Multivariate Calculus
MANUSCRIPT

William F. Barnes [1]

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Chapter 1

Multivariate Calculus

1 Surfaces and Solids

Before getting into heavy jargon, we'll do a brief tour of the extension of the curve $y = f(x)$ into more dimensions.

1.1 Surfaces

The natural extension of a single-input function $f(x)$ is one that takes two arguments. In analogy to $y = f(x)$, we may also write

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

where $f(x, y)$ requires two independent inputs x and y. The domain of f is part (or all) of the Cartesian plane on which x and y occur. The range variable z may be regarded as the 'height above' the plane at (x, y).

If $f(x, y)$ is continuous in both variables, the set of all z-points constitutes a surface. In the same sense that a curve is a continuous arrangement of points in the Cartesian plane, surfaces may are like 'sheets' in a Cartesian volume.

Level Curves

Fixing z constant on a surface restricts the freedom in the xy-plane at height z to a *level curve*. A level curve is the same as a contour line seen on a topographical (not topological) map, or on various weather maps. A small ring surrounds a local minimum or a local maximum. Level curves intersect at a saddle point.

Critical Points

As two-dimensional creatures, surfaces have three kinds of critical points. A maxima in the surface is when both the x- and the y-variables reach a high point simultaneously. The same comment applies to a minima on the surface.

Another kind of critical point is called a *saddle point*, which has one of the variables x, y is a maxima, and the other a minima.

1.2 Solids

Adding another variable into the mix, we can have functions of three variables

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

where F is most generally called a *scalar field*. The temperature or air density in a room qualifies as a scalar field. Holding any variable F constant produces a *level surface*, the generalization of the level curve.

We'll stave off the discussion of critical points within scalar fields, or if you see it coming, vector fields, until after a few developments are made.

Topological Remarks

If the field F describes a finite solid, then the notion of minima, maxima, and saddle points on the surface of the solid are given the respective labels 'pits', 'peaks', and 'passes'. It's possible to show using arguments from topology that the following is always true:

$$\text{peaks} - \text{passes} + \text{pits} = 2$$

To understand this, consider an ice cream cone with one scoop of ice cream, supposed spherical. There are two peaks in this situation - the top of the ice cream, and the bottom of the cone, so $2 = 2$ checks out. Press your thumb into the ice cream to introduce a pit and a pass simultaneously. Then you get $2 - 1 + 1 = 2$.

The relationship between critical points has an analogous formula with respect volumes with flat faces and sharp edges. If V is the number of vertices, E is the number of edges, and F is the number of faces, it's possible to prove, much like the above:

$$V - E + F = 2$$

2 Multiple Integration

2.1 Single Integral

The workhorse of integral calculus is the fundamental theorem

$$f(x_1) - f(x_0) = \int_{x_0}^{x_1} f'(t)\, dt \ ,$$

where $f'(x)$ is the derivative df/dx.

The integral calculates the area under the curve $y(x) = f'(x)$ between the endpoints x_0, x_1 and hands us the answer in the form $A = f(x_1) - f(x_0)$. A concise way to express the area under such a curve is

$$A = \int_{x_0}^{x_1} y(x)\, dx \ .$$

2.2 Double Integral

The standard area integral calculates the sum of an infinite number of heights $y(x)$ above the x-axis. It stands to reason that $y(x)$ itself could be the result of an integral:

$$y(x) = \int_0^{y(x)} dy$$

The lower limit need not be zero if we take $y(x)$ as the vertical length trapped between two curves $y_0(x)$, $y_1(x)$, or:

$$y(x) = \int_{y_0(x)}^{y_1(x)} dy$$

Inserting this form for $y(x)$ into the one dimensional area integral yields a *double integral*:

$$A = \int_{x_0}^{x_1} \int_{y_0(x)}^{y_1(x)} dy\, dx$$

Notice that the *inner* integration limits are functions of the *outer* integration variable.

Supposing $y_0(x)$, $y_1(x)$ are easily inverted, the same area can be expressed with the integration variables reversed:

$$A = \int_{y_0}^{y_1} \int_{x_0(y)}^{x_1(y)} dx\, dy$$

Order of Integration

Note that in any multiple integral, it's always implied that the order of integration goes from the inner-most to the outer-most, not unlike like simplifying expressions with parentheses.

Integration Region

The curves $y_0(x)$, $y_1(x)$ are called *bounding functions*. The same comment apples to their inverted counterparts $x_0(y)$, $x_1(y)$.

The total information contained in the integration limits, including bounding functions, is called the *integration region*, denoted $\mathcal{D}$. With this we can express the double integral in a less definite form:

$$A = \int \int_{\mathcal{D}} dx\, dy \ .$$

By obscuring the product $dx\, dy$ into an area element dA, the above can be written free of the Cartesian coordinate system:

$$A = \int \int_{\mathcal{D}} dA$$

Volume Integral

The double integral apparatus can be used to calculate the volume trapped between the xy-plane and a given surface $z = f(x, y)$. For this, we simply write

$$V = \int\int_{\mathcal{D}} f(x, y)\, dx\, dy\ .$$

Integrating Functions

Supposing we need to calculate something more abstract than an area, the double integral apparatus takes any reasonable function in its integrand

$$B = \int\int_{\mathcal{D}} f(x, y)\, dx\, dy\ ,$$

where $f(x, y)$ is a generalized surface.

2.3 Polar Integral

To work a specific case, the differential area element in polar coordinates reads

$$dA = r\, dr\, d\theta\ ,$$

which means

$$A = \int\int_{\mathcal{D}} r\, dr\, d\theta$$

Note that the r-variable is usually a function of θ, which means the r-integral should be solved first. In detail,

$$A = \int \left(\int r\, dr \right) d\theta\ ,$$

where the integration limits are left in indefinite form.

Now, even if there were an additional function $f(\theta)$ in the integrand, thus changing the integral to

$$B = \int \left(\int r\, dr \right) f(\theta)\, d\theta\ ,$$

notice how $f(\theta)$ has no r-dependence, and is situated outside the r-integral.

We're thus free to evaluate the inner r-integral, and the above becomes

$$B = \frac{1}{2} \int r^2 f(\theta)\, d\theta\ .$$

This is a nifty result, as if $f(\theta)$ weren't there, then the integral is simply the area under $r(\theta)$ in polar coordinates:

$$A = \frac{1}{2} \int r^2\, d\theta$$

Area of a Circular Arc

Calculating the area of the circular arc in polar coordinates is as easy as

$$A = \int_{\theta_0}^{\theta_1} \int_0^R r\, dr\, d\theta = \frac{1}{2} (\theta_1 - \theta_0) R^2\ ,$$

which is the entire story.

For a bit of self-torture, let us do the same calculation in Cartesian coordinates using double integration. To set up, consider a pair of points (x_0, y_0), (x_1, y_1) with $x_0 > x_1$ that define the endpoints of the arc:

$$\begin{aligned} R\cos(\theta_0) &= x_0 \\ R\sin(\theta_0) &= y_0 \\ R\cos(\theta_1) &= x_1 \\ R\sin(\theta_1) &= y_1 \end{aligned}$$

Note also that the points (x_0, y_0), (x_1, y_1) define straight lines through the origin (no y-intercept), with respective slopes:

$$\begin{aligned} m_0 &= \frac{y_0}{x_0} \\ m_1 &= \frac{y_1}{x_1} \end{aligned}$$

The area of the circular arc will be calculated in two parts, one that resolves to a triangle with all straight edges, and another to handled the curved region. Working this out carefully, find:

$$A = \int_0^{x_1} \int_{m_0 x}^{m_1 x} dy\, dx + \int_{x_1}^{x_0} \int_{m_0 x}^{\sqrt{R^2 - x^2}} dy\, dx$$

The first integral can be evaluated fully with ease, but the second needs to chipped away at. Doing a round of simplifying, reach the intermediate step

$$\begin{aligned} A = &\frac{x_1^2}{2} (m_1 - \cancel{m_0}) \\ &+ \int_{x_0}^{x_1} \sqrt{R^2 - x^2}\, dx \\ &- \frac{m_0}{2} \left(x_0^2 - \cancel{x_1^2} \right)\ . \end{aligned}$$

The remaining integral can be solved with a sine substitution, which has the general solution:

$$\begin{aligned} \int \sqrt{R^2 - x^2}\, dx = &\frac{x\sqrt{R^2 - x^2}}{2} \\ &+ \frac{R^2}{2} \arctan\left(\frac{x}{\sqrt{R^2 - x^2}} \right) + C \end{aligned}$$

For the problem on hand, this means

$$\int \sqrt{R^2 - x^2}\, dx = \frac{m_0 x_0^2 - m_1 x_1^2}{2} + \frac{R^2}{2}\left(\arctan\left(\frac{x_0}{y_0}\right) - \arctan\left(\frac{x_1}{y_1}\right)\right) .$$

The x- and m-terms all cancel, and the area reads

$$A = \frac{R^2}{2}\left(\arctan\left(\frac{x_0}{y_0}\right) - \arctan\left(\frac{x_1}{y_1}\right)\right) .$$

From trigonometry, note in general that

$$\arctan\left(\cot\left(u\right)\right) = \frac{\pi}{2} - u ,$$

and the area becomes

$$A = \frac{R^2}{2}\left(\frac{\pi}{2} - \theta_0 - \frac{\pi}{2} + \theta_1\right) ,$$

and finally,

$$A = \frac{1}{2}\left(\theta_1 - \theta_0\right) R^2 ,$$

in agreement with the previous answer.

Gaussian Integral

Consider the definite integral

$$I_1 = \int_{-\infty}^{\infty} e^{-ax^2}\, dx ,$$

which has no elementary solution. Instead of turning to a numerical approximation, which would ordinarily be the case for such an integral, consider the same exact integral with a swap of variables:

$$I_1 = \int_{-\infty}^{\infty} e^{-ay^2}\, dy$$

If this analysis doesn't seem insane yet, multiply each copy of the integral together to get to what seems like a dead end,

$$I_1^2 = \left(\int_{-\infty}^{\infty} e^{-ax^2}\, dx\right)\left(\int_{-\infty}^{\infty} e^{-ay^2}\, dy\right) ,$$

and melt the notation down:

$$I_1^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a\left(x^2+y^2\right)}\, dx\, dy$$

Now, one must be very careful when doing this, but it just happens that the x, y variables can be regarded as locations on the Cartesian plane, which lends to polar coordinates. Switching to polar, the above integral is

$$I_1^2 = \int_0^{2\pi}\int_0^{\infty} e^{-a\rho^2}\, \rho\, d\rho\, d\phi .$$

Observe how the region of integration (the infinite plane) makes the limits on each integral easy to write.

The ϕ-integral is trivial and resolves to 2π. The remaining ρ-integral can is solved straightforwardly by u-substitution. Chugging through each, we find $I_1^2 = \pi/a$, or

$$I_1 = \int_{-\infty}^{\infty} e^{-ax^2}\, dx = \sqrt{\frac{\pi}{a}} .$$

This cheat works on several I_1-like problems called *Gaussian integrals.* Let us work through

$$I_2 = \int_{-\infty}^{\infty} e^{-ax^2+bx}\, dx .$$

Completing the square within the exponential leads to:

$$I_2 = e^{b^2/4a}\frac{1}{\sqrt{a}}\int_{-\infty}^{\infty} e^{-u^2}\, du = \sqrt{\frac{\pi}{a}}\, e^{b^2/4a}$$

Yet another Gaussian integral

$$I_3 = \int_{-\infty}^{\infty} x^2\, e^{-ax^2}\, dx$$

can be solved by taking the derivative of $-I_1$ with respect to a (not x). In detail:

$$\frac{d}{da}\left(-I_1\right) = I_3 = -\frac{d}{da}\left(\sqrt{\frac{\pi}{a}}\right) = \sqrt{\frac{\pi}{4a^3}}$$

2.4 Triple Integral

The apparatus for multiple integration readily generalizes for three and more dimensions. For three dimensions, the idea of a bounding function becomes a *bounding surface*, and we have a *triple integral*:

$$V = \int_{x_0}^{x_1}\int_{y_0(x)}^{y_1(x)}\int_{z_0(x,y)}^{z_1(x,y)} dz\, dy\, dx$$

In the special case $z_0\left(x, y\right) = 0$, the above reduces to a standard volume integral.

The order of integration has greater significance as the dimension of the integral increases. Supposing the required bounding functions and surfaces are easily attained, the triple integral can be written several more ways, for instance:

$$V = \int_{y_0}^{y_1} \int_{z_0(y)}^{z_1(y)} \int_{x_0(y,z)}^{x_1(y,z)} dx\, dz\, dy$$

$$V = \int_{z_0}^{z_1} \int_{x_0(z)}^{x_1(z)} \int_{y_0(z,x)}^{y_1(z,x)} dy\, dx\, dz$$

Or, in terms of an integration region:

$$V = \int \int \int_{\mathcal{D}} dx\, dy\, dz$$

Of course, the triple integral can involve functions in the integrand. For a three-variable function $f(x, y, z)$, sometimes called a *scalar field*, we can calculate things like

$$B = \int \int \int_{\mathcal{D}} f(x, y, z)\, dx\, dy\, dz\ .$$

Non-Cartesian Volume Elements

To go from three-dimensional Cartesian coordinates to a different system, the volume element and specification of the integration need to be changed. For cylindrical coordinates, we may have

$$V = \int_{z_0}^{z_1} \int_{\phi_0(z)}^{\phi_1(z)} \int_{\rho_0(\phi,z)}^{\rho_1(\phi,z)} \rho\, d\rho\, d\phi\, dz\ ,$$

and for spherical coordinates:

$$V = \int_{\phi_0}^{\phi_1} \int_{\theta_0(\phi)}^{\theta_1(\phi)} \int_{r_0(\theta,\phi)}^{r_1(\theta,\phi)} r^2 \sin(\theta)\ dr\, d\theta\, d\phi$$

Like the two-dimensional case, the volume element and integration region can be generalized (a fancy word for 'obscured'):

$$V = \int \int \int_{\mathcal{D}} dV$$

Hurricane Problem

In a simplified model of a hurricane, the velocity of the wind is taken to be purely in the circumferential direction and of magnitude

$$v(\rho, z) = \Omega\, \rho\, e^{-z/h - \rho/a}\ ,$$

where ρ and z are cylindrical coordinates measured from the eye of the hurricane at sea level, and Ω, h, a are positive constants. The density of the atmosphere is approximated by

$$d(z) = d_0\, e^{-z/h}\ .$$

Find the total kinetic energy of the motion.

As an integral, the kinetic energy is given by

$$T = \int \frac{1}{2} v^2\, dm\ .$$

This can be converted to a volume integral via the relation

$$\frac{dm}{dV} = d(z)\ ,$$

where dV is the volume element in cylindrical coordinates. The kinetic energy integral becomes

$$T = \int_0^{\infty} \int_0^{2\pi} \int_0^{\infty} \frac{1}{2} d(z) \left(v(\rho, z)\right)^2 dV\ ,$$

or

$$T = \frac{d_0 \Omega^2}{2} \int_0^{\infty} \int_0^{2\pi} \int_0^{\infty} e^{-z/h} \rho^2\, e^{-2z/h - 2\rho/a} \rho\, d\rho\, d\phi\, dz\ .$$

The integral can be broken apart into three separate integrals

$$T = \frac{d_0 \Omega^2}{2} \left(\int_0^{\infty} e^{-3z/h}\, dz\right) \left(\int_0^{2\pi} d\phi\right) \left(\int_0^{\infty} \rho^3 e^{-2\rho/a} d\rho\right)\ ,$$

each straightforwardly evaluated:

$$T = \frac{d_0 \Omega^2}{2} \left(\frac{h}{3}\right) (2\pi) \left(\frac{3a^4}{8}\right) = \frac{\pi}{8} \Omega^2 d_0 h a^4$$

2.5 Shell Theorem

Newton's law of gravitation tells us that every particle in the universe is trying to pull every other particle toward itself with a force proportional to the masses involved and inversely proportional to the square of the separation, and this is duly used to calculate the force onto planets, moons, satellites, and so on.

Using triple integration and spherical coordinates, something Newton didn't have, we finally address an assumption made early in gravitational analysis, namely *why* we're allowed to represent voluminous objects as single points located at the center of mass. This is called the shell theorem, and entails two important proofs.

Outside a Sphere

Consider a solid sphere of radius R, total mass M, and uniform density λ. Also let there be a test particle of mass m somewhere in space. Without loss of generality, place the test particle on the z-axis at the point $\vec{D} = D\,\hat{z}$. The length D is the distance from the test particle to the center of the sphere.

In order to 'properly' calculate the gravitational attraction between the test mass and the sphere, a volume integral over there entire sphere must be calculated. Choose any element of volume dV inside the sphere at location $\vec{r}$, which is located distance r from the center, at an angle θ from the z-axis.

Let vector $\vec{q}$ denote the line connecting $\vec{D}$ to $\vec{r}$ such that

$$\vec{r} + \vec{q} = D\,\hat{z} \, ,$$

and also let α be the angle between $\hat{z}$ and $\hat{q}$. From the law of cosines, we can say:

$$q^2 = r^2 + D^2 - 2rD\cos(\theta)$$
$$r^2 = q^2 + D^2 - 2qD\cos(\alpha)$$

The total force on the test particle is the vector $\vec{F}$. However, due to the ϕ-symmetry of this picture, only the z-component of the force will have a net effect on the particle. All xy-components cancel equally and oppositely:

$$F = \int_{\mathcal{D}} d\vec{F} \cdot \hat{z} = \int\int\int_{\text{volume}} dF\cos(\alpha)$$

The differential force is

$$dF = \frac{-Gm}{q^2}dm \, ,$$

where dm is the mass of the differential volume element influencing the test particle. The mass term can be replaced using the density

$$\frac{dm}{dV} = \frac{M}{4\pi R^3/3} = \lambda \, ,$$

where it is appropriate to replace dV with the volume element in spherical coordinates.

The force integral now is

$$F = -Gm\lambda \int_0^{2\pi}\int_0^{\pi}\int_0^{R} \frac{\cos(\alpha)}{q^2} r^2 \sin(\theta)\, dr\, d\theta\, d\phi \, ,$$

which, after substituting and simplifying a bit, becomes:

$$F = -Gm\lambda\frac{2\pi}{2D}\int_0^{\pi}\int_0^{R} \left(\frac{1}{q} + \frac{D^2 - r^2}{q^3}\right) r^2 \sin(\theta)\, dr\, d\theta$$

Perform implicit differentiation on the q^2 equation to find, remembering r and θ are independent,

$$q\,dq = rD\sin(\theta)\,d\theta \, ,$$

and rewrite the integral with the intent of integrating over r last. Make you you know why the limits are now changed:

$$F = -Gm\lambda\frac{\pi}{D^2}\int_0^{R}\int_{(D-r)}^{(D+r)} \left(1 + \frac{D^2 - r^2}{q^2}\right) r\, dq\, dr$$

The whole q-integral treats r as a constant and resolves to $4r$, so

$$F = -Gm\lambda\frac{\pi}{D^2}\int_0^{R} 4r^2\, dr \, ,$$

and the r-integral is elementary. Simplifying everything gives

$$F = -Gm\left(\frac{3M}{4\pi R^3}\right)\frac{\pi}{D^2}\frac{4}{3}R^3 = \frac{-GMm}{D^2} \, .$$

Conveniently, the force acts as if *all* of its mass were concentrated at the center. This result is also true in general, where the notion of 'center' means center of mass, not necessarily the center of the volume.

Inside a Shell

Another interesting question that arises in the course of studying gravity is, what does it feel like inside a hollow uniform shell? To pursue this question, suppose we have a thin spherical shell of radius R and thickness $2a$ that is much less than R, and the test particle is inside anywhere within the shell.

This setup borrows all of the geometry from the previous setup, except this time we have $D < R$, which is the important part. Setting up the same integral and doing the same simplifications, we can jump to

$$F = -Gm\lambda\frac{\pi}{D^2}\int_{R-a}^{R+a}\int_{(r-D)}^{(D+r)} \left(1 + \frac{D^2 - r^2}{q^2}\right) r\, dq\, dr \, .$$

Most notably, the lower integration in the q-integral is swapped to accommodate $D < R$. This causes the q-integral to resolve to zero, and we find

$$F = 0$$

inside the shell.

3 Partial Derivative

Returning to the definition of a function, recall that a function f depends on an input variable x in the function's domain. Given any input value, the output of the function is written $y = f(x)$, and there is only one y for a given x. The set of all y-values constitute the function's range. A 'curve' given by function $y = f(x)$ may exhibit a myriad of features: asymptotic behavior, periodicity, singularities, critical points, inflection points, etc.

Derivative

One star result from the analysis of curves gives the slope of the function at a point x_0, namely

$$\frac{d}{dx} f(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} .$$

Taylor's Theorem

The so-called derivative turns out to be just the first-order version of something more general we known as Taylor's theorem. Near the point x_0, we have:

$$f(x) \approx f(x_0) + \sum_{q=1}^{\infty} \frac{1}{q!} f^{(q)}(x_0)(x - x_0)^q$$

3.1 Slope on a Surface

The technical definition of the derivative generalizes to surfaces. For this, we require the surface $z = f(x, y)$ to be differentiable both in the x-direction and the y-direction, meaning that the slope of the surface at a point (x_0, y_0) has two answers: a slope along x, and a slope along y.

To express the slope on a surface at the point (x_0, y), we write the usual slope formula treating x as the 'active' variable with y as a constant:

$$\frac{\partial}{\partial x} f(x_0, y) = \lim_{x \to x_0} \frac{f(x, y) - f(x_0, y)}{x - x_0} \tag{1.1}$$

Meanwhile, the slope at the point (x, y_0) allows y to vary while x is constant:

$$\frac{\partial}{\partial y} f(x, y_0) = \lim_{y \to y_0} \frac{f(x, y) - f(x, y_0)}{y - y_0} \tag{1.2}$$

The familiar d/dx-notation is replaced by $\partial/\partial x$. The symbol ∂ denotes the *partial derivative.*

3.2 Mixed Partial Derivatives

One issue that needs to be settled right away is the idea of *mixed* partial derivatives. For the surface $z = f(x, y)$, let us find out whether

$$\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial z}{\partial y}\right) \tag{1.3}$$

is true. Using brute force, start with

$$\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right) = \frac{\partial}{\partial y}\left(\lim_{x \to x_0} \frac{f(x, y) - f(x_0, y)}{x - x_0}\right) ,$$

which becomes

$$\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right) = \lim_{y \to y_0} \lim_{x \to x_0} \frac{f(x, y) - f(x_0, y) - f(x, y_0) + f(x_0, y_0)}{(y - y_0)(x - x_0)} .$$

Now, it takes little to imagine doing a similar calculation with the y-partial derivative first to have

$$\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial y}\right) = \frac{\partial}{\partial x}\left(\lim_{y \to y_0} \frac{f(x, y) - f(x, y_0)}{y - y_0}\right) ,$$

which then simplifies to something nearly identical to the above, save one difference, which that the *order* of the limits is swapped. The task boils down to showing in this context that

$$\lim_{x \to x_0} \lim_{y \to y_0} \leftrightarrow \lim_{y \to y_0} \lim_{x \to x_0}$$

can be assumed.

To prove this, define two new functions

$$\begin{aligned} X(x, y) &= f(x, y) - f(x_0, y) \\ Y(x, y) &= f(x, y) - f(x, y_0) \ , \end{aligned}$$

and notice the following equality:

$$X(x, y) - X(x, y_0) = Y(x, y) - Y(x_0, y)$$

The left- and right-hand sides of the above each represent the endpoints of a secant line on the surface. By the mean value theorem, each can be replaced by partial derivatives as

$$(y - y_0)\frac{\partial}{\partial y} X(x, b) = (x - x_0)\frac{\partial}{\partial x} Y(a, y) \ ,$$

where

$$\begin{aligned} x_0 &< a < x \\ y_0 &< b < y \ . \end{aligned}$$

Keep simplifying to write

$$(y - y_0)\left(\frac{\partial}{\partial y} f(x, b) - \frac{\partial}{\partial y} f(x_0, b)\right) = (x - x_0)\left(\frac{\partial}{\partial x} f(a, y) - \frac{\partial}{\partial x} f(a, y_0)\right) ,$$

and use the mean value theorem a second time on each side to write

$$(y - y_0)(x - x_0) \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} f(\alpha, b) \right) = (x - x_0)(y - y_0) \frac{\partial}{\partial y} \left(\frac{\partial}{\partial x} f(a, \beta) \right) ,$$

where

$$\begin{aligned} x_0 &< \alpha < x \\ y_0 &< \beta < y \, . \end{aligned}$$

Closing the limits tighter, we see that the pair a, α tend to x_0, and also the pair b, β tend to y_0. In the differential limit, the left and right sides are equal and the proof is done.

3.3 Partial Derivative Operator

Like the ordinary derivative operator d/dx, the partial derivative operator is written $\partial/\partial x$. For shorthand, the same operator is often written with one 'partial' symbol and a subscript:

$$\frac{\partial}{\partial x} = \partial_x$$

In this notation, the mixed partial derivative Equation (1.3) is simply written

$$\partial_{yx} f(x, y) = \partial_{xy} f(x, y) \ ,$$

or with just the operators,

$$\partial_{yx} = \partial_{xy} \, .$$

Yet another nomenclature for partial derivatives involves placing a subscript with the function itself:

$$\frac{\partial}{\partial x} f(x, y) = f_x$$

Second Derivative

With the notion of partial derivatives, the idea of the second derivative of a function can go three ways. Each of the following is a second derivative operator

$$\partial_{xx} \qquad \partial_{xy} \qquad \partial_{yy}$$

and each produces, in the general case, a different result.

The partial derivative operator obeys the same algebraic rules as the ordinary derivative operator. Without abusing the notation, we can establish things like:

$$\begin{aligned} (\partial_x + \partial_y)(\partial_x - \partial_y) &= \partial_{xx} - \partial_{xy} + \partial_{yx} - \partial_{yy} \\ &= \partial_{xx} - \partial_{yy} \end{aligned}$$

Third Derivative

The equivalency of the mixed partial derivative extends to any depth. From Equation (1.3), we reason that

$$\partial_{yxx} \qquad \partial_{xyx} \qquad \partial_{xxy}$$

yield the same result. For this reason, it turns out there four *unique* third derivative operations:

$$\partial_{xxx} \qquad \partial_{xxy} \qquad \partial_{yyx} \qquad \partial_{yyy}$$

The notation can be condensed once more by using exponent notation on repeated derivatives:

$$\begin{aligned} \partial_{xxx} &= \partial_{x^3} \\ \partial_{xxy} &= \partial_{x^2 y} \\ \partial_{yyx} &= \partial_{xy^2} \\ \partial_{yyy} &= \partial_{y^3} \end{aligned}$$

3.4 Total Derivative

The notion of 'regular' derivative still survives the jump to more dimensions, and is given the name *total* derivative.

For a function $f(x, y, z)$ the total derivative with respect to a variable t sums across each partial derivative:

$$\frac{d}{dt} f(x, y, z) = \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt}$$

The Differential

Stripping away the dt-variable by the chain rule yields the so-called 'differential of' $f(x, y, z)$:

$$df(x, y, z) = \frac{\partial f}{\partial x} \, dx + \frac{\partial f}{\partial y} \, dy + \frac{\partial f}{\partial z} \, dz$$

3.5 Variable Integration Limits

It's possible for an integral to have variable limits, which can make a mess of things like integration by parts. Consider a function $y(x)$ and a two-variable function $f(x, y(x))$. By the fundamental theorem, this setup implies integrals of the form

$$F(x) = \int_{a(x)}^{b(x)} f(x, t) \, dt \, .$$

To attack this, define a helper function

$$G(x, y) = \int_{t_0}^{y} f(x, t) \, dt \, ,$$

so then $F(x)$ reads

$$F(x) = \int_{t_0}^{b(x)} f(x,t)\,dt - \int_{t_0}^{a(x)} f(x,t)\,dt \\ = G(x, b(x)) - G(x, a(x)) \ .$$

Take the total derivative of $F(x)$:

$$\frac{d}{dx}F(x) = \frac{\partial}{\partial x}G(x,b(x)) - \frac{\partial}{\partial x}G(x,a(x)) \\ + \frac{\partial}{\partial y}G(x,b(x))\frac{db}{dx} \\ - \frac{\partial}{\partial y}G(x,a(x))\frac{da}{dx}$$

The first two terms combine to make $\partial F/\partial x$. To handle the $\partial G/\partial y$ factors, define Δy such that

$$G(x, y+\Delta y) = \int_{t_0}^{y+\Delta y} f(x,t)\,dt$$

Unpack the right side and divide through by Δy to find

$$\frac{G(x,y+\Delta y) - G(x,y)}{\Delta y} = \frac{1}{\Delta y}\int_{y}^{y+\Delta y} f(x,t)\,dt \ .$$

In the limit $\Delta y \to 0$, the left side is $\partial G/\partial x$. The right simplifies to $f(x,y)$. In other words:

$$\frac{\partial}{\partial y}G(x,y) = f(x,y)$$

Putting the whole answer together, we have found

$$\frac{d}{dx}\int_{a(x)}^{b(x)} f(x,t)\,dt = \\ f(x,b(x))\frac{db}{dx} - f(x,a(x))\frac{da}{dx} \\ + \frac{\partial}{\partial x}\int_{a(x)}^{b(x)} f(x,t)\,dt \tag{1.4}$$

as the chief result, called the *Leibniz integral rule.*

Finally, since the operator ∂_x doesn't touch the y-variable, the last integral obeys:

$$\frac{\partial}{\partial x}\int_{a(x)}^{b(x)} f(x,t)\,dt = \int_{a(x)}^{b(x)} \frac{\partial}{\partial x} f(x,t)\,dt$$

<u>Problem 1</u>

Prove the following:

$$\frac{d}{dx}\int_0^x e^{xt^2}\,dt = e^{x^3} + \int_0^x \frac{\partial}{\partial x}e^{xt^2}\,dt$$

3.6 Two-Variable Taylor's Theorem

Taylor's theorem generalizes readily to surfaces. To get started, consider a fixed point (x_0, y_0) in the domain of a surface $z = f(x,y)$. Deviations from the fixed point are tracked by two quantities

$$\Delta x = x - x_0 \\ \Delta y = y - y_0 \ .$$

Like the one-dimensional Taylor's theorem, we're allowed to frame the final answer as an infinite sum. To do this, first notice that the one-dimensional case contains every whole number power of the quantity $x - x_0 = \Delta x$. Then, for two dimensions, we ought to need every whole number power of $\Delta x \Delta y$.

Of course, the factor $f^{(q)}(x_0)/q!$ that appears in the one-dimensional case can't work for two dimensions. Without knowing what to replace this with, let a set of unknown coefficients $\{C_{jk}\}$ stand in for now. With all this, the two-dimensional Taylor's theorem looks like:

$$f(x,y) \approx f(x_0,y_0) \\ + C_{10}\Delta x + C_{01}\Delta y \\ + C_{20}\Delta x^2 + C_{11}\Delta x\Delta y + C_{02}\Delta y^2 \\ + C_{30}\Delta x^3 + C_{21}\Delta x^2\Delta y + C_{12}\Delta x\Delta y^2 + C_{03}\Delta y^3 \\ + \cdots$$

Now we have the problem of determining each unknown coefficient C_{jk}. Begin by applying the ∂_x operator across the whole equation, and then evaluate the equation at (x_0, y_0). With almost no effort, we can see that any terms containing Δx^2 or higher power will zero out, and the whole result is

$$\partial_x f(x_0,y_0) = C_{10} \ .$$

Applying the ∂_y instead and doing the exercise again leads to a similar result

$$\partial_y f(x_0,y_0) = C_{01} \ .$$

For the next 'row' of coefficients, apply the ∂_{xx}, ∂_{xy}, ∂_{yy} operators respectively, and evaluate at (x_0, y_0). This saps all but the order-two terms in the equation, from which we find:

$$\partial_{xx} f(x_0,y_0) = 2 \cdot C_{20} \\ \partial_{xy} f(x_0,y_0) = C_{11} \\ \partial_{yy} f(x_0,y_0) = 2 \cdot C_{02}$$

Solving for the order-three coefficients means using the four operators ∂_{x^3}, ∂_{x^2y}, ∂_{xy^2}, ∂_{y^3} to $f(x,y)$

and evaluate at (x_0, y_0). This gives four new equations:

$$\begin{aligned}
\partial_{x^3} f(x_0, y_0) &= 3 \cdot 2 \cdot C_{30} \\
\partial_{x^2 y} f(x_0, y_0) &= 2 \cdot C_{21} \\
\partial_{xyy} f(x_0, y_0) &= 2 \cdot C_{12} \\
\partial_{yyy} f(x_0, y_0) &= 3 \cdot 2 \cdot C_{03}
\end{aligned}$$

To summarize and condense notation once more, use using the general shorthand

$$z_{x^j y^k} = \partial_{x^j y^k} f(x_0, y_0) \ ,$$

and we have found

$$\begin{aligned}
C_{10} &= z_x \\
C_{01} &= z_y
\end{aligned}$$

$$\begin{aligned}
C_{20} &= z_{x^2}/2 \\
C_{11} &= z_{xy} \\
C_{02} &= z_{y^2}/2
\end{aligned}$$

$$\begin{aligned}
C_{30} &= z_{x^3}/3! \\
C_{21} &= z_{x^2 y}/2 \\
C_{12} &= z_{xy^2}/2 \\
C_{03} &= z_{y^3}/3!
\end{aligned}$$

The two-dimensional Taylor's theorem now looks like:

$$\begin{aligned}
&f(x, y) \approx f(x_0, y_0) \\
&+ z_x \Delta x + z_y \Delta y \\
&+ \frac{z_{x^2} \Delta x^2 + 2 z_{xy} \Delta x \Delta y + z_{y^2} \Delta y^2}{2} \\
&+ \frac{z_{x^3} \Delta x^3 + 3 z_{x^2 y} \Delta x^2 \Delta y + 3 z_{xy^2} \Delta x \Delta y^2 + z_{y^3} \Delta y^3}{3!} \\
&+ \cdots
\end{aligned}$$

Look for a moment at the pattern in the numerical coefficients in the numerator of each term written so far. Jotting these down:

$$\begin{array}{ccccccc}
 & & & 1 & & & \\
 & & 1 & & 1 & & \\
 & 1 & & 2 & & 1 & \\
1 & & 3 & & 3 & & 1
\end{array}$$

The pattern is clearly that of the binomial coefficients, i.e. the entries of Pascal's triangle. This means that the terms in the infinite sum can be regrouped as binomials with the help of the partial derivative operator. For instance, the order-two terms are written

$$\begin{aligned}
&z_{x^2} \Delta x^2 + 2 z_{xy} \Delta x \Delta y + z_{y^2} \Delta y^2 \\
&\qquad = (\Delta x \, \partial_x + \Delta y \, \partial y)^2 f(x_0, y_0) \ ,
\end{aligned}$$

and similarly for all orders.

Switching to summation notation, we finally have the two-dimensional Taylor's theorem

$$\begin{aligned}
&f(x, y) \approx f(x_0, y_0) \\
&\qquad + \sum_{q=1}^{\infty} \frac{1}{q!} (\Delta x \, \partial_x + \Delta y \, \partial y)^q f(x_0, y_0)
\end{aligned} \tag{1.5}$$

For a sanity check, you can see that if all $y = 0$ then the above reduces to the familiar one-dimensional form.

3.7 Error Analysis

In any experiment, a measured quantity A should always be accompanied by a window of uncertainty ΔA such that the working value is $A \pm \Delta A$. The same goes for any other measured quantity B, which is alone meaningless without writing $B \pm \Delta B$.

Supposing we're interested in the product $P = AB$ of two measured values, we write

$$\begin{aligned}
P + \Delta P &= (A \pm \Delta A)(B \pm \Delta B) \\
&= AB + A \Delta B + B \Delta A + \Delta A \Delta B \, .
\end{aligned}$$

If the uncertainties ΔA, ΔB are much less than the principal values A, B, then the product $\Delta A \Delta B$ is very small compared to the other terms and is effectively zero. Thus, the uncertainty in P is

$$\pm \Delta P = A \Delta B + B \Delta A \, ,$$

simplifying to

$$\pm \frac{\Delta P}{P} = \left(\frac{\Delta A}{A} + \frac{\Delta B}{B} \right) \ ,$$

or, again because $\Delta A \Delta B$ is negligible:

$$\frac{\Delta P}{P} = \sqrt{\left(\frac{\Delta A}{A} \right)^2 + \left(\frac{\Delta B}{B} \right)^2}$$

Interestingly, the same form arises from the first-order Taylor's theorem in two dimensions. For a general function $F = F(A \pm \Delta A, B \pm \Delta B)$, we find

$$(\Delta F)^2 \approx \left(\frac{\partial F}{\partial A} \right)^2 (\Delta A)^2 + \left(\frac{\partial F}{\partial B} \right)^2 (\Delta B)^2 \ ,$$

which readily generalizes for more variables. In the following we bloom out the expansion for ΔF for common scenarios.

Sums and Differences

Consider three measured quantities A, B, C such that

$$F = A + B - C\,.$$

The above trivially delivers

$$\Delta F = \sqrt{\Delta A^2 + \Delta B^2 + \Delta C^2}\,.$$

Products

For the product $P = AB$, we already found that the uncertainty in P is given by

$$\frac{\Delta P}{P} = \sqrt{\left(\frac{\Delta A}{A}\right)^2 + \left(\frac{\Delta B}{B}\right)^2}\,.$$

For example, if the dimensions of a box are given by $L \pm \Delta L$, $W \pm \Delta W$, $H \pm \Delta H$, then the uncertainty in the volume $V = LWH$ is

$$\Delta V = V\sqrt{\frac{\Delta L^2}{L^2} + \frac{\Delta W^2}{W^2} + \frac{\Delta H^2}{H^2}}\,.$$

The surface area of one L-face is approximated to first order via

$$L^2 + 2L\Delta L = A_L + \Delta A_L\,.$$

and similar for the W- and H-faces. Thus the uncertainty in the total surface area

$$S = 2\left(A_L + A_W + A_H\right)$$

is

$$\Delta S = 4\sqrt{L^2\Delta L^2 + W^2\Delta W^2 + H^2\Delta H^2}\,.$$

Ratios

As it turns out, the same uncertainty formula applies to thje product $P = AB$ and to the ratio $R = A/B$. In detail:

$$\begin{aligned}
(\Delta R)^2 &= \frac{1}{B^2}(\Delta A)^2 + \frac{A^2}{B^4}(\Delta B)^2 \\
\frac{(\Delta R)^2}{R^2} &= \frac{(\Delta A)^2}{A^2} + \frac{(\Delta B)^2}{B^2} \\
\frac{\Delta R}{R} &= \frac{\Delta P}{P}
\end{aligned}$$

Exponents

For the quantity $F = A^p B$, where p is an exponent with no uncertainty, it's straightforwardly shown that

$$\frac{\Delta F}{F} = \sqrt{\left(\frac{p\Delta A}{A}\right)^2 + \left(\frac{\Delta B}{B}\right)^2}\,.$$

Electrical Resistors

Two electrical resistors R_1, R_2 can be arranged in series to form an effective resistor

$$R_S = R_1 + R_2\,,$$

or arranged in parallel such that

$$R_P = \frac{1}{1/R_1 + 1/R_2}\,.$$

Of course, electrical resistors are always imperfect, thus we should introduce uncertainties ΔR_1, ΔR_2 to get a sense of ΔR_S, ΔR_P.

For ΔR_S, we simply write

$$\Delta R_S = \sqrt{\Delta R_1^2 + \Delta R_2^2}$$

without any hard work. For ΔR_P, we eventually find

$$\begin{aligned}
\Delta R_P &= \sqrt{\left(\frac{\partial R_P}{\partial R_1}\right)^2 \Delta R_1^2 + \left(\frac{\partial R_P}{\partial R_2}\right)^2 \Delta R_2^2} \\
&= R_P^2\sqrt{\frac{\Delta R_1^2}{R_1^4} + \frac{\Delta R_2^2}{R_2^4}}\,.
\end{aligned}$$

4 Numerical Methods

4.1 Regression Analysis

Regression analysis is an attempt to derive meaningful patterns from numerical data. To introduce the subject, we'll explore the scenario of fitting a curve $y = f(x)$ to a set of given data points $\{(x_j, y_j)\}$ in various ways.

Linear Fit

Suppose we're provided with the following set of ordered pairs:

x_j	0.6	1.8	2.8	3.6	4.2	5.6
y_j	1.6	1.6	2.6	2.0	4.0	3.6

Take each pair (x_j, y_j) with $j = 1, 2, \ldots, n$ as a point in the Cartesian plane. Further, suppose there was reason to believe that the pattern in the provided points is described by a straight line in the plane

$$y = mx + b\,,$$

where the slope m and y-intercept b are unknown, and to be found using the data provided.

To advance on the problem, move all variables to one side, and consider n instances of the equation

$$h_j(m, b) = mx_j + b - y_j\,.$$

That is, h_j measures the vertical distance between the point $mx_j + b$ and y_j. If the approximate line passes directly through (x_j, y_j), then $h_j(m, b) = 0$ for that point.

As defined, $h_j(m, b)$ could be a positive or a negative value, which would mean negative errors cancel out positive ones. To avoid this, let us work with the square of the vertical distance represented by h_j and call this a new function $F_j(m, b)$:

$$F_j(m, b) = (mx_j + b - y_j)^2$$

The total vertical distance from each point (x_j, y_j) to the line $y = mx + b$ is the sum of all F_j:

$$F(m, b) = \sum_{j=1}^{n} F_j(m, b) = \sum_{j=1}^{n} (mx_j + b - y_j)^2$$

Now comes the new idea. The ideal m and b for the data provided should correspond to a minimum in $F(m, b)$. That is, set the partial derivatives of F with respect to these variables to zero, and the correct m, b are implicated. We then have

$$\frac{\partial F}{\partial m} = 0 = \sum_{j=1}^{n} 2x_j (mx_j + b - y_j)$$

$$\frac{\partial F}{\partial b} = 0 = \sum_{j=1}^{n} 2(mx_j + b - y_j) \ .$$

To keep the algebra contained, define the quantity

$$X^\alpha Y^\beta = \sum_{j=1}^{n} x_j^\alpha y_j^\beta \ ,$$

which isn't treated as regular algebraic variable, for instance $(X)(X) \not= X^2$, and $(X)(Y) \not= XY$. Note for this example we have α, β never exceeding one.

In terms of the sums X, Y, etc., the minimization of $F(m, b)$ gives a system of two equations with two unknowns:

$$bn + mX = Y$$

$$bX + mX^2 = YX$$

The solution is straightforward using matrix methods or traditional:

$$m = \frac{(n)(XY) - (X)(Y)}{(n)(X^2) - (X)(X)}$$

$$b = \frac{(Y)(X^2) - (X)(XY)}{(n)(X^2) - (X)(X)}$$

To finish the example on hand, use a calculator to find $X = 18.6$, $Y = 15.4$, $XY = 55.28$, $X^2 = 73.4$. The final answer is:

$$m \approx 0.479$$

$$b \approx 1.082$$

Exponential Fit

Consider another set of points $\{(x_j, y_j)\}$ in the Cartesian plane that would be best approximated by an exponential fit

$$y(x) = A\, e^{mx} \ ,$$

where the scaling constant A and exponential parameter m are to be determined form the data given.

For this problem, let $A = \ln(b)$, where b is another constant, and the equation becomes $y = e^{mx+b}$. Take the natural log of both sides to write

$$\ln(y) = mx + b \ .$$

From here, the problem is completely analogous to the straight-line fit, except all y_j are substituted for $\ln(y_j)$. One b is known, reverse the logarithm to solve for A.

Polynomial Fit

For any set of of n total points (x_j, y_j) in the Cartesian plane, we can try a polynomial of order $m < n$ to fit the data:

$$y(x) = A_0 + A_1 x + A_2 x^2 + \cdots + A_m x^m$$

Similar to the straight-line fit, define a vertical distance $h_j(\{A_m\})$ such that

$$h_j = A_0 + A_1 x_j + A_2 x_j^2 + \cdots + A_m x_j^m - y_j \ .$$

Square this distance and sum over all n data points:

$$F(\{A_m\}) = \sum_{j=1}^{n} h_j^2$$

$$= \sum_{j=1}^{n} \left(A_0 + A_1 x_j + \cdots + A_m x_j^m - y_j\right)^2$$

The best-fitting polynomial is the one that that minimizes F with respect to all A_j simultaneously. Writing these out, one finds

$$\frac{\partial F}{\partial A_0} = 2\sum_{j=1}^{n} \left(A_0 + A_1 x_j + \cdots + A_m x_j^m - y_j\right)$$

$$\frac{\partial F}{\partial A_1} = 2\sum_{j=1}^{n} x_j \left(A_0 + A_1 x_j + \cdots + A_m x_j^m - y_j\right)$$

$$\frac{\partial F}{\partial A_2} = 2\sum_{j=1}^{n} x_j^2 \left(A_0 + A_1 x_j + \cdots + A_m x_j^m - y_j\right) \ ,$$

availing the pattern

$$\frac{\partial F}{\partial A_k} = 2\sum_{j=1}^{n} x_j^k \left(A_0 + A_1 x_j + \cdots + A_m x_j^m - y_j\right) ,$$

for any $k \le m$.

Each derivative is zero on the left, and the universal factor of 2 drops out. Not forgetting to distribute the x_j^k term into each sum, all of the above information is best written in matrix notation. In particular, we have

$$M = \begin{bmatrix} n & X & X^2 & \cdots & X^m \\ X & X^2 & X^3 & \cdots & X^{m+1} \\ X^2 & X^3 & X^4 & \cdots & X^{m+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ X^m & X^{m+1} & X^{m+2} & \cdots & X^{2m} \end{bmatrix} ,$$

such that

$$M \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \cdots \\ A_m \end{bmatrix} = \begin{bmatrix} Y \\ YX \\ YX^2 \\ \cdots \\ YX^m \end{bmatrix} .$$

There is a lot of information to juggle with if you're insane enough to do this by hand. Regardless, system can be solved by finding the row-reduced echelon form of:

$$\begin{bmatrix} n & X & X^2 & \cdots & X^m & Y \\ X & X^2 & X^3 & \cdots & X^{m+1} & YX \\ X^2 & X^3 & X^4 & \cdots & X^{m+2} & YX^2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ X^m & X^{m+1} & X^{m+2} & \cdots & X^{2m} & YX^m \end{bmatrix}$$

For one example, consider the following list of $n = 11$ ordered pairs:

x_j	0	1	2	3	4	5
y_j	1	6	17	34	57	86

x_j	6	7	8	9	10
y_j	121	162	209	262	321

Supposing there were reason to choose $m = 3$ for a quadratic approximation, we would then write

$$\begin{bmatrix} n & X & X^2 \\ X & X^2 & X^3 \\ X^2 & X^3 & X^4 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} Y \\ YX \\ YX^2 \end{bmatrix} ,$$

which, using the numbers on hand, evaluates to

$$\begin{bmatrix} 11 & 55 & 385 \\ 55 & 385 & 3025 \\ 385 & 3025 & 25333 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} 1276 \\ 9900 \\ 82434 \end{bmatrix} .$$

By standard means, we ultimately find $A_0 = 1$, $A_1 = 2$, $A_2 = 3$, or:

$$y(x) = 1 + 2x + 3x^2$$

4.2 Interpolation

In regression analysis, a set of n total data points $\{(x_j, y_j)\}$, leads to a best-fit polynomial (or other curve) that passes near, but not necessarily through each data point. By a more powerful process called *interpolation*, it's possible to find a curve that passes through each data point. With some effort, such a curve can be made continuous and smooth in its domain.

Rectangle Approximation

The crudest interpolation of the provided data points is the rectangular approximation, which draws a horizontal line for all $n - 1$ points spanning from x_j to x_{j+1} such that

$$f_0(x_j \le x < x_{j+1}) = y_j$$

Of course, we can also draw lines to the left instead of the right by a shift of index:

$$f_0(x_j \le x < x_{j+1}) = y_{j+1}$$

Connect the Dots

A slightly more informative approximation to the provided data points is the linear interpolation, which is a fancy name for connect the dots. By standard straight line methods, successive data points are connect by lines given by

$$f_1(x) = y_j + (x - x_j)\left(\frac{y_{j+1} - y_j}{x_{j+1} - x_j}\right) .$$

This has the appearance of a first terms of a Taylor approximation and also the form $y = mx + b$. All of these are equivalent to linear order.

There is another way to express the line $f_1(x)$ that appears mighty peculiar at first:

$$f_1(x) = y_j\left(\frac{x_{j+1} - x}{x_{j+1} - x_j}\right) + y_{j+1}\left(\frac{x - x_j}{x_{j+1} - x_j}\right)$$

Make sure the two expressions for $f_1(x)$ are equivalent.

Quadratic Interpolation

The linear interpolation can be improved by including an x^2-like term in $f(x)$, giving a quadratic interpolation in terms of undermined coefficients:

$$f_2(x) = A_0 + A_1 x + A_2 x^2$$

One way to find the unknown coefficients is to pick three consecutive points, such as (x_j, y_j) with $j = 0, 1, 2$. This generates three equations and three unknowns, which can be solved by standard means.

For a different approach to the problem, let us recite a trick named after Lagrange, which extends the 'peculiar' straight line method written above. The quadratic approximation is called the *Lagrange integrating polynomial*, and is given by

$$f_2(x) = y_0 L_0(x) + y_1 L_1(x) + y_2 L_2(x) \ ,$$

where the $L_j(x)$ are called the *Lagrange interpolating basis functions*:

$$\begin{aligned} L_0 &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \\ L_1 &= \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \\ L_2 &= \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} \end{aligned}$$

This can be straightforwardly reconciled with a traditional attack on the problem. In the original function $f_2(x)$, observe that A_2 is exactly one half of the second derivative of the function.

From ordinary calculus, we know the second derivative can be expressed via

$$f''(x) = \lim_{h \to 0} \frac{f(x - h) - 2f(x) + f(x + h)}{h^2} \ .$$

This formula is a bit oversimplifying in the sense that h doesn't necessarily equal any given pair $x_j - x_k$, never mind the limit.

Proceed by differentiating $f_2(x)$ twice (only the x^2 term survives). To keep the algebra sane, define

$$\Delta x_{jk} = x_j - x_k \ ,$$

and we have

$$\frac{1}{2} f_2''(x) = \frac{y_0}{\Delta x_{01} \Delta x_{02}} + \frac{y_1}{\Delta x_{10} \Delta x_{12}} + \frac{y_2}{\Delta x_{20} \Delta x_{21}} \ .$$

Establish a common denominator and rewrite:

$$\frac{1}{2} f_2''(x) = \frac{y_0 \Delta x_{12} - y_1 \Delta x_{02} + y_2 \Delta x_{01}}{\Delta x_{01} \Delta x_{02} \Delta x_{12}}$$

This is technically as far as the comparison can go. To an approximation though, we can have

$$h = x_1 - x_0 = x_2 - x_1 = \frac{x_2 - x_0}{2}$$

and the two second derivative formulas agree.

Higher Orders

The Lagrange interpolating basis functions readily generalize to higher orders. With the products

$$\begin{aligned} Q_n(x) &= \prod_{j \neq n} (x - x_j) \\ R_n(x) &= \prod_{j \neq n} (x_n - x_j) \ , \end{aligned}$$

the nth function is

$$L_n(x) = \frac{Q_n(x)}{R_n(x)} \ .$$

In therms of he Lagrange interpolating basis functions, the corresponding $y_n(x)$ is

$$y_n(x) = \sum_{j=0}^{n} y_j L_j(x) \ .$$

4.3 Spline

There is a handy method that combines polynomial interpolation with derivative matching. That is, if we have a set of n points $\{(x_j, y_j)\}$, where $j = 1, 2, 3, \ldots, n$, it's possible to come up with a curve that connects all of the points continuously and smoothly.

Cubic Approximation

In the domain $x_j < x < x_{j+1}$, a cubic interpolation going through the points x_j, x_{j+1} is assumed, taking generic form

$$f_j(x) = \sum_{j=0}^{3} A_j x^j \ .$$

Continuity Conditions

For continuity across the entire function f, we must have

$$\begin{aligned} f_{j-1}(x_j) &= f_j(x_j) \\ f_j(x_{j+1}) &= f_{j+1}(x_{j+1}) \ , \end{aligned}$$

which says the same thing twice. (Substitute $j \to j + 1$ in the first equation to recover the second.)

For continuity in derivative of f, differentiate each of the above once with respect to x

$$f'_{j-1}(x_j) = f'_j(x_j)$$
$$f'_j(x_{j+1}) = f'_{j+1}(x_{j+1}) \ ,$$

and then once more:

$$f''_{j-1}(x_j) = f''_j(x_j)$$
$$f''_j(x_{j+1}) = f''_{j+1}(x_{j+1}) \ ,$$

If there are n total points provided, there must be $n-1$ polynomials in the total interpolation, with a total of $4(n-1)$ unknowns. However, only $4(n-2)$ equations come from continuity arguments, and we need four more.

At the first point $j=1$ and the last point $j=n$, we set

$$f_1(x_1) = y_1$$
$$f_{n-1}(x_n) = y_n \ .$$

With the leftover freedom to impose two more equations, choose the second derivative to be zero at each endpoint:

$$f''_1(x_1) = 0$$
$$f''_{n-1}(x_n) = 0$$

This setup is called the *natural spline.*

Second Derivative Continuity

This is enough to assemble the whole curve. Begin with the abbreviation

$$k_j = f''_{j-1}(x_j) = f''_j(x_j) \ .$$

Between neighboring k_j, k_{j+1}, the second derivative of $f''_j(x)$ is a straight line connecting the two. Express this line as a two-point Lagrange system:

$$f''_j(x) = k_j\left(\frac{x-x_{j+1}}{x_j-x_{j+1}}\right) + k_{j+1}\left(\frac{x-x_j}{x_{j+1}-x_j}\right)$$

Integrate the above in the x-variable once to get an equation for $f'_j(x)$

$$f'_j(x) = \int f''_j(x)\,dx + C \ ,$$

where C is an integration constant. Substituting the above and carrying out the integral, one finds

$$f'_j(x) = \frac{k_j}{(x_j-x_{j+1})}\frac{(x-x_{j+1})^2}{2} + \frac{k_{j+1}}{(x_{j+1}-x_j)}\frac{(x-x_j)^2}{2} + C \ .$$

Integrate again to get an equation for $f_j(x)$

$$f_j(x) = \frac{k_j}{(x_j-x_{j+1})}\frac{(x-x_{j+1})^3}{3\cdot 2} + \frac{k_{j+1}}{(x_{j+1}-x_j)}\frac{(x-x_j)^3}{3\cdot 2} + Cx + D \ ,$$

where D is another integration constant.

The substitutions

$$C = A - B$$
$$D = -Ax_{j+1} + Bx_j$$

makes the above be slightly easier to work with:

$$f_j(x) = \frac{k_j}{(x_j-x_{j+1})}\frac{(x-x_{j+1})^3}{3\cdot 2} - \frac{k_{j+1}}{(x_j-x_{j+1})}\frac{(x-x_j)^3}{3\cdot 2} + A(x-x_{j+1}) - B(x-x_j)$$

Integration Constants

The integration constants need to be determined before moving on. Evaluate $f_j(x_j)$ to find

$$y_j = \frac{k_j}{(x_j-x_{j+1})}\frac{(x_j-x_{j+1})^3}{3\cdot 2} + A(x_j-x_{j+1}) \ ,$$

or

$$A = \frac{y_j}{(x_j-x_{j+1})} - k_j\frac{(x_j-x_{j+1})}{3\cdot 2} \ .$$

Evaluate $f_j(x_{j+1})$ to find

$$y_{j+1} = \frac{k_{j+1}}{(x_j-x_{j+1})}\frac{(x_j-x_{j+1})^3}{3\cdot 2} + B(x_j-x_{j+1}) \ ,$$

or

$$B = \frac{y_{j+1}}{(x_j-x_{j+1})} - k_{j+1}\frac{(x_j-x_{j+1})}{3\cdot 2} \ .$$

Putting the whole solution together:

$$f_j(x) = \frac{k_j}{6}\left(\frac{(x-x_{j+1})^3}{(x_j-x_{j+1})} - (x-x_{j+1})(x_j-x_{j+1})\right) - \frac{k_{j+1}}{6}\left(\frac{(x-x_j)^3}{(x_j-x_{j+1})} - (x-x_{j+1})(x_j-x_{j+1})\right) + \frac{y_j(x-x_{j+1}) - y_{j+1}(x-x_j)}{x_j-x_{j+1}}$$

First Derivative Continuity

What remains is to determine the terms k_j in terms of $\{(x_j, y_j)\}$. Write out the derivatives $f'_j(x_j)$ and $f'_{j-1}(x_j)$ and set them equal (as agreed earlier). For an updated $f'_j(x)$, we have

$$\begin{aligned} f'_j(x) = & \\ & \frac{k_j}{6}\left(\frac{3(x-x_{j+1})^2}{(x_j-x_{j+1})} - (x_j - x_{j+1})\right) \\ & - \frac{k_{j+1}}{6}\left(\frac{3(x-x_j)^2}{(x_j-x_{j+1})} - (x_j - x_{j+1})\right) \\ & + \frac{y_j - y_{j+1}}{x_j - x_{j+1}} \end{aligned}$$

and also, shifting index,

$$\begin{aligned} f'_{j-1}(x) = & \\ & \frac{k_{j-1}}{6}\left(\frac{3(x-x_j)^2}{(x_{j-1}-x_j)} - (x_{j-1} - x_j)\right) \\ & - \frac{k_j}{6}\left(\frac{3(x-x_{j-1})^2}{(x_{j-1}-x_j)} - (x_{j-1} - x_j)\right) \\ & + \frac{y_{j-1} - y_j}{x_{j-1} - x_j} . \end{aligned}$$

For shorthand, define

$$\begin{aligned} \Delta x_{j+} &= x_j - x_{j+1} \\ \Delta x_{j-} &= x_j - x_{j-1} \end{aligned}$$

and similar for the y-variables. Then evaluate each derivative equation at x_j and equate the results to get the continuity equation

$$\begin{aligned} & k_{j+1}\Delta x_{j+} + 2k_j(\Delta x_{j+} - \Delta x_{j-}) \\ & \qquad - k_{j-1}\Delta x_{j-} = 6\left(\frac{\Delta y_{j-}}{\Delta x_{j-}} - \frac{\Delta y_{j+}}{\Delta x_{j+}}\right) . \end{aligned}$$

Creating a System

For yet another shorthand, define the coefficients

$$\begin{aligned} \alpha_j &= -\Delta x_{j-} \\ \beta_j &= 2(\Delta x_{j+} - \Delta x_{j-}) \\ \gamma_j &= \Delta x_{j+} \\ \delta_j &= 6\left(\frac{\Delta y_{j-}}{\Delta x_{j-}} - \frac{\Delta y_{j+}}{\Delta x_{j+}}\right) \end{aligned}$$

which are all known in terms of the provided points. Then, the above can be written

$$\alpha_j k_{j-1} + \beta_j k_j + \gamma_j k_{j+1} = \delta_j ,$$

which has three unknowns in general, and we already decided $k_1 = k_n = 0$. Thus only the cases $j = 2, 3, 4, \ldots, n-1$ need be written out.

Example n=5

Choosing a modest example with $n = 5$ points provided, the above becomes:

$$\begin{aligned} \alpha_2 0 + \beta_2 k_2 + \gamma_2 k_3 &= \delta_2 \\ \alpha_3 k_2 + \beta_3 k_3 + \gamma_3 k_4 &= \delta_3 \\ \alpha_4 k_3 + \beta_4 k_4 + \gamma_4 0 &= \delta_4 \end{aligned}$$

This is a system of three equations and three unknowns k_2, k_3, k_4, and the problem has been reduced to a regular $A\vec{x} = \vec{b}$-like system.

In general, the spline calculation leads to a hefty augmented matrix with $n-2$ rows and $n-1$ columns.

4.4 Newton's Method

In one dimension, Newton's method is a reliable means for estimating the roots of an equation $g(x)$, which is to say finding the x-value(s) that solve $g(x) = 0$.

The formula for Newton's method comes from a first-order approximation of $g(x)$, namely

$$g_1(x) = g(x_0) + g'(x_0)(x - x_0) .$$

Providing an initial guess x_0 and letting $g_1(x_1) = 0$ implicates a new x_1 that should be an improvement over x_0. This can be continued recursively via the formula

$$x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)} .$$

Multivariate Newton's Method

Newton's method readily generalizes to multiple dimensions, which is to say, to systems of n equations with n unknowns. We assume the system is prepared such that the jth equation obeys

$$g_j\left(x^1, x^2, \ldots, x^n\right) = 0 ,$$

where the index j runs from 1 to n. For convenience, define a vector

$$\vec{x} = \left(x^1, x^2, \ldots, x^n\right)$$

so the above is concisely written $g_j(\vec{x}) = 0$.

Choosing an arbitrary x^k and expanding g_j to first order via Taylor expansion leads to

$$g_j\left(x^k\right) \approx g_j\left(x_0^k\right) + \sum_{k=1}^{n} \left.\frac{\partial g_j(\vec{x})}{\partial x^k}\right|_{x_0^k} \left(x^k - x_0^k\right) .$$

Proceed by defining a vector

$$\vec{g} = \left(g_1\left(\vec{x}\right), g_2\left(\vec{x}\right), \ldots, g_n\left(\vec{x}\right)\right) \ ,$$

along with a matrix J such that

$$J_{jk} = \left.\frac{\partial g_j\left(\vec{x}\right)}{\partial x^k}\right|_{\vec{x}_0} \ ,$$

so the above becomes

$$\vec{g}\left(\vec{x}\right) \approx \vec{g}\left(\vec{x}_0\right) + J\left(\vec{x} - \vec{x}_0\right) \ .$$

Analogous to the one-dimensional case, we take $\vec{x}_0 \rightarrow \vec{x}_n$ as an intial guess and set the left side to zero. Then, we can 'solve' for $\vec{x}_{n+1}$ in terms of the inverse of J:

$$\vec{x}_{n+1} = \vec{x}_n - J^{-1}\vec{g}\left(\vec{x}_n\right)$$

There is another way to proceed without calculating the inverse J^{-1}. Instead of solving for $\vec{x}_{n+1}$ directly, write

$$J\vec{x}_{n+1} = J\vec{x}_n - \vec{g}\left(\vec{x}_n\right) \ ,$$

and observe the right side is completely determined in terms of $\vec{x}_n$. Storing this result in a vector $\vec{b}_n$, we have a system

$$J\vec{x}_{n+1} = \vec{b}_n \ .$$

As an $A\vec{x} = \vec{b}$-like linear system, the above can be solved by finding the row-reduced echelon form (RREF) of the augmented matrix $J|\vec{b}_n$.

Example

Consider the nonlinear system of equations

$$\begin{aligned} 2x^2 + 3y &= 1 \\ 4x - 7y &= 3 \ , \end{aligned}$$

which, for the sake of this example, has two solutions attainable by standard means:

$$(x, y) = \begin{cases} (-1.58032, -1.33161) \\ (0.72318, -0.0153259) \end{cases}$$

Using Newton's method formalism, the above system reads

$$\begin{aligned} g_1\left(x\right) &= 2x^2 + 3y - 1 \\ g_2\left(x\right) &= 4x - 7y - 3 \ . \end{aligned}$$

Computing partial derivatives of $g_{1,2}\left(x\right)$, we attain the matrix components of matrix J, required for both the inverse method involving J^{-1} and the RREF method involving $J|\vec{b}_n$ as described. For this we have $J_{11} = 4x$, $J_{12} = 3$, $J_{21} = 4$, $J_{22} = -7$, or

$$J = \begin{bmatrix} 4x & 3 \\ 4 & -7 \end{bmatrix} \ .$$

It's also necesary to provide an initial guess $\vec{x}_0$ for each solution we're shooting for. In this case, the system represented is the intersection of a line and a parabola, thus there are at most two solutions to attain, and we'll work with the initial values:

$$(x_0, y_0) = \begin{cases} (1, 1) \\ (-1, -1) \end{cases}$$

Proceeding with the inverse method, we first establish

$$J^{-1} = \frac{1}{-28x - 12}\begin{bmatrix} -7 & -3 \\ -4 & 4x \end{bmatrix}$$

by standard means. Next write

$$\begin{aligned} \vec{x}_{n+1} &= \vec{x}_n \\ &\quad - \frac{1}{-28x_n - 12}\begin{bmatrix} -7 & -3 \\ -4 & 4x_n \end{bmatrix}\begin{bmatrix} 2x_n^2 + 3y_n - 1 \\ 4x_n - 7y_n - 3 \end{bmatrix} \end{aligned}$$

for both initial values $\vec{x}_0$.

Starting with $\vec{x}_0 = (-1, -1)$, the above calculation recursively proceeds as

$$\begin{bmatrix} -1 \\ -1 \end{bmatrix} \rightarrow \begin{bmatrix} -1.875 \\ -1.5 \end{bmatrix} \rightarrow \begin{bmatrix} -1.610 \\ -1.349 \end{bmatrix} \rightarrow \begin{bmatrix} -1.581 \\ -1.332 \end{bmatrix} \ ,$$

which is surely converging to the reported solution $(-1.58, -1.33)$. Repeating for $\vec{x}_0 = (1, 1)$, we correspondingly find

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} -0.75 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0.723 \\ -0.0152 \end{bmatrix} \rightarrow \begin{bmatrix} 0.723 \\ -0.0153 \end{bmatrix} \ ,$$

which converges to the other stated solution $(0.723, -0.0153)$.

For another approach, we calculate the $\vec{x}_{n+1}$th iteration from $J|\vec{b}_n$ using the augmented matrix

$$\begin{bmatrix} 4x_n & 3 & J_{11}x_n + J_{12}y_n - g_1\left(x_n, y_n\right) \\ 4 & -7 & J_{21}x_n + J_{22}y_n - g_2\left(x_n, y_n\right) \end{bmatrix} \ ,$$

simplifying to a structure that can be used recursively:

$$\begin{bmatrix} 4x_n & 3 & 2x_n^2 + 1 \\ 4 & -7 & 3 \end{bmatrix}$$

Inserting $\vec{x}_0 = (-1, -1)$, use row operations to attain the RREF matrix

$$\begin{bmatrix} 1 & 0 & -1.875 \\ 0 & 1 & -1.5 \end{bmatrix} \ ,$$

and the right-most column reveals $x_1 = -1.875$, $y_1 = -1.5$. Notice that this is the same $\vec{x}_1$ yielded by the previous approach to the solution. In fact, all subsequent $\vec{x}_n$ for the two methods come out the same.

Finally trying $\vec{x}_0 = (1, 1)$ and turning the crank, the solution $\vec{x}_1$ is read from

$$\begin{bmatrix} 1 & 0 & 0.75 \\ 0 & 1 & 0 \end{bmatrix} .$$

Again, we attain the same $\vec{x}_1$ produced by the previous method, and all subsequent $\vec{x}_n$ are also the same.

5 Vectors and Surfaces

5.1 Basis Vectors as Derivatives

In three-dimensional space, there are always three basis vectors from which everything is oriented. In Cartesian coordinates, these are just $\hat{x}$, $\hat{y}$, $\hat{z}$, and are fixed in space. In other systems, such as cylindrical coordinates $\hat{\rho}$, $\hat{\phi}$, $\hat{z}$, and spherical coordinates $\hat{r}$, $\hat{\theta}$, $\hat{\phi}$, each basis vector depends on the coordinates themselves.

In each system mentioned, the respective position vector is:

$$\begin{aligned} \vec{r} &= x\,\hat{x} + y\,\hat{y} + z\,\hat{z} \\ \vec{r} &= \rho\cos(\phi)\,\hat{x} + \rho\sin(\phi)\,\hat{y} + z\,\hat{z} \\ \vec{r} &= r\sin(\theta)\left(\cos(\phi)\,\hat{x} + \sin(\phi)\,\hat{y}\right) + r\cos(\theta)\,\hat{z} \end{aligned}$$

It's customary using geometry to work out the basis vectors for each system, namely $\hat{\rho}$, $\hat{\phi}$, $\hat{z}$, and also $\hat{r}$, $\hat{\theta}$, $\hat{\phi}$.

Having suffered the tedious derivations once, you're entitled to a secret from the math department. Let q represent any parameter whatsoever - it could be x, or z, or ϕ, etc. It turns out that the basis vector $\hat{q}$ is the normalized q-derivative of the position vector. That is:

$$\hat{q} = \frac{1}{|\partial\vec{r}/\partial q|}\frac{\partial\vec{r}}{\partial q} \tag{1.6}$$

For example, if we want $\hat{\theta}$ from spherical coordinates, write

$$\frac{\partial\vec{r}}{\partial\theta} = r\cos(\theta)\left(\cos(\phi)\,\hat{x} + \sin(\phi)\,\hat{y}\right) - r\sin(\theta)\,\hat{z} ,$$

whose magnitude is r. Dividing this out delivers the result promised:

$$\frac{1}{r}\frac{\partial\vec{r}}{\partial\theta} = \hat{\theta}$$

5.2 Surface Tangent Vectors

Parametric Surface Tangents

In the same way that curves $y = f(x)$ can be represented with vectors and parameters, the story is similar for surfaces $z = f(x, y)$. In a generic case, a surface requires two parameters u, v such that

$$\vec{r}(u, v) = x(u, v)\,\hat{x} + y(u, v)\,\hat{y} + z(u, v)\,\hat{z} ,$$

which doesn't necessarily need to framed in the Cartesian system.

Choosing any fixed point (u_0, v_0) on a parameterized surface, there exist a pair of embedded tangent vectors we'll call $\vec{u}$, $\vec{v}$ straightforwardly calculated directly from $\vec{r}(u, v)$:

$$\begin{aligned} \vec{u}(u_0, v_0) &= \left(\frac{\partial}{\partial u}\vec{r}(u, v_0)\right)\Big|_{u_0} \\ \vec{v}(u_0, v_0) &= \left(\frac{\partial}{\partial v}\vec{r}(u_0, v)\right)\Big|_{v_0} \end{aligned}$$

Like all vectors, the tangents $\vec{u}$, $\vec{v}$ can be converted to normal vectors by dividing out the magnitude:

$$\begin{aligned} \hat{u} &= \vec{u}/u \\ \hat{v} &= \vec{v}/v \end{aligned}$$

Level Curve Tangents

The tangent vectors to a level curve of $z = f(x, y)$ are trickier to determine. To begin, propose choose a point (x_0, y_0) and write the pair of vectors

$$\begin{aligned} \vec{u}(x_0, y_0) &= u_x\,\hat{x} + u_z\,\hat{z} \\ \vec{v}(x_0, y_0) &= v_y\,\hat{y} + v_z\,\hat{z} , \end{aligned}$$

where without loss of generality, $\vec{u}$ lacks a y-component and $\vec{v}$ lacks an x-component.

The ratios u_z/u_x, v_z/v_y, receptively, are the partial derivatives in disguise, as

$$\begin{aligned} \frac{u_z}{u_x} &= \left(\frac{\partial}{\partial x}f(x, y_0)\right)\Big|_{x_0} \\ \frac{v_z}{v_y} &= \left(\frac{\partial}{\partial y}f(x_0, y)\right)\Big|_{y_0} , \end{aligned}$$

which allows the vectors $\vec{u}$, $\vec{v}$ to be written in terms of partial derivatives:

$$\begin{aligned} \vec{u}(x_0, y_0) &= u_x\left(\hat{x} + \left(\frac{\partial}{\partial x}f(x, y_0)\right)\Big|_{x_0}\hat{z}\right) \\ \vec{v}(x_0, y_0) &= v_y\left(\hat{y} + \left(\frac{\partial}{\partial y}f(x_0, y)\right)\Big|_{y_0}\hat{z}\right) \end{aligned}$$

For shorthand, denote the fully-evaluated partial derivatives as $f_x(x_0, y_0)$, $f_y(x_0, y_0)$, respectively. Dividing each vector by its own magnitude gives the normalized version of each:

$$\hat{u} = \frac{\hat{x} + f_x\,\hat{z}}{\sqrt{1 + f_x^2}}$$
$$\hat{v} = \frac{\hat{y} + f_y\,\hat{z}}{\sqrt{1 + f_y^2}}$$

5.3 Surface Normal Vector

With a pair of surface tangent vectors $\vec{u}$, $\vec{v}$ in hand for a given point, the cross product of the two yields the vector $\vec{n}$ that is normal to the surface:

$$\vec{n} = \vec{u} \times \vec{v}$$

Parametric Surface Normal

For the parametric surface $\vec{r}(u, v)$, the surface normal is straightforwardly calculated from

$$\vec{n}(u_0, v_0) = \vec{u}(u_0, v_0) \times \vec{v}(u_0, v_0) \ ,$$

which suggests a normalized version

$$\hat{n} = \frac{\vec{u}(u_0, v_0) \times \vec{v}(u_0, v_0)}{|\vec{u}(u_0, v_0) \times \vec{v}(u_0, v_0)|} \ .$$

Of course, there is no need to normalize if we use unit vectors only:

$$\hat{n} = \hat{u} \times \hat{v}$$

Cartesian Surface Normal

The normal vector to the surface $z = f(x, y)$ at a point (x_0, y_0) is the cross product of the tangent vectors $\vec{u}(x_0, y_0)$, $\vec{v}(x_0, y_0)$. Explicitly, this is:

$$\vec{n}(x_0, y_0) = \vec{u} \times \vec{v} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ u_x & 0 & u_x f_x \\ 0 & v_y & v_y f_y \end{vmatrix} \ ,$$

or

$$\vec{n} = u_x v_y \left(-f_x\,\hat{x} - f_y\,\hat{y} + \hat{z}\right) \ .$$

Eliminate the stray coefficients by normalizing:

$$\hat{n} = \frac{-f_x\,\hat{x} - f_y\,\hat{y} + \hat{z}}{\sqrt{1 + f_x^2 + f_y^2}}$$

5.4 Tangent Plane

In either picture, whether it be parametric or Cartesian, the tangent vectors $\vec{u}$, $\vec{v}$ imply the existence of a *tangent plane* to the surface at a given point, much in the same way the slope at a point implies a straight line in the one-dimensional case. The normal vector $\vec{n}$ is always perpendicular to the tangent plane.

If the point (x_0, y_0, z_0) is the base from which the tangent vectors and normal vector are drawn, and (x, y, z) is any other point in space, then the equation of the tangent plane is:

$$\vec{n} \cdot \Delta\vec{x} = 0 \ ,$$

where

$$\Delta\vec{x} = \langle x, y, z\rangle - \langle x_0, y_0, z_0\rangle \ .$$

From what we know about planes, we can also write

$$ax + by + cz + d = 0$$

to represent the tangent plane. To reconcile this with the vector definition, write out the full dot product:

$$n_x(x - x_0) + n_y(y - y_0) + n_z(z - z_0) = 0 \ ,$$

or

$$n_x x + n_y y + n_z z + d = 0 \ ,$$

with

$$d = -n_x x_0 - n_y y_0 - n_z z_0 \ .$$

We can say a bit more about the Cartesian case, as

$$n_x = -f_x$$
$$n_y = -f_y$$
$$n_z = 1$$

would mean

$$-f_x(x - x_0) - f_y(y - y_0) + (z - z_0) = 0 \ .$$