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 functions f of two or three variables. Note that the derivative from one dimensional case generalizes to the gradient ∇F and the integral to the line integral.

Plane vector functions. Consider a vector function $\vec{f} = (P, Q)$ such that the derivatives of P and Q are continuous. We shall say that $\vec{f}$ is **conservative** vector field if and only if it is gradient of some scalar function $F(t)$,

$$\vec{f} = \nabla F.$$

In this case, the scalar function F is call a **potential function** of $\vec{f}$. If $\vec{f} = (P, Q)$, the condition $\vec{f} = \nabla F$ gives us that $P = F_x$ and $Q = F_y$. Since $F_{xy} = F_{yx}$ if F is twice differentiable function, this gives us that $P_y = Q_x$. Conversely, it can be shown that if $P_y = Q_x$ the vector function is conservative assuming that the domain of $\vec{f}$ is simply-connected (intuitively, the domain is connected and has no holes). Thus

<u>to check if $\vec{f} = (P, Q)$ is conservative, it is sufficient to check if $P_y = Q_x$.</u>

For a given conservative vector field $\vec{f} = (P, Q)$, a potential function F can be found on the following way:

1. $F_x = P \Rightarrow$ integrate P with respect to x. Denote the integration constant by $g(y)$. Thus $F = \int P dx + g(y)$.

2. $F_y = Q \Rightarrow$ differentiate F from previous step with respect to y and equate the derivative F_y with Q. Solve for $g(y)$.

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

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

is **independent of path** if and only if $\vec{f} = (P, Q)$ is conservative (i.e. if $P_y = Q_x$). In this case, if $\vec{f} = \nabla F$,

$$\int_C P dx + Q dy = \int_C \vec{f}(t) d\vec{r} = \int_C \nabla F d\vec{r} = F(\vec{r}(b)) - F(\vec{r}(a))$$

Space vector functions. Consider the vector function $\vec{f} = (P, Q, R)$. Assume that all the derivatives of P, Q and R are continuous. Similarly as in the two dimensional case, we say that $\vec{f}$ is

conservative vector field if and only if it is gradient of some scalar function $F(t)$, $\vec{f} = \nabla F$, called a **potential function** of $\vec{f}$. If $\vec{f} = (P, Q, R)$, this condition gives us that $P = F_x$, $Q = F_y$ and $R = F_z$. Since $F_{xy} = F_{yx}$, $F_{xz} = F_{zx}$, and $F_{yz} = F_{zy}$ for F a twice differentiable function, this gives us that $P_y = Q_x$, $P_z = R_x$ and $Q_z = R_y$. Conversely, it can be shown that if these three conditions hold that the vector function is conservative under the assumption that the domain of $\vec{f}$ is simply-connected. Thus

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

For a given conservative vector field $\vec{f} = (P, Q, R)$, a potential function F can be found on the following way:

1. $F_x = P \Rightarrow$ integrate P with respect to x. Denote the integration constant by $g(y, z)$. Thus $F = \int P dx + g(y, z)$.
2. $F_y = Q \Rightarrow$ differentiate F from the previous step with respect to y and equate the derivative F_y to Q. Solve for $g(y, z)$. Denote the integration constant by $h(z)$. Thus $g(y, z) = G(y, z) + h(z)$ where the function G is completely determined. Thus, $F = \int P dx + G(y, z) + h(z)$.
3. $F_z = R \Rightarrow$ differentiate F from the previous step with respect to z and equate the derivative F_z to R. Solve for $h(z)$. This determines F up to integration constant.

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 endpoints $\vec{r}(a) = (x(a), y(a), z(a))$ and $\vec{r}(b) = (x(b), y(b), z(b))$. Then the line integral $\int_C P dx + Q dy + R dz = \int_C \vec{f}(t) d\vec{r}$ is independent of path if and only if $\vec{f} = (P, Q, R)$ is conservative. In this case, if $\vec{f} = \nabla F$,

$$\int_C P dx + Q dy + R dz = \int_C \vec{f}(t) d\vec{r} = \int_C \nabla F d\vec{r} = F(\vec{r}(b)) - F(\vec{r}(a))$$

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 $x = \sqrt{t}$, $y = 1 + t^3$, $0 \leq t \leq 1$.
   (b) $\vec{f} = \langle y, x + z, y \rangle$, C is any path from $(2, 1, 4)$ to $(8, 3, -1)$.
   (c) $\vec{f} = \langle 2xz + \sin y, x \cos y, x^2 \rangle$, C is the helix $x = \cos t$, $y = \sin t$ $z = t$, for $0 \leq t \leq 2\pi$.

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 $P_y \neq Q_x$, 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. The potential function can be found as $F = \int Pdx = \int x^3y^4dx = \frac{1}{4}x^4y^4 + g(y)$. 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 $Q_z = 1 = R_y$.

   $F = \int Pdx = \int ydx = xy + g(y, z)$. Find F_y and set it equal to Q. $F_y = x + g_y = Q = x + z \Rightarrow g_y = z \Rightarrow g = \int zdy = yz + h(z)$. 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 $Q_z = 0 = R_y$.

   $F = \int Pdx = \int(2xz + \sin y)dx = x^2z + x\sin y + g(y, z)$. Find F_y and set it equal to Q. $F_y = x\cos y + g_y = Q = x\cos y \Rightarrow g_y = 0 \Rightarrow g = 0 + h(z)$. Thus $F = x^2z + x\sin y + h(z)$. Finally, find F_z and set it equal to R. $F_z = x^2 + h' = x^2 \Rightarrow h' = 0 \Rightarrow h = c$. Thus $F = x^2z + x\sin y + c$.

   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 $F(1, 0, 2\pi) - F(1, 0, 0) = 2\pi - 0 = 2\pi$.

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.

   The potential is $F = \int Pdx = x^2\sin y + g(y)$. $F_y = x^2\cos y + g'(y) = Q = x^2\cos y - 3y^2 \Rightarrow g' = -3y^2 \Rightarrow g = -y^3 + c$. 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 the potential F as $F = \int Pdx = \int(2xy + z^2)dx = x^2y + z^2x + g(y, z)$. 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 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.