

Oct. 14 2005: **Lecture 12:**

Multivariable Calculus

Reading:

Kreyszig Sections: §8.5 (pp:428–33) , §8.8 (pp:444–446) §8.9 (pp:446–452)

The Calculus of Curves

In the last lecture, the derivatives of a vector that varied continuously with a parameter, $\vec{r}(t)$, were considered. It is natural to think of $\vec{r}(t)$ as a curve in whatever space the vector \vec{r} is defined. In this way, a curve is represented by N coordinates as a *single* value takes on a range of numbers.

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Curves, Tangents, Surfaces

Visualizing a curve

Because the derivative of a curve with respect to its parameter is a tangent vector, the unit tangent can be defined immediately:

$$\hat{u} = \frac{\frac{d\vec{r}}{dt}}{\left\| \frac{d\vec{r}}{dt} \right\|} \quad (12-1)$$

It is convenient to find a new parameter, $s(t)$, that would make the denominator in Eq. 12-1 equal to one. This parameter, $s(t)$, is the arc-length:

$$\begin{aligned} s(t) &= \int_{t_o}^t ds \\ &= \int_{t_o}^t \sqrt{dx^2 + dy^2 + dz^2} \\ &= \int_{t_o}^t \sqrt{\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2 + \left(\frac{dz}{dt}\right)^2} dt \\ &= \int_{t_o}^t \sqrt{\left(\frac{d\vec{r}}{dt}\right) \cdot \left(\frac{d\vec{r}}{dt}\right)} dt \end{aligned} \quad (12-2)$$

and with s instead of t ,

$$\hat{u}(s) = \frac{d\vec{r}}{ds} \quad (12-3)$$

This is natural because $\|\vec{r}\|$ and s have the same units (i.e., meters and meters, fots and feet, etc) instead of, for instance, time, t , that makes $d\vec{r}/dt$ a velocity and involving two different kinds of units (e.g., furlongs and hours).

With the arc-length s , the magnitude of the curvature is particularly simple,

$$\kappa(s) = \left\| \frac{d\hat{u}}{ds} \right\| = \left\| \frac{d^2\vec{r}}{ds^2} \right\| \quad (12-4)$$

as is its interpretation—the curvature is a measure of how rapidly the unit tangent is changing direction.

Furthermore, the rate at which the unit tangent changes direction is a vector that must be normal to the tangent (because $d(\hat{u} \cdot \hat{u} = 1) = 0$) and therefore the unit normal is defined by:

$$\hat{p}(s) = \frac{1}{\kappa(s)} \frac{d\hat{u}}{ds} \quad (12-5)$$

There two unit vectors that are locally normal to the unit tangent vector $\hat{u}'(s)$ and the curve unit normal $\hat{p}(s) \times \hat{u}$ and $\hat{u}(s) \times \hat{p}$. This last choice is called the unit binormal, $\hat{b} \equiv \hat{u}(s) \times \hat{p}$ and the three vectors together form a nice little moving orthogonal axis pinned to the curve. Furthermore, there are convenient relations between the vectors and differential geometric quantities called the Frenet equations.

☹ *Using Arc-Length as a Curve's Parameter*

However, it should be pointed out that—although re-parameterizing a curve in terms of its arc-length makes for simple analysis of a curve—achieving this re-parameterization is not necessarily simple.

Consider the steps required to represent a curve $\vec{r}(t)$ in terms of its arc-length:

integration The integral in Eq. 12-2 may or may not have a closed form for $s(t)$.

If it does then we can perform the following operation:

inversion $s(t)$ is typically a complicated function that is not easy to invert, i.e., solve for t in terms of s to get a $t(s)$ that can be substituted into $\vec{r}(t(s)) = \vec{r}(s)$.

These difficulties usually result in treating the problem symbolically and the resorting to numerical methods of achieving the integration and inversion steps.

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Calculating arclength

Finding arc-length s of a curve and using as parameter

Scalar Functions with Vector Argument

In materials science and engineering, the concept of a spatially varying function arises frequently:

For example:

Concentration $c_i(x, y, z) = c_i(\vec{x})$ is the number (or moles) of chemical species of type i *per unit volume* located at the point \vec{x} .

Density $\rho(x, y, z) = \rho(\vec{x})$ mass *per unit volume* located at the point \vec{x} . a point $\rho(x, y, z) = \rho(\vec{x})$.

Energy Density $u(x, y, z) = u(\vec{x})$ energy *per unit volume* located at the point \vec{x} .

The examples above are spatially dependent densities of “extensive quantities.”

There are also spatially variable intensive quantities:

Temperature $T(x, y, z) = T(\vec{x})$ is the temperature which would be measured at the point \vec{x} .

Pressure $P(x, y, z) = P(\vec{x})$ is the pressure which would be measured at the point \vec{x} .

Chemical Potential $\mu_i(x, y, z) = \mu_i(\vec{x})$ is the chemical potential of the species i which would be measured at the point \vec{x} .

Each example is a scalar function of space—that is, the function associates a scalar with each point in space.

A topographical map is a familiar example of a graphical illustration of a scalar function (altitude) as a function of location (latitude and longitude).

☹ How Confusion Can Develop in Thermodynamics

However, there are many other types of scalar functions of several arguments, such as the state function: $U = U(S, V, N_i)$ or $P = P(V, T, N_i)$. It is sometimes useful to think of these types of functions a scalar functions of a “point” in a thermodynamics space.

However, this is often a source of confusion: notice that the internal energy is used in two different contexts above. One context is the value of the energy, say 128.2 Joules. The other context is the function $U(S, V, N_i)$. While the two symbols are identical, their meanings are quite different.

The root of the confusion lurks in the question, “What are the variables of U ?” Suppose that there is only one (independent) chemical species, then $U(\cdot)$ has three variables, such as $U(S, V, N)$. “But what if $S(T, P, \mu)$, $V(T, P, \mu)$, and $N(T, P, \mu)$ are known functions, what are the variables of U ?” The answer is, they are any three independent variables, one could write $U(T, P, \mu) = U(S(T, P, \mu), V(T, P, \mu), N(T, P, \mu))$ and there are six other natural choices.

The trouble arises when variations of a function like U are queried—then the variables that are varying must be specified.

For this reason, it is either a good idea to keep the functional form explicit in thermodynamics, i.e.,

$$\begin{aligned} dU(S, V, N) &= \frac{\partial U(S, V, N)}{\partial S} dS + \frac{\partial U(S, V, N)}{\partial V} dV + \frac{\partial U(S, V, N)}{\partial N} dN \\ dU(T, P, \mu) &= \frac{\partial U(T, P, \mu)}{\partial T} dT + \frac{\partial U(T, P, \mu)}{\partial P} dP + \frac{\partial U(T, P, \mu)}{\partial \mu} d\mu \end{aligned} \quad (12-6)$$

or use, the common thermodynamic notation,

$$\begin{aligned} dU &= \left(\frac{\partial U}{\partial S} \right)_{V, N} dS + \left(\frac{\partial U}{\partial V} \right)_{S, N} dV + \left(\frac{\partial U}{\partial N} \right)_{S, V} dN \\ dU &= \left(\frac{\partial U}{\partial T} \right)_{P, \mu} dT + \left(\frac{\partial U}{\partial P} \right)_{T, \mu} dP + \left(\frac{\partial U}{\partial \mu} \right)_{T, P} d\mu \end{aligned} \quad (12-7)$$

Total and Partial Derivatives, Chain Rule

There is no doubt that a great deal of confusion arises from the following question, “What are the variables of my function?”

For example, suppose we have a three-dimensional space (x, y, z) , in which there is an embedded surface $(x(w, v), y(w, v), z(w, v))$ $\vec{x}(w, v) = \vec{x}(\vec{u})$ where $\vec{u} = (v, w)$ is a vector that lies in the surface, and an embedded curve $(x(s), y(s), z(s)) = \vec{x}(s)$. Furthermore, suppose there is a curve that lies within the surface $(w(t), v(t)) = \vec{u}(t)$.

Suppose that $\mathcal{E} = f(x, y, z)$ is a scalar function of (x, y, z) .

Here are some questions that arise in different applications:

1. How does \mathcal{E} vary as a function of position?
2. How does \mathcal{E} vary along the surface?
3. How does \mathcal{E} vary along the curve?
4. How does \mathcal{E} vary along the curve embedded in the surface?

uous first and second partial derivatives near the point $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_n)$ is:

$$\begin{aligned}
 f(\xi_1, \xi_2, \dots, \xi_n) &= f(x_1, x_2, \dots, x_n) \\
 &+ \left. \frac{\partial f}{\partial x_1} \right|_{\vec{\xi}} (\xi_1 - x_1) + \left. \frac{\partial f}{\partial x_2} \right|_{\vec{\xi}} (\xi_2 - x_2) + \dots + \left. \frac{\partial f}{\partial x_n} \right|_{\vec{\xi}} (\xi_n - x_n) \\
 &+ \frac{1}{2} \left[\right. \\
 &\quad \left. \frac{\partial^2 f}{\partial x_1^2} \right|_{\vec{\xi}} (\xi_1 - x_1)^2 + \frac{\partial^2 f}{\partial x_1 \partial x_2} \Big|_{\vec{\xi}} (\xi_1 - x_1)(\xi_2 - x_2) + \dots + \frac{\partial^2 f}{\partial x_1 \partial x_n} \Big|_{\vec{\xi}} (\xi_1 - x_1)(\xi_n - x_n) \\
 &\quad + \frac{\partial^2 f}{\partial x_2 \partial x_1} \Big|_{\vec{\xi}} (\xi_2 - x_2)(\xi_1 - x_1) + \frac{\partial^2 f}{\partial x_2^2} \Big|_{\vec{\xi}} (\xi_2 - x_2)^2 + \dots + \frac{\partial^2 f}{\partial x_2 \partial x_n} \Big|_{\vec{\xi}} (\xi_2 - x_2)(\xi_n - x_n) \\
 &\quad \vdots \qquad \qquad \qquad \vdots \\
 &\quad + \frac{\partial^2 f}{\partial x_n \partial x_1} \Big|_{\vec{\xi}} (\xi_n - x_n)(\xi_1 - x_1) + \frac{\partial^2 f}{\partial x_n \partial x_2} \Big|_{\vec{\xi}} (\xi_n - x_n)(\xi_2 - x_2) + \dots + \frac{\partial^2 f}{\partial x_n^2} \Big|_{\vec{\xi}} (\xi_n - x_n)^2 \\
 &\quad \left. \right] \\
 &+ \mathcal{O}[(\xi_1 - x_1)^3] + \mathcal{O}[(\xi_1 - x_1)^2(\xi_2 - x_2)] + \mathcal{O}[(\xi_1 - x_1)(\xi_2 - x_2)^2] + \mathcal{O}[(\xi_2 - x_2)^3] \\
 &+ \dots + \mathcal{O}[(\xi_1 - x_1)^2(\xi_n - x_n)] + \mathcal{O}[(\xi_1 - x_1)(\xi_2 - x_2)(\xi_n - x_n)] + \dots + \mathcal{O}[(\xi_n - x_n)^3] \\
 &\qquad \qquad \qquad (12-8)
 \end{aligned}$$

or in a vector shorthand:

$$f(\vec{x}) = f(\vec{\xi}) + \nabla_{\vec{x}} f|_{\vec{x}=\vec{\xi}} \cdot (\vec{\xi} - \vec{x}) + (\vec{\xi} - \vec{x}) \cdot (\nabla_{\vec{x}} \nabla_{\vec{x}} f)|_{\vec{x}=\vec{\xi}} \cdot (\vec{x} - \vec{\xi}) + \mathcal{O}[\|\vec{\xi} - \vec{x}\|^3] \quad (12-9)$$

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Approximating Surfaces

Example of turning a function of two variables, $f(x, y)$ into an approximating function of four variables:

1. Start with a function $f(x, y)$ and expand it about a point (ξ, η) to second order—use MATHEMATICA[®]’s Normal function to convert from series representation to a parabolic representation.
2. The expansion is now a function of four variables—the first two variables are the point the function is expanded around, and the second two are the variable of the parabolic approximation at that point:

$$f_{\text{appx}}(\xi, \eta; x, y) = f(x, y) + \left. \frac{\partial f}{\partial x} \right|_{x,y} (\xi - x) + \left. \frac{\partial f}{\partial y} \right|_{x,y} (\eta - y) + \mathcal{Q}$$

where

$$\mathcal{Q} \equiv \frac{1}{2} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x,y} (\xi - x)(\xi - x) + \left. \frac{\partial^2 f}{\partial x \partial y} \right|_{x,y} (\xi - x)(\eta - y) + \frac{1}{2} \left. \frac{\partial^2 f}{\partial y^2} \right|_{x,y} (\eta - y)(\eta - y)$$

or

$$f_{\text{appx}}(\xi, \eta, x, y) = f(x, y) + \nabla f \cdot \begin{pmatrix} \xi - x \\ \eta - y \end{pmatrix} + \frac{1}{2} \mathcal{Q}_{\text{form}}$$

where

$$\mathcal{Q}_{\text{form}} \equiv (\xi - x, \eta - y) \begin{pmatrix} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x,y} & \left. \frac{\partial^2 f}{\partial x \partial y} \right|_{x,y} \\ \left. \frac{\partial^2 f}{\partial y \partial x} \right|_{x,y} & \left. \frac{\partial^2 f}{\partial y^2} \right|_{x,y} \end{pmatrix} \begin{pmatrix} \xi - x \\ \eta - y \end{pmatrix}$$

3. Plot the function $f_{\text{appx}}(\xi, \eta, x, y)$ for $|\xi - x| < \delta$ and $|\eta - y| < \delta$ for a selected number of points (x, y) .

Just a few of many examples of instances where Taylor’s expansions are used are:

linearization Examining the behavior of a model near a point where the model is understood.

Even if the model is wildly non-linear, a useful approximation is to make it linear by evaluating near a fixed point.

approximation If a model has a complicated representation in terms of unfamiliar functions, a Taylor expansion can be used to characterize the ‘local’ model in terms of a simple polynomials.

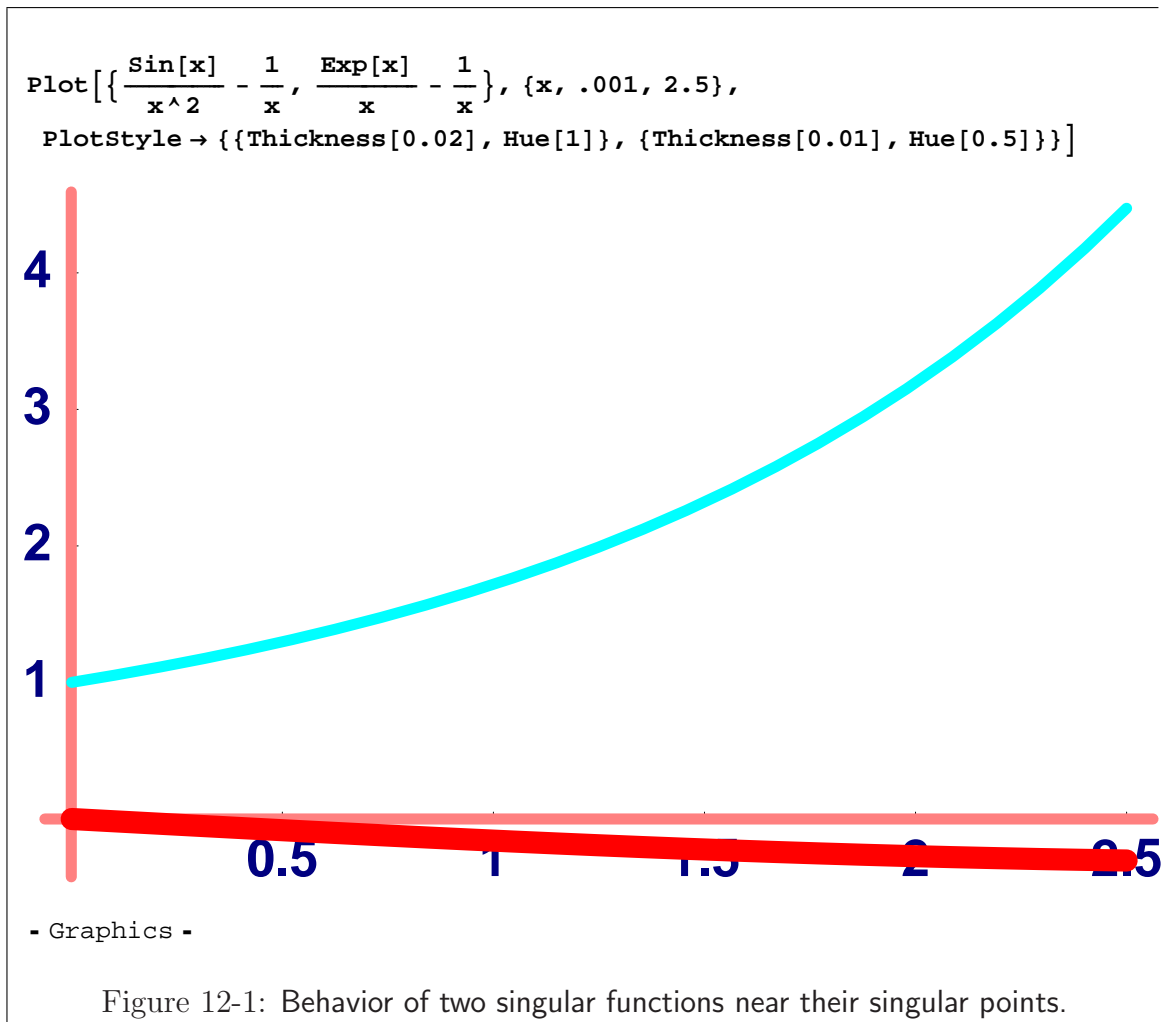
asymptotics Even when a system has singular behavior (e.g, the value of a function becomes infinite as some variable approaches a particular value), *how* the system becomes singular is very important. At singular points, the Taylor expansion will have leading order terms that are singular, for example near $x = 0$,

$$\frac{\sin(x)}{x^2} = \frac{1}{x} - \frac{x}{6} + \mathcal{O}(x^3) \quad (12-10)$$

The singularity can be subtracted off and it can be said that this function approaches ∞ "linearly" from below with slope $-1/6$. Comparing this to the behavior of another function that is singular near zero:

$$\frac{\exp(x)}{x} = \frac{1}{x} + 1 + \frac{x}{2} + \frac{x^2}{6} + \mathcal{O}(x^3) \quad (12-11)$$

shows that the e^x/x behavior is "more singular."



stability In the expansion of energy about a point is obtained, then the various orders of expansion can be interpreted:

zero-order The zeroth-order term in a local expansion is the energy of the system at the point evaluated. Unless this term is to be compared to another point, it has no particular meaning (if it is not infinite) as energy is always arbitrarily defined up to a constant.

first-order The first-order is related to the driving force to change the state of the system. Consider:

$$\Delta E = \nabla E \cdot \delta \vec{x} = -\vec{F} \cdot \delta \vec{x} \quad (12-12)$$

If force exists, the system can decrease its energy linearly by picking a particular change $\delta\vec{x}$ that is anti-parallel to the force.

For a system to be stable, it **is a necessary first condition that the forces (or first order expansion coefficients) vanish**.

second order If a system has no forces on it (therefore satisfying the necessary condition of stability), then where the system is stable or unstable depends on whether a small $\delta\vec{x}$ can be found that decreases the energy:

$$\begin{aligned}\Delta E &= \frac{1}{2} \delta\vec{x} \cdot \nabla - \vec{F} \cdot \delta\vec{x} \\ &= \frac{1}{2} \cdot \nabla \nabla E \cdot \delta\vec{x} \\ &= \frac{1}{2} \left. \frac{\partial^2 E}{\partial x_i \partial x_j} \right|_{x_1, x_2, \dots, x_n} \delta x_i \delta x_j\end{aligned}\tag{12-13}$$

where the summation convention is used above and the point (x_1, x_2, \dots, x_n) is one for which ∇E is zero.

numerics Derivatives are often obtained numerically in numerical simulations. The Taylor expansion provides a formula to approximate numerical derivatives—and provides an estimate of the numerical error as a function of quantities like numerical mesh size.

Gradients and Directional Derivatives

Scalar functions $F(x, y, z) = F(\vec{x})$ have a natural vector field associated with them—at each point \vec{x} there is a direction $\hat{n}(\vec{x})$ pointing in the direction of the most rapid increase of F . Associating the *magnitude* of a vector in the direction of steepest increase with the *rate of increase* of F defines the gradient.

The gradient is therefore a vector function with a vector argument (\vec{x} in this case) and it is commonly written as ∇F .

Here are some natural examples:

Meteorology The “high pressure regions” are commonly displayed with weather reports—as are the “isobars” or curves of constant barometric pressure. Thus displayed, pressure is a scalar function of latitude and longitude.

At any point on the map, there is a direction that points to local high pressure center—this is the direction of the gradient. The rate at which the pressure is increasing gives the magnitude of the gradient.

The gradient of pressure should be a vector that is related to the direction and the speed of wind.

Mosquitoes It is known that hungry mosquitoes tend to fly towards sources (or local maxima) of carbon dioxide. Therefore, it can be hypothesized that mosquitoes are able to determine the gradient in the concentration of carbon dioxide.

Heat In an isolated system, heat flows from high-temperature ($T(\vec{x})$) regions to low-temperature regions.

The Fourier empirical law of heat flow states that the rate of heat flows is proportional to the local *decrease* in temperature.

Therefore, the local rate of heat flow should be a proportional to the vector which is *minus* the gradient of $T(\vec{x})$: $-\nabla T$

☹ Finding the Gradient

☹ Potentials and Force Fields

Force is a vector. Force projected onto a displacement vector \vec{dx} is the rate at which work, dW , is done *on* an object $dW = -\vec{F} \cdot \vec{dx}$.

If the work is being supplied by an external agent (e.g., a charged sphere, a black hole, a magnet, etc.), then it may be possible to ascribe a potential energy ($E(\vec{x})$, a scalar function with vector argument) to the agent associated with the position at which the force is being applied.⁴ This $E(\vec{x})$ is the potential for the agent and the force field due to the agent is $\vec{F}(\vec{x}) = -\nabla E(\vec{x})$.

Sometimes the force (and therefore the energy) scale with the “size” of the object (i.e., the object’s total charge in an electric potential due to a fixed set of charges, the mass of an object in the gravitational potential of a black hole, the magnetization of the object in a magnetic potential, etc.). In these cases, the potential field can be defined in terms of a unit size (per unit charge, per unit mass, etc.). One can determine whether such a scaling is applied by checking the units.

⁴As with any energy, there is always an arbitrary constant associated with the position (or state) at which the energy is taken to be zero. There is no such ambiguity with force. Forces are, in a sense, more fundamental than energies. Energy appears to be fundamental because all observations of the first law of thermodynamics demonstrate that there is a conserved quantity which is a state function and is called energy.