_____Oct. 12 2005: **Lecture 11:** _____

Geometry and Calculus of Vectors

Reading:
Kreyszig Sections: §8.1 (pp:401–06) , §8.2 (pp:408–413) §8.3 (pp:414–21) §8.4 (pp:423–27)

_____ **Vector Products** _____

The concept of vectors as abstract objects representing a collection of data has already been presented. Every student at this point has already encountered vectors as representation of points, forces, and accelerations in two and three dimensions.

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Solution to 2D Diffusion Equation for Point Source Initial Conditions

Flux as a vector field derived from concentration

$$\vec{J} = -D(\frac{\partial C}{\partial x}, \frac{\partial C}{\partial y})$$

Visualizing vector fields

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  👀 _Review: The Inner (dot) product of two vectors and relation to projection_ ....

An inner (or dot-) project is multiplication of two vectors that produces a scalar.

$$
\begin{aligned}
\vec{a} \cdot \vec{b} &\equiv \\
&\equiv a_i b_i \\
&\equiv a_i b_j \delta_{ij} \text{ where } \delta_{ij} \equiv \begin{cases} 1 \text{ if } i = j \\ 0 \text{ otherwise} \end{cases} \\
&\equiv (a_1, a_2, \ldots a_N) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} \\
&\equiv (b_1, b_2, \ldots b_N) \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}
\end{aligned}
\tag{11-1}
$$

The inner product is:

linear, distributive $(k_1 \vec{a} + k_2 \vec{b}) \cdot \vec{c} = k_1 \vec{a} \cdot \vec{c} + k_2 \vec{b} \cdot \vec{c}$

symmetric $\vec{a} \cdot \vec{b} = \vec{b} \cdot \vec{a}$

satifies Schwarz inequality $\|\vec{a} \cdot \vec{b}\| \leq \|\vec{b}\| \|\vec{a}\|$

satifies triangle inequality $\|\vec{a} + \vec{b}\| \leq \|\vec{b}\| + \|\vec{a}\|$

  If the vector components are in a cartesian (i.e., cubic lattice) space, <u>then</u> there is a useful equation for the angle between two vectors:

$$
\cos \alpha = \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \|\vec{b}\|} = \hat{n}_a \cdot \hat{n}_b
\tag{11-2}
$$

where $\hat{n}_i$ is the unit vector that shares a direction with i. <u>_Caution:_</u> _when working with vectors in non-cubic crystal lattices (e.g, tetragonal, hexagonal, etc.) the angle relationship above does not hold. One must convert to a cubic system first to calculate the angles._

The projection of a vector onto a direction $\hat{n}_b$ is a scalar:

$$p = \vec{a} \cdot \hat{n}_b \tag{11-3}$$

> ☻ *Review: Vector (or cross-) products* ....

The vector product (or cross ×) differs from the dot (or inner) product in that multiplication produces a vector from two vectors. One might have quite a few choices about how to define such a product, but the following idea proves to be useful (and standard).

normal Which way should the product vector point? Because two vectors (usually) define a plane, the product vector might as well point away from it.

   The exception is when the two vectors are linearly dependent; in this case the product vector will have zero magnitude.

   The product vector is normal to the plane defined by the two vectors that make up the product. A plane has two normals, which normal should be picked? By convention, the "right-hand-rule" defines which of the two normal should be picked.

magnitude Given that the product vector points away from the two vectors that make up the product, what should be its magnitude? We already have a rule that gives us the cosine of the angle between two vectors, a rule that gives the sine of the angle between the two vectors would be useful. Therefore, the cross product is defined so that its magnitude for two unit vectors is the sine of the angle between them.

   This has the extra utility that the cross product is zero when two vectors are linearly-dependent (i.e., they do not define a plane).

   This also has the utility, discussed below, that the triple product will be a scalar quantity equal to the volume of the parallelepiped defined by three vectors.

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Example of a Cross Product

Matrix form of cross product

$$\vec{a} \times \vec{b} = \det \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix}$$

The triple product,

$$\vec{a} \cdot (\vec{b} \times \vec{c}) = (\vec{a} \times \vec{b}) \cdot \vec{c} =$$
$$\|\vec{a}\|\|\vec{b}\|\|\vec{c}\| \sin \gamma_{b-c} \cos \gamma_{a-bc} = \tag{11-4}$$
$$\|\vec{a}\|\|\vec{b}\|\|\vec{c}\| \sin \gamma_{a-b} \cos \gamma_{ab-c}$$

where γ_{i-j} is the angle between two vectors i and j and γ_{ij-k} is the angle between the vector k and plane spanned by i and j. is equal to the parallelepiped that has $\vec{a}$, $\vec{b}$, and $\vec{c}$, emanating from its bottom-back corner.

If the triple product is zero, the volume between three vectors is zero and therefore they must be linearly dependent.

Derivatives Vectors

Consider a vector, $\vec{p}$, as a point in space. If that vector is a function of a real continuous parameter for instance, t, then $\vec{p}(t)$ represents the loci as a function of a parameter.

If $\vec{p}(t)$ is continuous, then it sweeps out a continuous curve as t changes continuously. It is very natural to think of t as time and $\vec{p}(t)$ as the trajectory of a particle—such a trajectory would be continuous if the particle does not disappear at one instant, t, and reappear an instant later, $t + dt$, some finite distance distance away from $\vec{p}(t)$.

If $\vec{p}(t)$ is continuous, then the limit:

$$\frac{d\vec{p}(t)}{dt} = \lim_{\Delta t \to 0} \frac{\vec{p}(t + \Delta t) - \vec{p}(t)}{\Delta t} \tag{11-5}$$

Notice that the numerator inside the limit is a vector and the denominator is a scalar; so, the derivative is also a vector. Think about the equation geometrically—it should be apparent that the vector represented by the derivative is locally tangent to the curve that is traced out by the points $\vec{p}(t - dt)$, $\vec{p}(t)$ $\vec{p}(t + dt)$, etc.

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Vector Derivatives

Visualizing a vector curve and its derivative

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👓 *Review: Partial and total derivatives* ....

One might also consider a time- and space-dependent vector field, for instance $\vec{E}(x,y,z,t) = \vec{E}(\vec{x},t)$ could be the force on a unit charge located at $\vec{x}$ at time t.

Here, there are many different things which might be varied and give rise to a derivative. Such questions might be:

1. How does the force on a unit charge differ for two nearby unit-charge particles, say at (x,y,z) and at $(x,y+\Delta y,z)$?

2. How does the force on a unit charge located at (x,y,z) vary with time?

3. How does the the force on a particle change as the particle traverses some path $(x(t),y(t),z(t))$ in space?

Each question has the "flavor" of a derivative, but each is asking a different question. So a different kind of derivative should exist for each type of question.

The first two questions are of the nature, "How does a quantity change if only one of its variables changes and the others are held fixed?" The kind of derivative that applies is the partial derivative.

The last question is of the nature, "How does a quantity change when all of its variables depend on a single variable?" The kind of derivative that applies is the total derivative. The answers are:

1.
$$\frac{\partial \vec{E}(x,y,z,t)}{\partial y} = \left(\frac{\partial \vec{E}}{\partial y}\right)_{\text{constant} x,z,t} \tag{11-6}$$

2.
$$\frac{\partial \vec{E}(x,y,z,t)}{\partial t} = \left(\frac{\partial \vec{E}}{\partial t}\right)_{\text{constant} x,y,z} \tag{11-7}$$
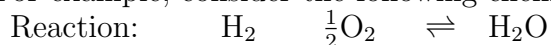
3.

$$\frac{d\vec{E}(x(t), y(t), z(t), t)}{dt} = \frac{\partial \vec{E}}{\partial x}\frac{dx}{dt} + \frac{\partial \vec{E}}{\partial y}\frac{dy}{dt} + \frac{\partial \vec{E}}{\partial z}\frac{dz}{dt} + \frac{\partial \vec{E}}{\partial t}\frac{dt}{dt} = \nabla \vec{E}(\vec{x}(t), t) \cdot \frac{d\vec{x}}{dt} + \frac{\partial \vec{E}}{\partial t} \quad (11\text{-}8)$$


☻ *All vectors are not spatial* ....

It is useful to think of vectors as spatial objects when learning about them—but one shouldn't get stuck with the idea that all vectors are points in two- or three-dimensional space. The spatial vectors serve as a good analogy to generalize an idea.

For example, consider the following chemical reaction:

Reaction:	H_2	$\frac{1}{2}O_2$	$\rightleftharpoons$	H_2O
Initial:	1	1	$\rightleftharpoons$	0
During Rx.:	$1 - \xi$	$1 - \frac{1}{2}\xi$	$\rightleftharpoons$	ξ

The composition could be written as a vector:
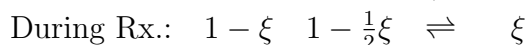
$$\vec{N} = \begin{pmatrix} \text{moles } H_2 \\ \text{moles } O_2 \\ \text{moles } H_2O \end{pmatrix} = \begin{pmatrix} 1 - \xi \\ 1 - \frac{1}{2}\xi \\ \xi \end{pmatrix} \quad (11\text{-}9)$$

and the variable ξ plays the role of the "extent" of the reaction—so the composition variable $\vec{N}$ lives in a reaction-extent (ξ) space of chemical species.