

Oct. 25 2006

## Lecture 14: Integrals along a Path

Reading:

Kreyszig Sections: 10.1, 10.2, 10.3 (pages 420–425, 426–432, 433–439)

### Integrals along a Curve

Consider the type of integral that everyone learns initially:

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


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The equation implies that  $f$  is integrable and

$$dE = f dx = \frac{dE}{dx} dx \quad (14-2)$$

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

$$E(b) - E(a) = \int_a^b dE \quad (14-3)$$

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)  $\vec{x}(t) = (x_1(t), x_2(t), \dots, x_n(t))$ .

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

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

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## 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.<sup>6</sup> 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:

$$\oint dU = \oint \nabla_{\vec{S}} U \cdot d\vec{S} = 0 \quad \oint dS = \oint \nabla_{\vec{S}} S \cdot d\vec{S} = 0 \quad \oint dG = \oint \nabla_{\vec{S}} G \cdot d\vec{S} = 0 \quad (14-5)$$

$$\oint dP = \oint \nabla_{\vec{S}} P \cdot d\vec{S} = 0 \quad \oint dT = \oint \nabla_{\vec{S}} T \cdot d\vec{S} = 0 \quad \oint dV = \oint \nabla_{\vec{S}} V \cdot d\vec{S} = 0 \quad (14-6)$$

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

$$\vec{0} = \nabla \times \vec{F} \quad (14-7)$$

or equivalently,

$$0 = \frac{\partial F_j}{\partial x_i} - \frac{\partial F_i}{\partial x_j} \quad (14-8)$$

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.

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<sup>6</sup>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.

## Lecture 14 MATHEMATICA® Example 1

### Path Dependence of Integration of Vector Function: Non-Conservative Example

Download notebooks, pdfs, or html from <http://pruffle.mit.edu/3.016-2006>.

The path dependence of a vector field with a non-vanishing curl ( $\vec{v}(\vec{x}) = xyz(\hat{i} + \hat{k} + \hat{z})$ ) is demonstrated with a family of closed curves.

- 1: *VectorFunction* ( $xyz, xyz, xyz$ ) is an example vector field that has a *non-vanishing curl*. The curl is computed with *Curl* which is in the *Calculus'VectorAnalysis'* package. Here, the particular coordinate system is specified with *Cartesian* argument to *Curl*.
- 2: The curl vanishes only at the origin—this is shown with *FindInstance* called with a list of equations corresponding to the vanishing curl.
- 3: This is the integrand  $\vec{v} \cdot d\vec{s}$  computed as indicated in the figure.  $P(\theta)$  represents any periodic function, but  $(x, y) = R(\cos \theta, \sin \theta)$  representing paths that wrap around cylinders.
- 4: *PathDepInt* is an integral for  $\vec{v}$  represented by *VectorFunction* an arbitrary path wrapping around the cylinder.
- 5: This is the second example of a computation by using a replacement for a periodic  $P(\theta)$  (i.e., each of the  $P(\theta)$  begin and end at the same point, but the path between differs). That the two results differ shows that  $\vec{v}$  is path-dependent—this is a general result for non-vanishing curl vector functions.

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1 << Calculus`VectorAnalysis`;
VectorFunction = {xyz, xyz, xyz}
CurlVectorFunction =
Simplify[Curl[VectorFunction, Cartesian[x, y, z]]]

2 ConditionsOfZeroCurl =
Table[0 == CurlVectorFunction[[i]], {i, 3}]

3 FindInstance[ConditionsOfZeroCurl, {x, y, z}]

For the integral of the vector potential ( $\oint \vec{v} \cdot d\vec{s}$ ) any curve
that wraps around a cylinder of radius R with an axis that
coincides with the z-axis can be parameterized as

(x(t), y(t), z(t)) = (R cos(t), R sin(t), A P_{2,z}(t))
where P_{2,z}(t) = P_{2,z}(t + 2\pi) and P_{2,z}(0) = P_{2,z}(2\pi).
Therefore
ds = (-R sin(t), R cos(t), A P'_{2,z}(t)) dt = (-y(t), x(t), A P'_{2,z}(t)) dt

4 vf =
VectorFunction.(-y, x, Amp D[P[t], t]) /. {x -> Radius Cos[t],
y -> Radius Sin[t], z -> Amp P[t]] // Simplify

5 PathDepInt = Integrate[vf, {t, 0, 2 Pi}]

6 PathDepInt /. P -> Sin

7 PathDepInt /. {P[t] -> t(t - 2 Pi), P'[t] -> D[t(t - 2 Pi), t]}

8 pdigen = PathDepInt /. {P[t] -> CosIn[t], P'[t] -> D[CosIn[t], t]}

9 Simplify[pdigen, n \in Integers]

10 thecurves = ParametricPlot3D[{Cos[t], Sin[t], Cos[3 t]},
{Cos[t], Sin[t], Cos[3 t]}, {t, 0, 2 Pi}]

11 Show[{Graphics3D[Thickness[0.01]],
Graphics3D[Hue[0.25, 0.5, 0.5]], thecurves}]

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## Lecture 14 MATHEMATICA® Example 2

### Examples of Path-Independence of Curl-Free Vector Fields and Curl-Free Subspaces

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A curl-free vector field can be generated from any scalar potential, in this case  $\vec{w} = \nabla e^{xyz} = \vec{w}(\vec{x}) = e^{xyz}(yz\hat{x} + zx\hat{y} + xy\hat{z})$ . To find a function that is curl-free on a restricted subspace (for example, the vector function  $\vec{v}(\vec{x}) = (x^2 + y^2 - R^2)\hat{z}$  vanishes on the surface of a cylinder) one needs to find a  $\vec{m}$  such that  $\nabla \times \vec{m} = \vec{v}$  (for this case

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

is one of an infinite number of such vector functions.)

- 1: To ensure that we will have a zero-curl, a vector field is generated from a gradient of a scalar potential. The curl vanishes because  $\nabla \times \nabla f = 0$ .
- 2: This is a demonstration that the curl does indeed vanish.
- 3: Here is the integrand for  $\oint \vec{v} \cdot d\vec{s}$  for the family of paths that wrap around a cylinder for the particular case of this conservative fields.
- 4: This is the general result for the family of curves indicated by  $P(\theta) \dots$
- 5: This demonstrates that the path integral closes for any periodic  $P(\theta)$ —which is the same as the condition that the curve is closed.
- 8: This demonstrates the method used to find the vector function which has a curl that vanishes on a cylinder.
- 11: This will demonstrate that the integral of the generally non-zero curl vector function is path independent *as long as the path lies on a surface where the curl of the vector function vanishes*.

```
Start with a scalar potential to ensure that we can generate a
curl-free vector field
1 temp = Grad[Exp[x y z], Cartesian[x, y, z]]
2 AnotherVFunction = {e^xyz y z, e^xyz x z, e^xyz x y}
Simplify[Curl[AnotherVFunction, Cartesian[x, y, z]]]
3 anotherv = AnotherVFunction.(-y, x, D[P[t], t])/
  {x → Radius Cos[t], y → Radius Sin[t], z → P[t]} // Simplify
4 PathDepInt = Integrate[anotherv, t]
5 (PathDepInt /. t → 2 Pi) - (PathDepInt /. t → 0)
Now we generate an example of a vector-valued function that is
not curl-free in general, but is path independent in a restricted
subspace where the curl vanishes.
6 VanishOnCylinder = x^2 + y^2 - Radius^2
7 CurlOfOneStooge = {0, 0, VanishOnCylinder}
8 Stooge = (-1/2 Integrate[VanishOnCylinder, y],
  1/2 Integrate[VanishOnCylinder, x], 0)
9 Simplify[Curl[Stooge, Cartesian[x, y, z]]]
10 WhyIOughta = Stooge.(-y, x, D[P[t], t])/
  {x → Radius Cos[t], y → Radius Sin[t]} // Expand
11 Integrate[WhyIOughta, {t, 0, 2 Pi}]
```

## 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	$r(x) = \int_{\alpha(x)}^{\beta(x)} g(\xi, x) d\xi$	$\frac{dr}{dx} = f(\beta(x)) \frac{d\beta}{dx} - f(\alpha(x)) \frac{d\alpha}{dx} + \int_{\alpha(x)}^{\beta(x)} \frac{\partial g(\xi, x)}{\partial x} d\xi$

## Using Jacobians to Change Variables in Thermodynamic Calculations

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.

#### 14-0.0.1 Example of a Multiple Integral: Electrostatic Potential above a Charged Region

This will be an 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 calculation superimposes the charges from each infinitesimal area by integrating a  $1/r$  potential from each point in space to each infinitesimal patch in the 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:

$$dE(x, y, z, \xi, \eta) = \frac{|e|\sigma(\xi, \eta)d\xi d\eta}{\vec{r}(x, y, z, \xi, \eta)} \tag{14-13}$$

for a patch with uniform charge,

$$dE(x, y, z, \xi, \eta) = \frac{|e|\sigma d\xi d\eta}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + z^2}} \tag{14-14}$$

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

$$E(x, y, z) \propto \int_{-\sqrt{3}/6}^{\sqrt{3}/2} \left( \int_{\eta - \sqrt{3}/2}^{\sqrt{3}/2 - \eta} \frac{d\xi}{\sqrt{(x - \xi)^2 + (y - \eta)^2 + z^2}} \right) d\eta \tag{14-15}$$

## Lecture 14 MATHEMATICA® Example 3

### Potential near a Charged and Shaped Surface Patch: Brute Force

Download notebooks, pdfs, or html from <http://pruffle.mit.edu/3.016-2006>.

A example of a multiple integral and its numerical evaluation for the triangular charged patch.

- 2: `Integrate`'s syntax is to integrate over the last integration iterator first, and the first iterator last.
- 3: This will show that the closed form of the above integral appears to be unknown to MATHEMATICA® ...
- 4: However, the energy can be integrated numerically. Here is a function that calls `NIntegrate` for a location given by its arguments.
- 6: This will be a very slow calculation on most computers, but it will show how the potential changes along a line segment of length 2 that runs through the origin at 45°.
- 7: Even slower, `ContourPlot` is used at sequential heights for use as an animation.

