Lecture 14: Integrals along a Path

Reading:
Kreyszig Sections: 10.1, 10.2, 10.3 (pages420–425, 426–432, 433–439)

Integrals along a Curve

Consider the type of integral that everyone learns initially:

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

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

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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.[6] 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.

[6] 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 of Integration of Vector Function: Non-Conservative Example

notebook (non-evaluated) pdf (evaluated) html (evaluated)

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`.

3: The curl vanishes only at the origin—this is shown with `FindInstance` called with a list of equations corresponding to the vanishing curl.

4: 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.

5: *PathDepInt* is an integral for $\vec{v}$ represented by *VectorFunction* an arbitrary path wrapping around the cylinder.

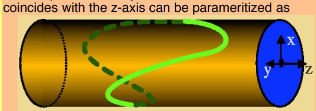
7: This is the second example of a computation by using a replacement for a periodic $P(\theta)$ (i.e., each of the $P(\theta)$ begin and end at the same point, but the path between differs). That the two results differ shows that $\vec{v}$ is path-dependent—this is a general result for non-vanishing curl vector functions.

```
1  << Calculus`VectorAnalysis`
   VectorFunction = {x y z, x y z , y x z}
   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 parameritized as



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

```
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] → Cos[n t], P'[t] → D[Cos[n t], t]}

9  Simplify[pdigen, n ∈ Integers]

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

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

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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 $\vec{w} = \nabla e^{xyz} = \vec{w}(\vec{x}) = e^{xyz}(yz\hat{i} + zx\hat{k} + xy\hat{z})$. To find a function that is curl-free on a restricted subpace (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 $P(\theta)$ . . .

5: This demonstrates that the path integral closes for any perioidic $P(\theta)$—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^(x y z) y z, e^(x y z) x z, e^(x y z) x y}
   Simplify[Curl[AnotherVFunction, Cartesian[x, y, z]]]

3  anothervf = AnotherVFunction.{-y, x, D[P[t], t]} /.
       {x → Radius Cos[t], y → Radius Sin[t], z → P[t]} // Simplify

4  PathDepInt = Integrate[anothervf, 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}]
```

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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:

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

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

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For example, the heat capacity at constant volume is:

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

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

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

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

. 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 infinitessimal area by integrating a $1/r$ potential from each point in space to each infinitessimal 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:

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

for a patch with uniform charge,

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

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

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

Potential near a Charged and Shaped Surface Patch: Brute Force

notebook (non-evaluated) pdf (evaluated) html (evaluated)

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

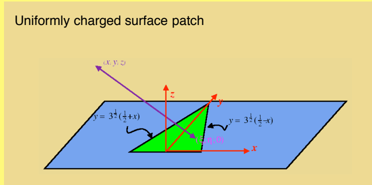
2: `Integrate`'s syntax is to integrate over the last integration iterator first, and the first iterator last.

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.




```
1  Integrate[Exp[3 x], {y, 0, 1}, {x, 0, y}]
   (Integrate[Exp[3 x], {x, 0, y}])
   Integrate[(Integrate[Exp[3 x], {x, 0, y}]), {y, 0, 1}]

2  ntegrate[Exp[3 x], {x, 0, y}, {y, 0, 1}]
   (Integrate[Exp[3 x], {y, 0, 1}])
   Integrate[ (Integrate[Exp[3 x], {y, 0, 1}]) , {x, 0, y}]
```

3 TrianglePotentialDirect = Integrate[$\frac{1}{\sqrt{(x-\xi)^2+(y-\eta)^2+z^2}}$, $\{\eta, 0, \frac{\sqrt{3}}{2}\}, \{\xi, \frac{\eta}{\sqrt{3}} - \frac{1}{2}, \frac{1}{2} - \frac{\eta}{\sqrt{3}}\}$, Assumptions → {x ∈ Reals, y ∈ Reals, z > 0}]

4 TrianglePotentialNumeric[x_, y_, z_] := NIntegrate[$\frac{1}{\sqrt{(x-\xi)^2+(y-\eta)^2+z^2}}$, $\{\eta, 0, \frac{\sqrt{3}}{2}\}, \{\xi, \frac{\eta}{\sqrt{3}} - \frac{1}{2}, \frac{1}{2} - \frac{\eta}{\sqrt{3}}\}$]

```
5  TrianglePotentialNumeric[1, 3, .01]

6  Plot[TrianglePotentialNumeric[x, x, 1/40], {x, -1, 1}]

7  Table[ContourPlot[TrianglePotentialNumeric[x, y, h], {x, -1, 1},
     {y, -0.5, 1.5}, Contours → Table[v, {v, .25, 2, .25}],
     ColorFunction → (Hue[1 - 0.66 * # / 2] &),
     ColorFunctionScaling -> False], {h, .025, .5, .025}]
```

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