FUNCTION AND VECTOR CALCULUS

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Last Update: 14/Feb/2019

1. Introduction

These course notes will details the basics of mutlivariate function and vector calculus, with the context of Game Physics in mind. Some knowledge of linear algebra (matrix multiplication, axis systems, linear transformations), and basic calculus (functions of one variable and their derivatives) will be assumed. We use the notation $\mathbf{x} \in \mathbb{R}^n$ to denote "a vector $\mathbf{x} = \{x_1, \ldots x_n\}$ of n scalars". We use bold letters $\mathbf{x}$ for vectors and regular x for scalars. Unless otherwise stated in this document, we treat vectors as column vectors. We denote a matrix as $A_{n\times m}$ with n rows and m columns. The identity matrix of size n is I_n. We denote unit-norm vectors as $\hat{x}$.

1.1. **Dot product.** We define the dot product between two vectors $\mathbf{u}$ and $\mathbf{v}$, both of size n as $\langle \mathbf{u}, \mathbf{v}\rangle = \sum_{i=1}^{n} u_i \cdot v_i$. In matrix multiplication notation, we have that $\langle \mathbf{u}, \mathbf{v}\rangle = \mathbf{u}^T \cdot \mathbf{v} = \mathbf{u}^T \cdot I_n \cdot \mathbf{v}$. The squared norm of a vector $\mathbf{u}$ is measured by a dot product with itself: $|\mathbf{u}|^2 = \langle u, u\rangle$. For general vectors $\mathbf{u}, \mathbf{v}$, we have $\langle \mathbf{u}, \mathbf{v}\rangle = |\mathbf{u}| \cdot |\mathbf{v}|\, cos(\theta)$, where θ is the convex angle between the two vectors. As such, orthogonal vectors have zero dot product.

1.2. **Cross product.** The cross product $\mathbf{u} \times \mathbf{v}$ is the vector which is orthogonal to both (or: the normal to the plane they span), where its specific orientation is given by the right-hand rule (so in the canonical axis system $\hat{x}, \hat{y}, \hat{z}$ we have that $\hat{z} = \hat{x} \times \hat{y}$). The norm is $|\mathbf{u} \times \mathbf{v}| = |\mathbf{u}| \cdot |\mathbf{v}|\, sin(\theta)$. As such, vectors that are parallel (and therefor their spanned plane is degenerate), have zero cross product.

2. Multivariate calculus

We work with *multivariate* functions of the type $f : \mathbb{R}^m \to \mathbb{R}^n$, taking m scalars to n scalars:

$$f\left(x_1, x_2, \ldots, x_m\right) = \left(y_1, y_2, \ldots y_n\right).$$

The simplest case is that of linear functions, represented by a matrix $A_{n\times m}$, so that $f(x) = y = A \cdot x$. if $m = n$ this function is often denoted as a *change of coordinates* or a *mapping*. In our course, they represent changes in the object like rotation, translation, or deformation. Like the case of single-values, single-variable function that you might have learned in high-school, we investigate the derivatives of f to understand local behaviour. For physics, that means how much does an object deforms locally.

2.1. **Single function of multiple variables.** We first study the case where $n = 1$. We define the partial derivative $\frac{\partial y}{\partial x_i}$ as the derivative of the function f with relation to the variable x_i, where the rest of the variables are considered as constants. For instance, consider the following function and derivatives, for $m = 2$.

$$\begin{aligned} f(x_1, x_2) = y &= (x_1)^3 + (x_2)^4 + 3x_1x_2 \\ \frac{\partial y}{\partial x_1} &= 3\,(x_1)^2 + 3x_2 \\ \frac{\partial y}{\partial x_2} &= 4\,(x_2)^3 + 3x_1 \end{aligned}$$

the partial derivative in x_i has a geometric meaning: consider the function as a height field, where y is the height. Then, $\frac{\partial y}{\partial x_i}$ is the slope of the function in the direction of the *coordinate* x_i.

2.1.1. *Gradient.* The gradient of the function f is the row vector ∇f of size m of all partial derivatives:

$$\nabla f = \left(\frac{\partial y}{\partial x_1}, \ldots, \frac{\partial y}{\partial x_m}\right)$$

.

The gradient also has a geometric meaning: it points towards the direction of *steepest ascent*. If you are at a point $\mathbf{x}$ and would like to climb up to the top of the (local) mountain, you best move in the direction of the gradient at each point of your hike. Consequently, *extremal* points like mountain tops, valley bottoms, and saddles have $\nabla f = 0$.

2.2. **Vector-valued functions.** We next consider again the general case of $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$. This function actually comprises n independent function y_i, where each has its own gradient row vector. We stack these rows in the $n \times m$ *Jacobian* matrix:

$$J_f = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_m} \end{pmatrix}$$

Note that the Jacobian of a linear function is simply $J_f = A$. A special case is rotation where $m = n = 3$, and the Jacobian is just the rotation matrix $R_{3\times 3}$ (it is the same for $m = n = 2$).

2.3. **First-order approximations.** In order to study what happens locally to an object under a mapping f, we need to look at a lower order approximation of it. For motivation, remember that for a single-variable function one approximates a function locally using a tangent line, to understand its slope. We are going to do the same in a more general way. The (Taylor) first-order approximation of a function at point $\mathbf{x}$ is:

$$f(\mathbf{x} + \delta\mathbf{x}) \approx f(\mathbf{x}) + J_f(\mathbf{x}) \cdot \delta\mathbf{x},$$

for any possible $\delta\mathbf{x} \rightarrow 0$, which denotes an *infinitesimal* direction away from $\mathbf{x}$. We would like to investigate the effect of the mapping f on two infinitesimally-closed points $\mathbf{x}$ and $\mathbf{x}+\delta\mathbf{x}$. For instance, how much the distance between them changes after the mapping f. That is important to understand stretching and compressions. We then have that:

$$|f(\mathbf{x}+\delta\mathbf{x}) - f(\mathbf{x})|^2 \approx |J_f(\mathbf{x}) \cdot \delta\mathbf{x}|^2 = \delta\mathbf{x}^T \cdot J_f^T \cdot J_f \cdot \delta\mathbf{x}.$$

The last step is just implementing the dot product $|u| =< u, u >$ as the multiplication of a row and column vectors $u^T \cdot u$.

If we subsequently define $M_f(\mathbf{x}) = J_f(\mathbf{x})^T \cdot J_f(\mathbf{x})$, we get a matrix of size $m \times m$ which implements a symmetric (by the construction) bilnear map (since it's a matrix). In addition, M is also positive semidefinite, as:

$$\forall\mathbf{u} \in \mathbb{R}^m, \mathbf{u}^T M_f \mathbf{u} = |J_f \cdot u|^2 \geq 0$$

As such, M_f is a *metric*. $M_f(\mathbf{x})$ encodes the local deformation of the function f at $\mathbf{x}$. Note that M can also measure *shear*: consider two original directions $\delta\mathbf{x}$ and $\delta\mathbf{x}'$, which had original dot product $\langle\delta\mathbf{x}, \delta\mathbf{x}'\rangle$ measuring the angles between them. The new dot product between them is now $\langle\delta\mathbf{x}, \delta\mathbf{x}'\rangle_M = \delta\mathbf{x}^T \cdot M \cdot \delta\mathbf{x}'$, which means the angles between them change according to $M_f(X)$.

To make this more intuitive, let us look at special examples:

(1) f is a rotation in $\mathbb{R}^3$, where then $J_f = R$, the rotation matrix. We have that for every $\mathbf{x}$, $M = R^T \cdot R = I_3$—the new metric is also an identity, which means no deformation of lengths or angles! that makes sense, as a rotation is a rigid transformation.
(2) f is a linear transformation $y = Ax$. In that case, $M = A^T \cdot A$ and does not depend on x (the change of lengths and angles is uniform throughout the object).
(3) f is an independent scaling in each dimension: $f(x_1, x_2) = \left(4x_1, \frac{1}{3}x_2\right)$. We get that

$$J_f = \begin{pmatrix} 4 & 0 \\ 0 & \frac{1}{3} \end{pmatrix}, M = \begin{pmatrix} 16 & 0 \\ 0 & \frac{1}{9} \end{pmatrix}.$$

We can see that M reflects the squared stretch in each dimension.

We will learn much more about deformation in the soft-body physics lecture. For now it is important to understand the calculus of metrics, jacobians, and gradients.

3. Vector Calculus

3.1. **Vector fields.** We treat vector fields in the plane $\mathbb{R}^2$ and in space $\mathbb{R}^3$. In the case of $\mathbb{R}^3$, vector fields are the assignment of a vector (x, y, z) to each point in $\mathbb{R}^3$, which is a special case of a vector-valued function $f : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ (if to be strictly formal, we should use $f : \mathbb{R}^3 \rightarrow \mathbb{E}^3$, but this is out of our scope to explain why). They appear in applications like fluid simulation, deformation and force fields, including electromagnetism. We identify several prominent features of fields:

(1) Sinks and sources, from which the field either diverges or converges into. If there is a material flowing through the field, then it wants to escape a source, and get drawn to a sink.
(2) Vortices, which would rotate material around them, like the eye of a hurricane.

We already investigated one type of vector field: the gradient ∇f. In the case of a height function, the sinks and sources are the mountain tops and valley bottoms. But there are no "mountain vortices", and not by chance, as we next see.

3.2. **Integration over a curve.** Integrating vector fields over curves (and surfaces and volumes) is our primary analysis tool to discover features in fields. Assume a curve parameterized by a "time" parameter $t \in [0,1]$, where its trace is $\mathbf{C}(t) = (x(t), y(t), z(t))$. In this parameterized form, it describes the transport of a particle along the positions of the curve. We denote the vector field at each point as $\mathbf{v}(x,y,z)$. We treat the vector field as a force field, and would like to compute the total *work* done on the particle along the curve by this field. Remember that the work done on a particle by a force $\mathbf{v}$ along some displacement $\Delta\mathbf{C}$ is $\mathbf{v} \cdot \Delta\mathbf{C}$. That means that if the vector field is orthogonal to the movement of the the particle, it does not do any work; alternatively, if the field is parallel to the curve, it does the most work possible at this point. Let us next make this more precise:

We consider the *differential* $d\mathbf{C}$ of the curve, which is an infinitesimal limit of our $\Delta\mathbf{C}$: a very small linear segment of the curve at each point. Intuitively, you get it as the limit of discretizing the curve into an increasingly fine polyline (a part of a polygon). Imagine we have such a polyline where every edge takes Δt time to travel. Then, the segments are just the vectors

$$\mathbf{C}(t+\Delta t) - \mathbf{C}(t) = \frac{\mathbf{C}(t+\Delta t) - \mathbf{C}(t)}{\Delta t} \cdot \Delta t \xrightarrow[\Delta t \to 0]{} \mathbf{C}'(t) \cdot dt = d\mathbf{C}.$$

Note that we use $\mathbf{C}'(t) = \frac{d\mathbf{C}}{dt}$. At each edge of the polyline, the work done is then (we assume the vector field is constant on the polyline edge) $\mathbf{v}\left(x(t), y(t), z(t)\right) \cdot C'(t)dt$, and the entire work done on the curve $\mathbf{C}$ by the vector field $\mathbf{v}$ is given by the following integral:

$$\int_{\mathbf{C}} v\left(x(t), y(t), z(t)\right) \cdot d\mathbf{C} = \int_0^1 \left[v\left(x(t), y(t), z(t)\right) \cdot \mathbf{C}'(t)\right] dt$$

.

3.3. **Conservative vector fields.** Suppose that the vector field v is indeed the gradient of some scalar potential f: $\mathbf{v} = \nabla f$. We get that the formula above converges into:

$$\int_0^1 \left[\nabla f \cdot \mathbf{C}'(t)\right] dt = f(1) - f(0).$$

The left-hand side is obtained with integration by parts which we leave as an exercise. We get quite a profound result: the integration does not depend on the curve $\mathbf{C}$ at all! we call this property *path-independence*. This makes sense when we investigate the meaning of f and the work done in such cases: f encodes a potential energy (like height of the mountain, or electric charge, or gravity of a star). ∇f is nothing but the force that the potential induces on the scene, which realizes the potential: when you move along the negative gradient, the energy reduces to zero. Consider climbing up a mountain: the gradient is always in the direction of steepest ascent. If you move in a direction which is not entirely the gradient, the force responsible for gaining height (potential) is only the part of your hike that ascends or descends. As a special case, if you move on a *level set* of the mountain (hike along its side), the force ∇f is always orthogonal to you, and you do not gain any height.

This is also correct if you climb up and down to the same height. More generally, if you move in a closed curve where you start and return to the same point, you get $\int_0^1 \left[\nabla f \cdot \mathbf{C}'(t)\right] dt = f(1) - f(0) = 0$.

We then call a gradient vector field ∇f a *conservative* vector field. Suppose that we are given a general vector field $\mathbf{v}$ which integrates to zero along closed curves, is it conservative? is there a function f to which it is a gradient? the answer is no, but "almost", as we see in the following.

3.4. **The curl operator.** Consider a closed infinitesimal curve $\mathbf{C}(t)$ where $\mathbf{C}(0) = \mathbf{C}(1)$ around a point $\mathbf{p} = (x, y, z)$, wrapping around an infinitesimal area A around it. The curve lies in a plane with normal $\hat{n}$. We define the *curl* operator $\nabla\times$ of a vector field $\mathbf{v}$ implicitly as follows:

$$(\nabla \times v) \cdot \hat{n} = \frac{1}{|A|} lim_{A \to 0} \oint_{\mathbf{C}} \mathbf{v}\left(\mathbf{p}\right) \cdot d\mathbf{C}(\mathbf{p})$$

In words, it is the integration of $\mathbf{v}$ around curve $\mathbf{C}$ in the plane defined by $\hat{n}$, weighted with the inverse area, as the curve converges to a single point. Note that our definition was implicit: we only gave the dot product of $\nabla \times v$ with a specific normal. We can instead use the explicit definition:

$$\nabla \times v = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \times \mathbf{v},$$

where the "$\times$" means a cross product. The curl operator produces a new vector field $\nabla \times \mathbf{v}$ from the original $\mathbf{v}$.

The curl operator has an intuitive geometric meaning: by looking at the definition, it measures how much work the field does on a particle orbiting around the point p, going around on the closed curve $\mathbf{C}$, normal to an axis $\hat{n}$. Alternatively, curl measures how much rotation, or *vorticity* is caused by the vector field around point $\mathbf{p}$.

By definition, and from the zero-integration properties of conservatives field, we get the identity:

$$\nabla \times \nabla f = 0$$

which is true for every function f. That means that conservative fields are *curl-free*, often also called *irrotational*. It is evident why a conservative field is irrotational: it is induced by a potential, and going around a curve returns to the same point and the same potential. Then we should ask the same question from above: is every curl-free field $\mathbf{v}$ also conservative, and is the gradient of some f? it is, if the domain is *simply-connected*. That is, the vector field is within a volume Ω without any "holes" in the inside. The point is that in simply-connected domains, every curve $\mathbf{C}$ can be shrunk to a point at the limit; in the presence of holes, you can wrap the hole with a curve where the field would not integrate to zero, but where it is still curl-free by definition—this is a complicated theory which is out of our scope.

3.5. **The divergence operator.** The curl operator teaches us about vortices, but we are yet to quantify sources and sinks. Consider an infinitesimal volumetric domain Ω around a point $\mathbf{p}$, with a boundary $\partial\Omega$, and the outward-pointing normal $\hat{n}(\partial\Omega)$ We define the divergence operator as follows:

$$\nabla \cdot v = lim_{\Omega \rightarrow \{\mathbf{p}\}} \frac{1}{|\Omega|} \oiint_{\partial \Omega} [\mathbf{v} \cdot \hat{n}]\, d(\partial \Omega)$$

This integral has some yet uninterpreted components. By $d(\partial\Omega)$ we mean an infinitesimal path of the surface, as if the surface is tessellated into very fine mesh (remember what we did for the polyline tesselation above). Then, $\mathbf{v} \cdot \hat{n}$ measures the *flow* of the field through the patch, or how much the field transports material away from Ω through this patch. For a two-dimensional field in the plane, our formulation reduces to a familiar form:

$$\nabla \cdot v = lim_{\Omega \rightarrow \{\mathbf{p}\}} \frac{1}{|\Omega|} \oint_{\partial \Omega} [\mathbf{v} \cdot \hat{n}]\, dl$$

This form is very similar to the formulation for curl. The difference is that for curl we use the $d\mathbf{C}$, which is the infinitesimal polyline edge, where for divergence we use $\hat{n} \cdot dl$, where dl is the *length* of dC, and $\hat{n}$ is the normal to this polyline. One can equivalently write $d\mathbf{C} = \hat{T}dl$, where $\hat{T}$ is the unit tangent vector to the curve, and dl is the infinitesimal length (the length of the edge of the very-fine polyline). From this, we see that $dC = R^{90}(\hat{n} \cdot dl)$ (a rotation by $90°$). So the only difference is that divergence integrates against the normal, where curl integrates against the tangent.

The divergence also has a differential definition:

$$\nabla \cdot v = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot \mathbf{v}.$$

Intuitively, divergence measures how much the vector field transports material away from the point $\mathbf{p}$. That is, how much $\mathbf{p}$ is a source. Negative divergence then identifies with a sink. Fields that are *divergence-free*, where $\nabla \cdot \mathbf{v} = 0$ are often called *solenoidal*. They are the dominant objects in fluid simulation, because they represent *incompressible* flows.

3.6. **The Laplacian.** We know that conservative fields are curl-free, but they are not in general divergence free; the potential function creates sources and sinks. Can a general field be curl-free and divergence-free at the same time? Yes. Such fields are called *harmonic*. But they do not appear in every domain. Usually, they appear in the presence of multiple boundaries and holes.

What is in general the divergence of a conservative field? Intuitively, this would measure how much the sources and sinks of the potential are strong—in the mountain metaphor, how steep the mountain is. This is measured by the *Laplacian* operator:

$$\Delta f = \nabla \cdot \nabla f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 l f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2},$$

Where "$\frac{\partial^2}{\partial x^2}$" means the second derivative of x, without loss of generality. The laplacian operator is widely used in image processing and graphics, as a measure o how much a function f at a point $\mathbf{p}$ is different from f in the local neighborhood of $\mathbf{p}$. This is used to create low-pass filters for denoising and edge detection. It is also used in physics to quantify heat diffusion, where a heat distribution f diffuses as follows: $\frac{df}{dt} = \nabla f$.

3.7. **Stokes Theorem.** Stokes theorem is the most fundamental principle in vector calculus, and one of the most profound principles of physics in general. The most general form is as follows: given a volumetric domain Ω with boundary $\partial\Omega$, and a quantity ω that goes through the boundary of the domain, we have that:

$$\int_{\Omega} d\omega = \int_{\partial\Omega} \omega$$

In words, the total change from the quantity ω within the domain equals to its total flow through the boundary. Avoiding formal definition of what ω is (a differential form), we have a very basic and intuitive principal: the sum of everything that goes in and out from the domain Ω through its boundary (the right-hand side integral) equals the change in the quantity on the inside (the left-hand side). When ω is expressed as a vector field, we have the following variants of Stokes Theorem:

(1) The integration over a curve of conservative fields: $\int_0^1 [\nabla f \cdot \mathbf{C}'(t)]\, dt = f(1) - f(0)$, if you consider Ω as the curve $\mathbf{C}$, and the endpoints $\mathbf{C}(0)$ and $\mathbf{C}(1)$ as its boundary $\partial\Omega$. As a special case, we have the single-variable Fundemental Theorem of Calculus: $\int_{x_0}^{x_1} F'(x)dx = F(x_1) - F(x_0)$.

(2) **Kelvin-Stokes theorem**: Gives a surface patch S, it relates the total curl on the surface to the work on the boundary curve. In fact, this is the non-infinitesimal version of the definition of curl:

$$\iint_S [\nabla \times v] \cdot dS = \oint_{\partial S} v \cdot d(\partial S)$$

.

(3) **Divergence theorem**: relates the flow on the boundary $\partial\Omega$ with normal $\hat{n}$ to the total change in material (divergence) inside a volumetric domain Ω. It is also a non-infinitesimal version of the definition of divergence:

$$\iiint_{\Omega} [\nabla \cdot v] d\Omega = \oiint_{\partial\Omega} [v \cdot \hat{n}] d(\partial\Omega)$$