred to as the **adjoint equation**.

Question:

- Can we show that boundary conditions on $\lambda(x,t)$ are satisfied by this "forward-backward" problem?