Calculus 3
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The Fundamental Theorem

If $y = f(x)$ is a continuous function on $[a, b]$, and F is the antiderivative of f (i.e. $F'(x) = f(x)$), recall that the Fundamental Theorem of Calculus states that

$$\int_a^b f(t)dt = \int_a^b F'(t)dt = F(t)|_a^b = F(b) - F(a)$$

We generalize this formula to line integrals of vector functions $\vec{f}$ of more than one variable.

Conservative vector fields. Consider a vector function $\vec{f} = \langle P, Q, R\rangle$ such that the derivatives of P, Q and R are continuous. Since the gradient replaces the concept of a derivative in this case, the condition that $F' = f$ from the one-dimensional case becomes

$$\nabla F = \vec{f} \quad \Rightarrow \quad \langle F_x, F_y, F_z\rangle = \langle P, Q, R\rangle.$$

Thus, the condition that F is an"antiderivative" of $\vec{f}$ is equivalent with three requirements

$$F_x = P, \quad F_y = Q, \quad \text{and} \quad F_z = R.$$

If there is a function F such that the above three equations hold, we say that $\vec{f}$ is a **conservative** vector field and that F is a **potential function** of $\vec{f}$.

It turns out there are vector fields which are conservative and vector fields which are not conservative. So, one would like to have a set of criteria which specify exactly when a given vector field is conservative and when it is not, and a procedure for determining a potential in case when the field is conservative.

If a vector field is conservative, differentiating the first equation above with respect to y and z, the second with respect to x and z and the third with respect to x and y produces the following.

$$\begin{array}{lll} F_x = P & \Rightarrow & F_{xy} = P_y, \quad F_{xz} = P_z, \\ F_y = Q & \Rightarrow & F_{yx} = Q_x, \quad F_{yz} = Q_z, \\ F_z = R & \Rightarrow & F_{zx} = R_z, \quad F_{zy} = R_y. \end{array}$$

If F is a twice-differentiable function, $F_{xy} = F_{yx}$, $F_{xz} = F_{zx}$, and $F_{yz} = F_{zy}$ and so

$$P_y = Q_x, \quad P_z = R_x, \quad \text{and} \quad Q_z = R_y.$$

Thus, every conservative vector field satisfies these three conditions. It turns out that the converse holds as well: if the above conditions hold, one can find a potential F so $\vec{f}$ is conservative. To show this, assume that the above three conditions holds and that the domain of $\vec{f}$ is simply-connected (intuitively, the domain is connected and has no holes). Three steps below describe the process of finding a potential F of $\vec{f}$.

1. Since $F_x = P$ holds, integrating P with respect to x determines F up to the terms which only have y and z in them. If $g(y, z)$ is the sum of all such terms, then $F = \int P dx + g(y, z)$.

2. Since $F_y = Q$, differentiating F from the previous step with respect to y and equating the derivative F_y with Q produces an equation in g_y. Thus integrating g_y with respect to y determines g up to the terms which only have z in them. If $h(z)$ is the sum of all such terms, then $g(y,z) = G(y,z) + h(z)$ for some function G we determined in this step and still unknown function h. Thus, $F = \int P dx + G(y,z) + h(z)$.

3. Since $F_z = R$, differentiating F from the previous step with respect to z and equating the derivative F_z with R, produces an equation in h'. Integrating with respect to z determines h up to an integration constant. Hence, we get to know all the terms of F up to an integration constant.

Note that the above process has three steps and that exactly one of the three equations $F_x = P$, $F_y = Q$, and $F_z = R$ is used in each step.

This shows that a vector field $\vec{f}$ is conservative exactly when the conditions $P_y = Q_x$, $P_z = R_x$, and $Q_z = R_y$ hold. Thus,

to check if $\vec{f} = \langle P, Q, R\rangle$ is conservative, check if $P_y = Q_x$, $P_z = R_x$, and $Q_z = R_y$.

Assume now that $\vec{f}$ is a vector function defined on a simply-connected region and that C is a smooth curve $\vec{r}(t) = (x(t), y(t), z(t))$ with the initial point $\vec{r}(a) = (x(a), y(a), z(a))$ and the terminal point $\vec{r}(b) = (x(b), y(b), z(b))$. Then the line integral

$$\int_C \vec{f}(t) \cdot d\vec{r} = \int_C P dx + Q dy + R dz$$

is **independent of path** if and only if $\vec{f} = \langle P, Q, R\rangle$ is conservative. In this case, if $\vec{f} = \nabla F$,

$$\int_C \vec{f}(t) \cdot d\vec{r} = \int_C \nabla F \; d\vec{r} = F(\vec{r}(b)) - F(\vec{r}(a)) = F(\text{end}) - F(\text{beginning})$$

Plane vector fields. If $\vec{f} = \langle P, Q\rangle$ is a plane vector field such that the derivatives of P and Q are continuous, then the absence of R and z in the process described above reduces checking if $\vec{f}$ is conservative to only checking if $P_y = Q_x$ and the conditions on relating F and $\vec{f}$ to only having that $F_x = P$ and $F_y = Q$.

Practice problems.

1. Check if the given vector functions are conservative. If they are, find their potential functions.

   (a) $\vec{f} = \langle xe^y, ye^x\rangle$ (b) $\vec{f} = \langle x^3y^4, x^4y^3 + 2y\rangle$.

2. Check that the given vector function is conservative, find its potential and use it to evaluate $\int_C \vec{f} d\vec{r}$ for given curve C.

   (a) $\vec{f} = \langle x^3y^4,\ x^4y^3 + 2y\rangle$, C is the curve with parametric equations $x = \sqrt{t}$ and $y = 1 + t^3$ for $0 \le t \le 1$.

   (b) $\vec{f} = \langle y,\ x + z,\ y\rangle$, C is any path from $(2, 1, 4)$ to $(8, 3, -1)$.

(c) $\vec{f} = \langle 2xz + \sin y,\ x\cos y + 3y^2 z,\ x^2 + y^3 + 6z\rangle$, C is the helix $x = \cos t$, $y = \sin t$, $z = t$ for $0 \le t \le 2\pi$.

3. Show that the line integral is independent of path and evaluate it.

(a) $\int_C 2x \sin y\, dx + (x^2 \cos y - 3y^2)\, dy$ where C is any path from (-1,0) to (5, 1).

(b) $\int_C (2xy + z^2)\, dx + (x^2 + 2yz + 2)\, dy + (y^2 + 2xz + 3)\, dz$ where C is any path from (1, 0, 2) to (0, 1, 4).

Solutions.

1. (a) $P = xe^y \Rightarrow P_y = xe^y$, and $Q = ye^x \Rightarrow Q_x = ye^x$. Since $P_y \ne Q_x$, the field is not conservative.

(b) $P = x^3y^4 \Rightarrow P_y = 4x^3y^3$, and $Q = x^4y^3 + 2y \Rightarrow Q_x = 4x^3y^3$. Since $P_y = Q_x$, the field is conservative. A potential function can be found as $F = \int P dx = \int x^3y^4 dx = \frac{1}{4}x^4y^4 + g(y)$. Finding F_y and setting it equal to Q yields that $x^4y^3 + g'(y) = x^4y^3 + 2y$. From here $g'(y) = 2y \Rightarrow g(y) = y^2 + c$. Thus, $F = \frac{1}{4}x^4y^4 + y^2 + c$.

2. (a) The vector function $\vec{f}$ is conservative by the the previous problem and its potential is $F = \frac{1}{4}x^4y^4 + y^2 + c$. In given parametrization of C, $t = 0$ corresponds to $(x, y) = (0, 1)$ and $t = 1$ to $(x, y) = (1, 2)$. So, $\int_C \vec{f} d\vec{r} = F(1, 2) - F(0, 1) = 4 + 4 + c - 0 - 1 - c = 7$.

(b) The vector field $\vec{f}$ is conservative since $P_y = 1 = Q_x$, $P_z = 0 = R_x$, and $Q_z = 1 = R_y$.

$F = \int P dx = \int y dx = xy + g(y, z)$. Find F_y and set it equal to Q. $F_y = x + g_y = Q = x + z \Rightarrow g_y = z \Rightarrow g = \int z dy = yz + h(z)$. Thus $F = xy + yz + h(z)$. Finally, find F_z and set it equal to R. $F_z = y + h' = y \Rightarrow h' = 0 \Rightarrow h = c$. Thus $F = xy + yz + c$. The integral $\int_C \vec{f} d\vec{r}$ is equal to $F(8, 3, -1) - F(2, 1, 4) = 21 - 6 = 15$.

(c) The vector field $\vec{f}$ is conservative since $P_y = \cos y = Q_x$, $P_z = 2x = R_x$, and $Q_z = 3y^2 = R_y$.

$F = \int P dx = \int (2xz + \sin y) dx = x^2z + x \sin y + g(y, z)$. Find F_y and set it equal to Q. $F_y = x \cos y + g_y = Q = x \cos y + 3y^2 z \Rightarrow g_y = 3y^2 z \Rightarrow g = \int 3y^2 z dy = y^3 z + h(z)$. Thus $F = x^2 z + x \sin y + y^3 z + h(z)$. Finally, find F_z and set it equal to R. $F_z = x^2 + y^3 + h' = x^2 + y^3 + 6z \Rightarrow h' = 6z \Rightarrow h = \int 6z dz = 3z^2 + c$. Thus $F = x^2 z + x \sin y + y^3 z + 3z^2 + c$.

In the given parametrization of C, $t = 0$ corresponds to $(x, y, z) = (1, 0, 0)$ and $t = 2\pi$ to $(x, y, z) = (1, 0, 2\pi)$. So, the integral $\int_C \vec{f} d\vec{r}$ is equal to $F(1, 0, 2\pi) - F(1, 0, 0) = 2\pi + 12\pi^2 - 0 \approx 124.72$.

3. (a) Let $\vec{f} = \langle P, Q\rangle$ with $P = 2x \sin y$ and $Q = x^2 \cos y - 3y^2$. Then $P_y = 2x \cos y = Q_x$ so the field is conservative.

A potential is $F = \int P dx = x^2 \sin y + g(y)$. $F_y = x^2 \cos y + g'(y) = Q = x^2 \cos y - 3y^2 \Rightarrow g' = -3y^2 \Rightarrow g = -y^3 + c$. Thus, $F = x^2 \sin y - y^3 + c$. The integral is $\int_C = F(5, 1) - F(-1, 0) = 25 \sin 1 - 1 - 0 = 20.04$

(b) Consider $\vec{f} = \langle P, Q, R\rangle$ with $P = 2xy + z^2, Q = x^2 + 2yz + 2$ and $R = y^2 + 2xz + 3$. Check that $P_y = 2x = Q_x$, $P_z = 2z = R_x$, and $Q_z = 2y = R_y$ so that $\vec{f}$ is conservative.

Find a potential F as $F = \int P dx = \int (2xy + z^2)dx = x^2y + z^2x + g(y, z)$. Equating F_y with Q obtain $F_y = x^2 + g_y = x^2 + 2yz + 2 \Rightarrow g_y = 2yz + 2 \Rightarrow g = \int (2yz + 2)dy = y^2z + 2y + h(z)$. Thus $F = x^2y + z^2x + y^2z + 2y + h$. Equating F_z with R obtain $F_z = 2zx + y^2 + h' = y^2 + 2xz + 3 \Rightarrow h' = 3 \Rightarrow h = 3z + c$. Thus $F = x^2y + z^2x + y^2z + 2y + 3z + c$.

The integral is $\int_C = F(0, 1, 4) - F(1, 0, 2) = 4 + 2 + 12 - 4 - 6 = 8$.

Independence of path in Physics and Chemistry.

The terminology used in chemistry and physics is sometimes slightly different. A **state function** is a function of the parameters of the system which only depends upon the parameters' values at the **endpoints of the path**. Thus, the change in a state function is a path independent. For example, the change of temperature is a state function. To illustrate that it is "path independent", consider that we can raise the temperature of water for 10 degrees on a few different ways: a) heat the water by 10 degrees, b) heat the water by 100 degrees and wait till it cools down to 10 degrees above the initial temperature, c) stir the water until the temperature gets raised by 10 degrees etc.

In thermodynamics, a state function, state quantity, or a function of state, is a property of a system that depends only on the current state of the system, not on the way in which the system got to that state. For example, internal energy, enthalpy and entropy are state quantities. In contrast, mechanical work and heat are process quantities because they describe quantitatively the transition between equilibrium states of thermodynamic systems.

When a system changes state continuously, it traces out a "path" in the state space. The path can be specified by noting the values of the state parameters as the system traces out the path, perhaps as a function of time, or some other external variable. Thus, we can treat state functions as vector functions.

Example. (from Wikipedia) Let us consider the pressure $P(t)$ and the volume $V(t)$ as functions of time t when t is between time t_0 and time t_1. If we wish to calculate the work done by the system from time t_0 to time t_1, we can calculate

$$W(t_0, t_1) = \int_{\text{state } 0}^{\text{state } 1} P\, dV = \int_{t_0}^{t_1} P(t) \frac{dV(t)}{dt}\, dt.$$

It is clear that in order to calculate the work W in the above integral, we will have to know the functions $P(t)$ and $V(t)$ at each time t, over the entire path. Thus, the work W is not a state function here.

Let us suppose now that we wish to calculate the work plus the integral of VdP over the path. We would have:

$$\Phi(t_0, t_1) = \int_{t_0}^{t_1} P \frac{dV}{dt}\, dt + \int_{t_0}^{t_1} V \frac{dP}{dt}\, dt = \int_{t_0}^{t_1} \frac{d(PV)}{dt}\, dt = P(t_1)V(t_1) - P(t_0)V(t_0).$$

It can be seen that the integrand can be expressed as the exact differential of the function $P(t)V(t)$ and that therefore, the integral can be expressed as the difference in the value of $P(t)V(t)$ at the end points of the integration. The product PV is therefore a state function of the system.

Thus, in order to determine if a given function is a state function or not, it is key to see when a line integral of a vector function is independent of path.