Oct. 21 2005:   Lecture 15:

Surface Integrals and Some Related Theorems

Reading:
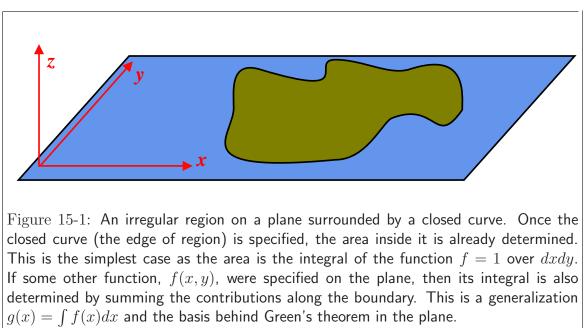Kreyszig Sections: §9.4 (pp:485–90) ,   §9.5 (pp:491–495)   §9.6 (pp:496–505)   §9.7 (pp:505–09)

Green's Theorem for Area in Plane Relating to its Bounding Curve

Reappraise the simplest integration operation, $g(x) = \int f(x)dx$. Temporarily ignore all the tedious mechanical rules of finding and integral and concentrate on what integration *does*.
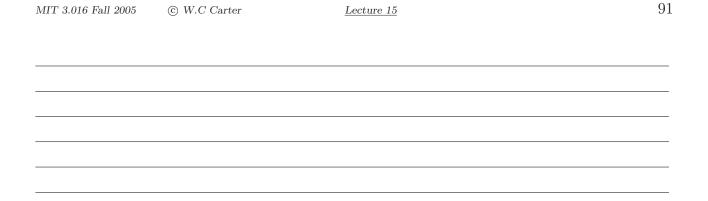
Integration replaces a fairly complex process—adding up all the contributions of a function $f(x)$—with a clever new function $g(x)$ that only needs end-points to return the result of a complicated summation.

It is perhaps initially astonishing that this complex operation on the interior of the integration domain can be incorporated merely by the domain's endpoints. However, careful reflection provides a counterpoint to this marvel. How could it be otherwise? The function $f(x)$ is specified and there are no surprises lurking along the x-axis that will trip up dx as it marches merrily along between the endpoints. All the facts are laid out and they willingly submit to the process their preordination by $g(x)$ by virtue of the endpoints.[6]

The idea naturally translates to higher dimensional integrals and these are the basis for Green's theorem in the plane, Stoke's theorem, and Gauss (divergence) theorem. Here is the idea:
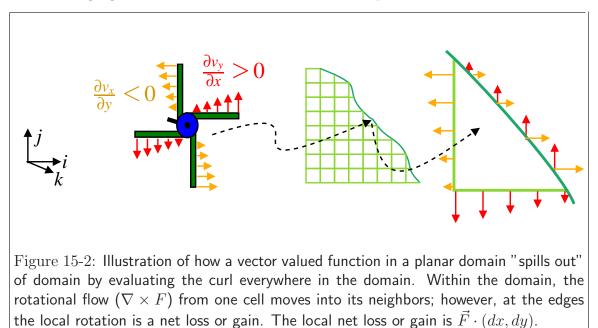

Figure 15-1: An irregular region on a plane surrounded by a closed curve. Once the closed curve (the edge of region) is specified, the area inside it is already determined. This is the simplest case as the area is the integral of the function $f = 1$ over $dxdy$. If some other function, $f(x, y)$, were specified on the plane, then its integral is also determined by summing the contributions along the boundary. This is a generalization $g(x) = \int f(x)dx$ and the basis behind Green's theorem in the plane.

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[6]I do hope you are amused by the evangelistic tone. I am a bit punchy from working non-stop on these lectures and wondering if anyone is really reading these notes. Sigh.

The analog of the "*Fundamental Theorem of Differential and Integral Calculus*"[7] for a region $\mathcal{R}$ bounded in a plane with normal $\hat{k}$ that is bounded by a curve $\partial\mathcal{R}$ is:

$$\int\int_{\mathcal{R}} (\nabla \times \vec{F}) \cdot \hat{k} dx dy = \oint_{\partial\mathcal{R}} \vec{F} \cdot d\vec{r} \tag{15-1}$$

The following figure motivates Green's theorem in the plane:

Figure 15-2: Illustration of how a vector valued function in a planar domain "spills out" of domain by evaluating the curl everywhere in the domain. Within the domain, the rotational flow $(\nabla \times F)$ from one cell moves into its neighbors; however, at the edges the local rotation is a net loss or gain. The local net loss or gain is $\vec{F} \cdot (dx, dy)$.

The generalization of this idea to a surface $\partial\mathcal{B}$ bounding a domain $\mathcal{B}$ results in Stokes' theorem, which will be discussed later.

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[7]This is the theorem that implies the integral of a derivative of a function is the function itself (up to a constant).

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Turing an integral over a domain into an integral over its boundary

Using Green's theorem in the plane to simplify the integration to find the potential above a triangular path that was evaluated in the last lecture.

Here we turn the two dimensional numerical integration which requires $\mathcal{O}(N^2)$ calculations into an integration around the boundary which requires $\mathcal{O}(N)$ evaluations for the same accuracy.

1. The integral in question is:

$$E(x,y,z) = \int\int_R \frac{d\xi d\eta}{\sqrt{(x-\xi)^2 + (y-\eta)^2 + z^2}}$$

2. Green's theorem in the plane is:

$$\int\int_R \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y}\right) dxdy = \int_{\partial R}(F_1 dx + F_2 dy)$$

3. Find a function $\vec{F} = (F_1, F_2)$ which matches the integral in questions. This can be done by simply setting $F_2 = 0$ and integrating to find F_1

$$F_1 = \int \frac{d\eta}{\sqrt{(x-\xi)^2 + (y-\eta)^2 + z^2}}$$

which not very difficult.

4. It remains to parameterize the three legs of the triangle as paths to integrate over (i.e., use $(x(t), y(t))$ from the three line segments and integrate over $(dx, dy) = (x'dt, y'dt)$.

5. The integral is still to complicated, however the numerical evaluation of this boundary integral is **much more efficient**.

_____ **Representations of Surfaces** _____

Integration over the plane $z = 0$ in the form of $\int f(x,y)dxdy$ introduces surface integration—over a planar surface—as a straightforward extension to integration along a line. Just as integration over a line was generalized to integration over a curve by introducing two or three variables that depend on a *single* variable (e.g., $(x(t), y(t), z(t))$), a surface integral can be conceived as introducing three (or more) variables that depend on two parameters (i.e., $(x(u,v), y(u,v), z(u,v))$).
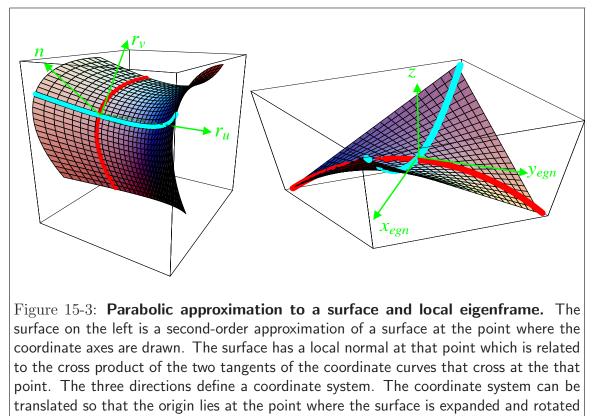
However, there are different ways to formulate representations of surfaces:

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Representations of Surfaces

Three representations in MATHEMATICA®

Surfaces and interfaces play fundamental roles in materials science and engineering. Unfortunately, the mathematics of surfaces and interfaces frequently presents a hurdle to materials scientists and engineering. The concepts in surface analysis can be mastered with a little effort, but there is no escaping the fact that the algebra is tedious and the resulting equations are onerous. Symbolic algebra and numerical analysis of surface alleviates much of the burden.

Most of the practical concepts derive from a second-order Taylor expansion of a surface near a point. The first-order terms define a tangent plane; the tangent plane determines the surface normal. The second-order terms in the Taylor expansion form a matrix and a quadratic form that can be used to formulate an expression for curvature. The eigenvalues of the second-order matrix are of fundamental importance.

The Taylor expansion about a particular point on the surface takes a particularly simple form if the origin of the coordinate system is located at the point and the z-axis is taken along the surface normal as illustrated in the following figure.

Figure 15-3: **Parabolic approximation to a surface and local eigenframe.** The surface on the left is a second-order approximation of a surface at the point where the coordinate axes are drawn. The surface has a local normal at that point which is related to the cross product of the two tangents of the coordinate curves that cross at the that point. The three directions define a coordinate system. The coordinate system can be translated so that the origin lies at the point where the surface is expanded and rotated so that the normal $\hat{n}$ coincides with the z-axis as in the right hand curve.

In this coordinate system, the Taylor expansion of $z = f(x, y)$ must be of the form

$$\Delta z = 0dx + 0dy + \frac{1}{2}(dx, dy) \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x^2} \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix}$$

If this coordinate system is rotated about the z-axis into its eigenframe where the off-diagonal components vanish, then the two eigenvalues represent the maximum and minimum curvatures. The sum of the eigenvalues is invariant to transformations and the sum is known as the *mean curvature* of the surface. The product of the eigenvalues is also invariant—this quantity is known as the *Gaussian curvature*.

The method in the figure suggests a method to calculate the normals and curvatures for a surface. Those results are tabulated below.

Level Set Surfaces: Tangent Plane, Surface Normal, and Curvature

$$F(x, y, z) = \text{const}$$

Tangent Plane $(\vec{x} = (x, y, z), \vec{\xi} = (\xi, \eta, \zeta))$

$$\nabla F \cdot (\vec{\xi} - \vec{x}) \text{ or } \frac{\partial F}{\partial x}(\xi - x) + \frac{\partial F}{\partial y}(\eta - y) + \frac{\partial F}{\partial z}(\zeta - z)$$

Normal

$$\frac{\xi - x}{\frac{\partial F}{\partial x}} = \frac{\eta - y}{\frac{\partial F}{\partial y}} = \frac{\zeta - z}{\frac{\partial F}{\partial z}}$$

Mean Curvature

$$\nabla \cdot \left(\frac{\nabla F}{\|\nabla F\|} \right) \text{ or}$$

$$\frac{\left[\begin{array}{c} \left(\frac{\partial^2 F}{\partial y^2} + \frac{\partial^2 F}{\partial z^2} \right)\left(\frac{\partial F}{\partial x}\right)^2 + \left(\frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial x^2} \right)\left(\frac{\partial F}{\partial y}\right)^2 + \left(\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} \right)\left(\frac{\partial F}{\partial z}\right)^2 \\ -2 \left(\frac{\partial F}{\partial x}\frac{\partial F}{\partial y}\frac{\partial^2 F}{\partial x \partial y} + \frac{\partial F}{\partial y}\frac{\partial F}{\partial z}\frac{\partial^2 F}{\partial y \partial z} + \frac{\partial F}{\partial z}\frac{\partial F}{\partial x}\frac{\partial^2 F}{\partial z \partial x} \right) \end{array} \right]}{{\frac{\partial F}{\partial x}}^2 + {\frac{\partial F}{\partial y}}^2 + {\frac{\partial F}{\partial z}}^{2}{}^{3/2}}$$

Parametric Surfaces: Tangent Plane, Surface Normal, and Curvature

$$\vec{x} = (p(u, v), q(u, v), s(u, v)) \text{ or } x = p(u, v) y = q(u, v) z = s(u, v)$$

Tangent Plane $(\vec{x} = (x, y, z), \vec{\xi} = (\xi, \eta, \zeta))$

$$(\vec{\xi} - \vec{x}) \cdot \left(\frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \right) \det \begin{pmatrix} \xi - x & \eta - y & \zeta - z \\ \frac{\partial p}{\partial u} & \frac{\partial q}{\partial u} & \frac{\partial s}{\partial u} \\ \frac{\partial p}{\partial v} & \frac{\partial q}{\partial v} & \frac{\partial s}{\partial v} \end{pmatrix} = 0$$

Normal

$$\frac{\xi - x}{\frac{\partial(q,s)}{\partial(u,v)}} = \frac{\eta - y}{\frac{\partial(s,p)}{\partial(u,v)}} = \frac{\zeta - z}{\frac{\partial(p,q)}{\partial(u,v)}}$$

Mean Curvature

$$\frac{\left(\frac{d\vec{x}}{du} \cdot \frac{d\vec{x}}{du} \right)\left(\frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \cdot \frac{d^2\vec{x}}{dv^2} \right) - 2\left(\frac{d\vec{x}}{du} \cdot \frac{d\vec{x}}{dv} \right)\left(\frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \cdot \frac{d^2\vec{x}}{dudv} \right) + \left(\frac{d\vec{x}}{dv} \cdot \frac{d\vec{x}}{dv} \right)\left(\frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \cdot \frac{d^2\vec{x}}{du^2} \right)}{\left(\frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \cdot \frac{d\vec{x}}{du} \times \frac{d\vec{x}}{dv} \right)^{3/2}}$$

Graph Surfaces: Tangent Plane, Surface Normal, and Curvature

$$z = f(x, y)$$

Tangent Plane $(\vec{x} = (x, y, z), \vec{\xi} = (\xi, \eta, \zeta))$

$$\frac{\partial f}{\partial x}(\xi - x) + \frac{\partial f}{\partial y}(\eta - y) = (\zeta - z)$$

Normal

$$\frac{\xi - x}{\frac{\partial f}{\partial x}} = \frac{\eta - y}{\frac{\partial f}{\partial y}} = \frac{\zeta - z}{-1}$$

Mean Curvature

$$\frac{(1 + \frac{\partial f}{\partial x}^2)\frac{\partial^2 f}{\partial y^2} - 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\frac{\partial^2 f}{\partial x \partial y} + (1 + \frac{\partial f}{\partial y}^2)\frac{\partial^2 f}{\partial x^2}}{\sqrt{1 + \frac{\partial f}{\partial x}^2 + \frac{\partial f}{\partial y}^2}}$$

_____ Integration over Surfaces _____

Integration of a function over a surface is a straightforward generalization of $\int \int f(x, y) dx dy = \int f(x, y) dA$. The set of all little rectangles $dxdy$ defines a planar surface. A non-planar surface $\vec{x}(u, v)$ is composed of a set of little parallelogram patches with sides given by the infinitesimal vectors

$$\begin{aligned} \vec{r_u} du &= \frac{\partial \vec{x}}{\partial u} du \\ \vec{r_v} du &= \frac{\partial \vec{x}}{\partial v} dv \end{aligned} \tag{15-2}$$

Because the two vectors $\vec{r_u}$ and $\vec{r_v}$ are not necessarily perpendicular, their cross-product is needed to determine the magnitude of the area in the parallelogram:

$$dA = \|\vec{r_u} \times \vec{r_v}\| du dv \tag{15-3}$$

and the integral of some scalar function, $g(u, v) = g(x(u, v), y(u, v)) = g(\vec{x}(u, v))$, on the surface is

$$\int g(u, v) dA = \int \int g(u, v) \|\vec{r_u} \times \vec{r_v}\| du dv \tag{15-4}$$

However, the operation of taking the norm in the definition of the surface patch dA indicates that some information is getting lost—this is the local normal orientation of the surface. There are two choices for a normal (inward or outward).

When calculating some quantity that does not have vector nature, only the magnitude of the function over the area matters (as in Eq. 15-4). However, when calculating a vector quantity, such as the flow through a surface, or the total force applied to a surface, the surface orientation matters and it makes sense to consider the surface patch as a vector quantity:

$$\begin{aligned} \vec{A}(u, v) &= \|\vec{A}\|\hat{n}(u, v) = A\hat{n}(u, v) \\ d\vec{A} &= \vec{r_u} \times \vec{r_v} \end{aligned} \tag{15-5}$$

where $\hat{n}(u,v)$ is the local surface unit normal at $\vec{x}(u,v)$.

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Integrals of Anisotropic Surface Energy

The surface energy of single crystals often depends on the surface orientation. This is especially the case for materials that have covalent and/or ionic bonds.

To find the total surface energy of such a single crystal, one has to integrate an *orientation-dependent* surface energy over the surface of a body.

This example compares the total energy of such an anisotropic surface energy integrated over a sphere and a cube that enclose the same volume.

1. Enter the parametric equation of the sphere in terms of longitude $v \in (0, 2\pi)$ and latitude $u \in (-\pi/2, \pi/2)$.

2. Calculate the tangent plane vectors $\vec{r_u}$ and $\vec{r_v}$

3. Calculate their cross product for subsequent use in the surface integral:

$$\int \int g(\hat{n}(u,v)) \| \vec{r_u} \times \vec{r_v} \| du dv$$

4. Use the vectors to calculate the local unit normal.

5. Integrate a model function:

$$\gamma_{anis}(\hat{n}) = 1 + \gamma_{111} n_1^2 n_2^2 n_3^3$$

over a sphere

6. Compare this result to the integration over a cube with the same volume.

The above calculation compares two fixed shapes—to find the surface which has the least energy for enclosing a given volume, one would employ a construction known as the *Wulff Theorem.*