Oct. 19 2005: Lecture 14:

Integrals along a Path

Reading:
Kreyszig Sections: §9.1 (pp:464–70) , §9.2 (pp:471–477) §9.3 (pp:478–484)

Integrals along a Curve

Consider the type of integral that everyone learns initially:

$$E(b) - E(a) = \int_a^b f(x)dx \tag{14-1}$$

The equation implies that f is integrable and

$$dE = f dx = \frac{dE}{dx} dx \tag{14-2}$$

so that the integral can be written in the following way:

$$E(b) - E(a) = \int_a^b dE \tag{14-3}$$

where a and b represent "points" on some *line* where E is to be evaluated.

Of course, there is no reason to restrict integration to a straight line—the generalization is the integration along a curve (or a path) $\vec{x}(t) = (x_1(t), x_2(t), \ldots, x_n(t))$.

$$E(b) - E(a) = \int_{\vec{x}(a)}^{\vec{x}(b)} \vec{f}(\vec{x}) \cdot d\vec{x} = \int_a^b g(x(\vec{t}))dt = \int_a^b \nabla E \cdot \frac{d\vec{x}}{dt} dt = \int_a^b dE \tag{14-4}$$

This last set of equations assumes that the gradient exists–i.e., there is some function E that has the gradient $\nabla E = \vec{f}$.

Path-Independence and Path-Integration

If the function being integrated along a simply-connected path (Eq. 14-4) is a gradient of some scalar potential, then the path between two integration points does not need to be specified: the integral is independent of path. It also follows that for closed paths, the integral of the gradient of a scalar potential is zero.[5] A simply-connected path is one that does not self-intersect or can be shrunk to a point without leaving its domain.

There are familiar examples from classical thermodynamics of simple one-component fluids that satisfy this property:

$$\oint dU = \oint \nabla_{\vec{\mathcal{S}}} U \cdot d\vec{\mathcal{S}} = 0 \qquad \oint dS = \oint \nabla_{\vec{\mathcal{S}}} S \cdot d\vec{\mathcal{S}} = 0 \qquad \oint dG = \oint \nabla_{\vec{\mathcal{S}}} G \cdot d\vec{\mathcal{S}} = 0 \tag{14-5}$$

$$\oint dP = \oint \nabla_{\vec{\mathcal{S}}} P \cdot d\vec{\mathcal{S}} = 0 \qquad \oint dT = \oint \nabla_{\vec{\mathcal{S}}} T \cdot d\vec{\mathcal{S}} = 0 \qquad \oint dV = \oint \nabla_{\vec{\mathcal{S}}} V \cdot d\vec{\mathcal{S}} = 0 \tag{14-6}$$

Where $\vec{\mathcal{S}}$ is any other set of variables that sufficiently describe the equilibrium state of the system (i.e, $U(S,V)$, $U(S,P)$, $U(T,V)$, $U(T,P)$ for U describing a simple one-component fluid).

The relation curl grad $f = \nabla \times \nabla f = 0$ provides method for testing whether some *general* $\vec{F}(\vec{x})$ is independent of path. If

$$\vec{0} = \nabla \times \vec{F} \tag{14-7}$$

or equivalently,

$$0 = \frac{\partial F_j}{\partial x_i} - \frac{\partial F_i}{\partial x_j} \tag{14-8}$$

for all variable pairs x_i, x_j, then $\vec{F}(\vec{x})$ is independent of path. These are the Maxwell relations of classical thermodynamics.

[5] In fact, there are some extra requirements on the domain (i.e., the space of all paths that are supposed to be path-independent) where such paths are defined: the scalar potential must have continuous second partial derivatives everywhere in the domain.

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Path Dependence, Curl, and Curl=0 subspaces

This example will show that the choice of path matters for a vector-valued function that does not have vanishing curl and that it doesn't matter when integrating a function with vanishing curl.

Path-dependent/Non-conserving Field

1. Verify that the function $\vec{v}(\vec{x}) = xyz(\hat{i} + \hat{k} + \hat{z})$ does not have vanishing curl.
2. Integrate $\vec{v}$ along a path that is wrapped around a cylinder of radius R, (e.g., $(x(t), y(t), z(t)) = (R\cos t, R\sin t, AP_{2\pi}(t))$, where $P_{2\pi}(t = 0) = P_{2\pi}(t = 2\pi)$)
3. Calculate the integral specifically for $P_{2\pi}(t) = \cos t$, $P_{2\pi}(t) = \sin t$, $P_{2\pi}(t) = t(t - 2\pi)$, and $P_{2\pi}(t) = \cos Nt$.

Path-independent/Conservative Field

1. Verify that, for the function $\vec{w}(\vec{x}) = e^{xyz}(yz\hat{i} + zx\hat{k} + xy\hat{z})$, $\nabla \times \vec{w} = 0$. In fact, $\vec{w} = \nabla e^{xyz}$.
2. Integrate $\vec{w}$ along the same cylindrical-type path as above and see that the integral always vanishes—it is path-independent.

Path independent on a Subspace

1. The vector function $\vec{v}(\vec{x}) = (x^2 + y^2 - R^2)\hat{z}$ only vanishes on the cylinder or radius R.
2. It is easy to find $\vec{w}$ such that $\vec{w} = \nabla \times v$:

$$\vec{w} = \frac{1}{2}\left(yR^2\left[1 - x^2 - \frac{y^2}{3}\right]\hat{x} + -xR^2\left[1 - y^2 - \frac{x^2}{3}\right]\hat{y}\right)$$

   In fact, because we could add any vector function that has vanishing curl to $\vec{w}$ there are an infinite number of $\vec{w}$ such that $\vec{w} = \nabla \times v$.

3. Therefore, if we integrate $\vec{w}$ along a path *that is restricted* to the cylinder it should be path independent.
4. Using the same methods as above, we find that the integral on the cylinder will be independent of P—the vector function $\vec{w}$ is independent of path as long as the path remains on the cylinder.

Multidimensional Integrals

Perhaps the most straightforward of the higher-dimensional integrations (e.g., vector function along a curve, vector function on a surface) is a scalar function over a domain such as, a rectangular block in two dimensions, or a block in three dimensions. In each case, the integration over a dimension is uncoupled from the others and the problem reduces to pedestrian integration along a coordinate axis.

Sometimes difficulty arises when the domain of integration is not so easily described; in these cases, the limits of integration become functions of another integration variable. While specifying the limits of integration requires a bit of attention, the only thing that makes these cases difficult is that the integrals become tedious and lengthy. MATHEMATICA® removes some of this burden.

A short review of various ways in which a function's variable can appear in an integral follows:

	The Integral	Its Derivative
Function of limits	$p(x) = \int_{\alpha(x)}^{\beta(x)} f(\xi) d\xi$	$\frac{dp}{dx} = f(\beta(x))\frac{d\beta}{dx} - f(\alpha(x))\frac{d\alpha}{dx}$
Function of integrand	$q(x) = \int_{a}^{b} g(\xi, x) d\xi$	$\frac{dq}{dx} = \int_{a}^{b} \frac{\partial g(\xi, x)}{\partial x} d\xi$
Function of both	$r(x) = \int_{\alpha(x)}^{\beta(x)} g(\xi, x) d\xi$	$\frac{dr}{dx} = f(\beta(x))\frac{d\beta}{dx} - f(\alpha(x))\frac{d\alpha}{dx} + \int_{\alpha(x)}^{\beta(x)} \frac{\partial g(\xi, x)}{\partial x} d\xi$

Extra Information and Notes

Potentially interesting but currently unnecessary

Changing of variables is a topic in multivariable calculus that often causes difficulty in classical thermodynamics.

This is an extract of my notes on thermodynamics: http://pruffle.mit.edu/3.00/

Alternative forms of differential relations can be derived by changing variables.

To change variables, a useful scheme using Jacobians can be employed:

$$\begin{aligned}\frac{\partial(u,v)}{\partial(x,y)} &\equiv \det\begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y}\end{vmatrix} \\ &= \frac{\partial u}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial u}{\partial y}\frac{\partial v}{\partial x} \\ &= \left(\frac{\partial u}{\partial x}\right)_y \left(\frac{\partial v}{\partial y}\right)_x - \left(\frac{\partial u}{\partial y}\right)_x \left(\frac{\partial v}{\partial x}\right)_y \\ &= \frac{\partial u(x,y)}{\partial x}\frac{\partial v(x,y)}{\partial y} - \frac{\partial u(x,y)}{\partial y}\frac{\partial v(x,y)}{\partial x}\end{aligned} \tag{14-9}$$

$$\begin{aligned}\frac{\partial(u,v)}{\partial(x,y)} = -\frac{\partial(v,u)}{\partial(x,y)} &= \frac{\partial(v,u)}{\partial(y,x)} \\ \frac{\partial(u,v)}{\partial(x,v)} &= \left(\frac{\partial u}{\partial x}\right)_v \\ \frac{\partial(u,v)}{\partial(x,y)} &= \frac{\partial(u,v)}{\partial(r,s)}\frac{\partial(r,s)}{\partial(x,y)}\end{aligned} \tag{14-10}$$

For example, the heat capacity at constant volume is:

$$\begin{aligned}C_V &= T\left(\frac{\partial S}{\partial T}\right)_V = T\frac{\partial(S,V)}{\partial(T,V)} \\ &= T\frac{\partial(S,V)}{\partial(T,P)}\frac{\partial(T,P)}{\partial(T,V)} = T\left[\left(\frac{\partial S}{\partial T}\right)_P\left(\frac{\partial V}{\partial P}\right)_T - \left(\frac{\partial S}{\partial P}\right)_T\left(\frac{\partial V}{\partial T}\right)_P\right]\left(\frac{\partial P}{\partial V}\right)_T \\ &= T\frac{C_P}{T} - T\left(\frac{\partial P}{\partial V}\right)_T\left(\frac{\partial V}{\partial T}\right)_P\left(\frac{\partial S}{\partial P}\right)_T\end{aligned} \tag{14-11}$$

Using the Maxwell relation, $\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P$,

$$C_P - C_V = -T\frac{\left[\left(\frac{\partial V}{\partial T}\right)_P\right]^2}{\left(\frac{\partial V}{\partial P}\right)_T} \tag{14-12}$$

which demonstrates that $C_P > C_V$ *because, for any stable substance, the volume is a decreasing function of pressure at constant temperature.*

MATHEMATICA® Example: (notebook) Lecture-14

Potential near a Charged and Shaped Surface Patch

Example calculation of the spatially-dependent energy of a unit point charge in the vicinity of a charged planar region having the shape of an equilateral triangle.

The energy of a point charge $|e|$ due to a surface patch on the plane $z = 0$ of size $d\xi d\eta$ with surface charge density $\sigma(x, y)$ is:

$$dE(x, y, z, \xi, \eta) = \frac{|e|\sigma(\xi, \eta)d\xi d\eta}{\vec{r}(x, y, z, \xi, \eta)}$$

for a patch with uniform charge,

$$dE(x, y, z, \xi, \eta) = \frac{|e|\sigma d\xi d\eta}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + z^2}}$$

For an equilateral triangle with sides of length one and center at the origin, the vertices can be located at $(0, \sqrt{3}/2)$ and $(\pm 1/2, -\sqrt{3}/6)$.

The integration becomes

$$E(x, y, z) \propto \int_{-\sqrt{3}/6}^{\sqrt{3}/2} \left(\int_{\eta-\sqrt{3}/2}^{\sqrt{3}/2-\eta} \frac{d\xi}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + z^2}} \right) d\eta$$

MATHEMATICA® 's syntax is to integrate over the last integration iterator first, and the first iterator last; i.e., the expression:
`Integrate[1/r[x,y,z], {x,a,b}, {y,f[x],g[x]}, {z,p[x,y],q[x,y]}]`
would integrate over z first, y second, and lastly x.

The closed form of the above integral appears to be unknown to MATHEMATICA® . However, the energy can be integrated numerically without difficulty and visualized.