Lecture 16: Integral Theorems

Reading:
Kreyszig Sections: 10.8, 10.9 (pages 463–467, 468–473)

Higher-dimensional Integrals

The fundamental theorem of calculus was generalized in a previous lecture from an integral over a single variable to an integration over a region in the plane. Specifically, for generalizing to Green’s theorem in the plane, a vector derivative of a function integrated over a line and evaluated at its endpoints was generalized to a vector derivative of a function integrated over the plane.

Figure 16-15: Illustrating how Green’s theorem in the plane works. If a known vector function is integrated over a region in the plane then that integral should only depend on the bounding curve of that region.
The Divergence Theorem

Suppose there is “stuff” flowing from place to place in three dimensions.
the box’s surface:

\[
\frac{d}{dt}(\text{amount of stuff in box}) = \frac{d}{dt} \int_{\text{box}} \left( \frac{\text{amount of stuff}}{\text{volume}} \right) dV
\]

\[
= \int_{\text{box}} \frac{d}{dt} \left( \frac{\text{amount of stuff}}{\text{volume}} \right) dV
\]

\[
= \int_{\text{box}} \left( \text{some scalar function related to } \vec{J} \right) dV
\]

\[
= \int_{\text{box}} \vec{J} \cdot d\vec{A} \tag{16-1}
\]

Figure 16-18: Integration of a vector function near a point and its relation to the change in that vector function. The rate of change of stuff is the integral of flux over the outside—and in the limit as the box size goes to zero, the rate of change of the amount of stuff is related to the sum of derivatives of the flux components at that point.

To relate the rate at which “stuff \( M \)” is flowing into a small box of volume \( \delta V = dx dy dz \) located at \((x, y, z)\) due to a flux \( \vec{J} \), note that the amount that \( M \) changes in a time \( \Delta t \) is:

\[
\Delta M(\delta V) = (M \text{ flowing out of } \delta V) - (M \text{ flowing in } \delta V)
\]

\[
= \vec{J}(x - \frac{dx}{2}) \hat{y} dy dz - \vec{J}(x + \frac{dx}{2}) \hat{y} dy dz + \vec{J}(y - \frac{dy}{2}) \hat{z} dz dx - \vec{J}(y + \frac{dy}{2}) \hat{z} dz dx + \vec{J}(z - \frac{dz}{2}) \hat{k} k dx dy - \vec{J}(z + \frac{dz}{2}) \hat{k} k dx dy
\]

\[
= -\left( \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right) \delta V \Delta t + O(dx^4) \tag{16-2}
\]

If \( C(x, y, z) = M(\delta V)/\delta V \) is the concentration (i.e., stuff per volume) at \((x, y, z)\), then in the limit of small volumes and short times:

\[
\frac{\partial C}{\partial t} = -\left( \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right) = -\nabla \cdot \vec{J} = -\text{div} \vec{J} \tag{16-3}
\]

For an arbitrary closed volume \( V \) bounded by an oriented surface \( \partial V \):

\[
\frac{dM}{dt} = \frac{d}{dt} \int_V C dV = \int_V \frac{\partial C}{\partial t} dV = -\int_V \nabla \cdot \vec{J} dV = -\int_{\partial V} \vec{J} \cdot d\vec{A} \tag{16-4}
\]
The last equality

\[ \int_V \nabla \cdot \vec{J} dV = \int_{\partial V} \vec{J} \cdot d\vec{A} \quad (16-5) \]

is called the Gauss or the divergence theorem.
London Dispersion Potential due to a Finite Body

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If the London interaction (i.e., energy between two induced dipoles) can be treated as a $1/r^6$ potential, then the potential due to a volume is an integration over each point in the volume and an arbitrary point in space. This calculation will be made much more efficient by turning the volume integral into a surface integral by using the divergence theorem.

1: To find a vector potential, $\vec{F}$ which has a divergence that is equal to $\nabla \cdot \vec{F} = -1/\|\vec{X} - \vec{CX}\|^6$, $PVecLondon$ is a ‘guess.’ The $\vec{CX}$ will vary over the solid body and $\vec{X}$ is an arbitrary point at which the potential is to be determined.

2: We will need $\nabla$ from the VectorAnalysis package.

3: this will show that the guess $PVecLondon$ is a correct vector function for the $1/r^6$ potential.

4: Our calculation will be for a cylinder of radius $R$ and aspect ratio $\lambda \equiv L/R$. We will use $R$ to scale all length variables and introduce dimensionless variables: $x = X/R$, $y = Y/R$, $z = Z/R$, $cx = CX/R$, $cy = CY/R$, and $cz = CZ/R$. The variables are scaled by introducing ScaleRules which are rules to be used in a replacement. Because the potential has a $1/(\text{length}^5)$ length scale, we multiply it by $R^5$ to remove that dimension. We use FullSimplify after the replacement with Assumptions of a positive radius to find the simplest possible form of the non-dimensionlized vector potential.
Cylinder Surface and Integrands

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We parameterize the cylinder surface and compute the local oriented surface area and then find the integrand which is to be used for the cylinder surface.

The following is a parametric representation of a cylinder surface that is coaxial with the z-axis (the cylinder ends will be included later).

CylSurf = \{(Cos[0], Sin[0], cz)\}

The infinitesimal surface vectors \(\vec{p}_c\) and \(\vec{p}_r\) for the cylinder surface are obtained by differentiation; they will be used to find the surface patch dl.

CylSurfNormal = Cross[CylSurf, 0]

The surface normal given by \(\vec{p}_c \times \vec{p}_r\) to the cylinder surface. Here for the following (multiplied by \(dz\)) is the infinitesimal oriented surface patch dl.

NormalVecCylSurf = Cross[CylSurfNormal, CylSurfR]

The integrand to be evaluated over the cylinder surface is the vector potential, dotted into the normal vector. Because of the cylindrical symmetry of the model, we can convert to cylindrical coordinates. One use of coordinates is in the cylindrical patch \(dz\) of the cylinder surface \(dz = dz\), \(\rho = 0\), \(\theta = 0\), \(\rho = 0\), \(\theta = 0\). We must evaluate \(d\vec{F} = A \times d\vec{r}\) in the cylindrical coordinates for which we will be testing the potential \((\rho, \theta, \phi, r, y, z)\). Because the potential must be independent of \(\phi\), we might as well set it to zero.

CylinderIntegrandθϕ = FullSimplify[
  (PwpsS5 / (x = Cos[θ], y = Sin[θ],
  x = ρ, y = ρ), NormalVecCylSurf)]]

We have a choice whether to integrate over \(\rho < r < \sqrt{l^2 - r^2}\) or \(r < \rho < \sqrt{l^2 - r^2}\).

1: This is the cylinder surface in terms of \(cz\) and \(\theta\)
2: These are the differential quantities that define the local tangent plane to the cylindrical surface.
3: This will be the multiplier elemental area for a parameterized cylindrical surface \(d\vec{r} = d\vec{r} \times d\vec{r} / dz\), this is the local normal to the surface; here it is the unit normal because we have scaled all length quantities by \(R\)
4: \(CylinderIntegrand\theta\phi\) is the integrand (i.e., the vector potential evaluated on the parameterized cylinder surface) for the cylindrical surface. Because of the cylindrical symmetry of the potential, the potential must be depend only on the normalized distance from the cylinder axis, \(\rho\), and the height above the mid-plane, \(z\): this conversion to cylindrical coordinates is effected by a rule-replacement operation.
Lecture 16 \textsc{Mathematica®} Example 3

Integrating over the Cylinder Surface

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We have a choice whether to integrate over $\theta \in (0, 2\pi)$ or over $z \in -\lambda/2, \lambda/2$ first. We calculate the integral over $cz$ first which will leave a form that we can numerically integrate over $\theta$. (Note: As of 23 Oct. 2007, I’ve determined that it is possible to find the definite integral over $\theta$ and then over $cz$; therefore, this integral does have a closed form solution. For purposes of this demonstration, we will leave the integral over $\theta$ to be computed by a numerical integration. To demonstrate the idea of reducing the triple numerical integration, over a single numerical integration, I’ll have to find a more complicated surface to integrate over in the future.)

1: Because of the mirror symmetry of the function about the $z = 0$ plane, we can restrict the integral to $z > 0$ and use this as an assumption to aid the definite integral over $cz$. (Note this is a time-consuming integral and simplification, in the notebook form distributed with these notes, there is a dialogue that allows the user to download a precomputed result.)

2: To determine whether we can use this integrand at the mid-plane ($z = 0$), we check to see if the limit as $z \to 0$ is the same as evaluating the integrand at $z = 0$ first, and then finding the integral that applies for $z = 0$. Here, we check the limit.

3: Here, we set $z = 0$ and integrate.

4: The limit and the case of $z = 0$ are the same, so we use the form of the integrand, $CylinderIntegrandUpperZ\theta$, calculated above. We turn the expression into a function by using \texttt{Evaluate} after the rule-replacement. This method of subverting the delayed evaluation, (:=), will work so long as the function’s variables have not been assigned. These methods will be discussed in a section below. In practice, it is probably safer to replace variables with temporary, undefined, symbols and then cut-and-paste. (It is difficult to demonstrate the cut-and-paste with static notes like these.)

5: The function defined above, $CylinderIntegrand\theta$, is used as the argument to the numerical integration, \texttt{NIntegrate}, over $\theta \in (0, 2\pi)$. The produces a function, $CylinderContribution$, that gives the contribution by integrating over the cylinder surface.
Lecture 16 Mathematica® Example 4

Integrating over the Cylinder’s Top Surface


We parameterize the cylinder’s top end-cap in terms of \( r \) (dimensionless \( r < 1 \)) and \( \theta \), and then find a closed-form solution for the double integral over the top surface.

\[
\text{TopSurf} = \{r \cos(\theta), r \sin(\theta), z/2\}
\]

\[
\text{TopSurfRr} = \frac{\partial}{\partial r}\text{TopSurf}, \; r
\]

\[
\text{NormalVecTopSurf} = \text{Cross}[\text{TopSurfRr}, \text{TopSurfRq}]
\]

\[
\text{TopIntegrand} = \text{FullSimplify}[\text{Cross[TopSurfRr, TopSurfRq]}]
\]

\[
\text{Integrate}\left[\text{TopIntegrand}, (0, 0, 2\pi), \text{Assumptions}\rightarrow\{0 < r < 1, \lambda > 0, \rho < 1, x > \lambda/2\}\right]
\]

\[
\text{TopPart} = \text{Integrate}[\text{TopIntegrand}, (r, 0, 1), \text{Assumptions}\rightarrow\{0 < r < 1, \lambda > 0, \rho < 1, x > \lambda/2\}]
\]

\[
\text{TopContribution} = \text{Evaluate}\left[\text{TopPart}/.\quad (z\rightarrow\text{dist}, \; \text{height} \rightarrow \text{AspectRat})\right]
\]

\(1\)–4: As in the case for the cylinder’s curved surface, the top surface is parameterized, then the local tangent is computed, and the local oriented surface differential element is computed. The integrand is produced with the inner-product with the vector potential evaluated at the cylinder’s top.

\(5\)–6: There is a singularity at the cylinder surface that produces a little extra work on our part to ensure that we don’t evaluate at this singularity. To get a closed form of the integral over \( \theta \), it is useful to divide space into four regions where the potential is to be measured: 1) Inside the cylinder radius and above the cylinder top; 2) Inside the cylinder radius and below the cylinder top; 3) Outside the cylinder radius and above the cylinder top; 4) Outside the cylinder radius and below the cylinder top. These give the same result, so long as we don’t evaluate at the cylinder’s surface.

\(7\): The top integrand in \( r \) can be integrated for \( r \in (0, 1) \) and produces a closed form.

\(8\): A function for the contribution of the upper disk, \( \text{TopContribution} \), is defined.
Integrating over the Cylinder’s Bottom Surface

We parameterize the cylinder’s bottom end-cap \((cz = -\lambda/2)\) in terms of \(r\) (dimensionless \(r < 1\)) and \(\theta\), and then find a closed-form solution for the double integral over the bottom surface.

1–4: As above for the cylinder’s outside and for its top surface, the bottom disk is parameterized, then the local tangent is computed, and the local oriented surface differential element is computed. The integrand is produced with the inner-product with the vector potential evaluated at the cylinder’s bottom.

5–6: Similar to our method of avoiding the singularity at the top surface To get a closed form of the bottom-disk integral over \(\theta\), space is divided into two regions where the potential is to be measured: 1) Inside the cylinder; 2) Outside the cylinder. These give the same result.

7: The bottom integrand in \(r\) can be integrated for \(r \in (0, 1)\) and produces a closed form.

8: A function for the contribution of the bottom disk, \(BotContribution\), is defined.

9: We can produce a function to compute the potential at any point in space by summing the contributions from all three cylinder surfaces. The first function is the most expensive because it contains a numerical integration over \(\theta\).

Efficiency and Speed Issues: When to Evaluate the Right-Hand-Side of a Function in Mathematica®.

The standard practice is to define functions in Mathematica with \(\texttt{:=}\). However, sometimes it makes sense to evaluate the right-hand-side when the function definition is made. These are the cases where the right hand side would take a long time to evaluate—each time the function is called, the evaluation would be needed again and again. The following example illustrates a case where it makes sense to use \texttt{Evaluate} in a function definition (or, equivalently defining the function with immediate assignment \(\texttt{=}\)).

As in the use of \(\texttt{=}\), this can result in errors if the function’s variables have been defined previously. In cases where it is desirable to create a function from an expression, it is probably safest to use rule-
replacement with undefined variables, observe the result, and then use cut-and-paste to define a function with a delayed evaluation in terms of these demonstrably undefined variables.

Lecture 16  MATHEMATICA® Example 6
To Evaluate or Not to Evaluate when Defining Functions

This example illustrates a case in which immediate evaluation = would be preferable to delayed evaluation :=

1: When a non-trivial integral is done for the first time, Mathematica loads various libraries. Notice the difference in timing between this first computation of \( \int \exp[\tan(x)]dx \) and the following one.

2: The second evaluation is faster. Now, a baseline time has been established for evaluating this integral symbolically.

3: Here, to make a function definition for the integral, the symbolic integral is obtained and so the function definition takes longer than it would if we had not used Evaluate.

4: Using an := is roughly equivalent to using Evaluate above and the time to make the function assignment should be approximately the same.

5: Here, the symbolic integration is delayed until the function is called (later). Therefore, the function assignment is very rapid.

6: We can use the ?-operator to investigate the stored forms of the three function definitions. The first two forms are roughly equivalent, except for the delayed versus immediate function definition. The third form uses the unevaluated integral in the definition. symbolic information.

7: The function evaluation is much faster in the case where the symbolic integration is not needed. This would be the preferred form if the function were to be called many times.

8: The relatively slow speed of the function which contains the unevaluated integral indicates that it would be a poor choice when numerical efficiency is an issue. Therefore, if we were to use ContourPlot, or some other function that would need to compute the result at many different points, then the integration would be done at each point, instead of having its closed form evaluated. Thus, the function with the embedded closed form is preferable.
We use the function that we have defined above as the argument to ContourPlot. Because the function is singular at the cylinder surface, we choose to plot the logarithm of the potential instead. Because the potential is negative outside of the cylinder, we must use an absolute value before taking the log. To remind ourselves of this fact, we use the function that we have defined above as the argument to ContourPlot. We use blue tones, LakeColors, to indicate the positive potential values.

1: We define a short-hand function to wrap around the potential function so that the log(|P|) is computed.

2–3: To get an idea of what the function looks like, we plot the potential first along the cylinder axis, and then for a distance within the mid-plane.

4: We break the contour-plots into an inner and an outer graphic. Here we use ContourPlot to plot (minus) the logarithm of the potential outside the cylinder. RegionFunction is used to to limit the region over which the plot is computed and displayed. Furthermore, the numerical integration is ill-behaved along lines that continue from the cylinder’s corner; we use Exclusions to avoid these regions. We use a green tone, AvocadoColors, to indicate the negative values.

5: Here, we produce the contour-plot for the region inside the cylinder. Again, we use the RegionFunction-option of ContourPlot. We use blue tones, LakeColors, to indicate the positive potential values.

6: We combine the inner and outer regions into a single plot by using Show.
We produce an equivalent visualization with *Plot3D*. From the form of these plots, it is clear that a non-polar molecule would be attracted to the cylinder, with a force that becomes unbounded in the vicinity of the cylinder. The barrier to cross into the cylinder is infinite at the cylinder surface. However, within a cylinder there is a force that pushes a foreign particle to the center of the cylinder. The Hamaker force would tend to push pores towards the middle of a dielectric cylinder.

Stokes’ Theorem

The final generalization of the fundamental theorem of calculus is the relation between a vector function integrated over an oriented surface and another vector function integrated over the closed curve that bounds the surface.

A simplified version of Stokes’s theorem has already been discussed—Green’s theorem in the plane.
can be written in full vector form:

\[
\int \int_R \left( \frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} \right) \ dxdy = \int \nabla \times \vec{F} \cdot d\vec{A}
\]

\[
= \oint_{\partial R} (F_1 dx + F_2 dy) = \oint_{\partial R} \vec{F} \cdot d\vec{r}
\]  

(16-6)

as long as the region \( R \) lies entirely in the \( z = \text{constant} \) plane.

In fact, Stokes’s theorem is the same as the full vector form in Eq. 16-6 with \( R \) generalized to an oriented surface embedded in three-dimensional space:

\[
\int \int_R \nabla \times \vec{F} \cdot d\vec{A} = \oint_{\partial R} \vec{F} \cdot d\vec{r}
\]  

(16-7)

Plausibility for the theorem can be obtained from Figures 16-15 and 16-16. The curl of the vector field summed over a surface “spills out” from the surface by an amount equal to the vector field itself integrated over the boundary of the surface. In other words, if a vector field can be specified everywhere for a \( \text{fixed} \) surface, then its integral should only depend on some vector function integrated over the boundary of the surface.

**Maxwell’s equations**

The divergence theorem and Stokes’s theorem are generalizations of integration that invoke the divergence and curl operations on vectors. A familiar vector field is the electromagnetic field and Maxwell’s equations depend on these vector derivatives as well:

\[
\begin{align*}
\nabla \cdot \vec{B} &= 0 \\
\nabla \times \vec{E} &= \frac{\partial \vec{B}}{\partial t} \\
\n\nabla \times \vec{H} &= \frac{\partial \vec{D}}{\partial t} + \vec{j} \\
\n\nabla \cdot \vec{D} &= \rho 
\end{align*}
\]  

(16-8)

in MKS units and the total electric displacement \( \vec{D} \) is related to the total polarization \( \vec{P} \) and the electric field \( \vec{E} \) through:

\[
\vec{D} = \vec{P} + \epsilon_o \vec{E}
\]  

(16-9)

where \( \epsilon_o \) is the dielectric permittivity of vacuum. The total magnetic induction \( \vec{B} \) is related to the induced magnetic field \( \vec{H} \) and the material magnetization through

\[
\vec{B} = \mu_o (\vec{H} + \vec{M})
\]  

(16-10)

where \( \mu_o \) is the magnetic permeability of vacuum.

**Ampere’s Law**

Ampere’s law that relates the magnetic field lines that surround a static current is a macroscopic version of the (static) Maxwell equation \( \nabla \times \vec{H} = \vec{j} \):
Gauss’ Law

Gauss’ law relates the electric field lines that exit a closed surface to the total charge contained within the volume bounded by the surface. Gauss’ law is a macroscopic version of the Maxwell equation \( \nabla \cdot \vec{D} = \rho \):