# VECTOR CALCULUS

For a function *f* = *f* (*x*, *y*) of two variables, we define the partial derivative of *f* with respect to *x*

as

*∂ f* = lim *f* (*x* + *h*, *y*) *− f* (*x*, *y*) ,

*∂x h→*0 *h*

and similarly for the partial derivative of *f* with respect to *y*. To take a partial derivative, take the derivative treating all other variables as constants. As an example, consider

*f* (*x*, *y*) = 2*x*3*y*2 + *y*3.

We have

*∂ f* = 6*x*2*y*2, *∂ f*

*∂x ∂y*

= 4*x*3*y* + 3*y*2.

Second derivatives are defined as the derivatives of the first derivatives, so we have

*∂*2 *f*

2 *∂*2 *f* 3

*∂x*2 = 12*xy* ,

*∂y*2 = 4*x*

+ 6*y*;

and for continuous differentiable functions, the mixed second partial derivatives are independent of the order in which the derivatives are taken,

*∂*2 *f*

*∂x∂y*

= 12*x*2*y* =

*∂*2 *f*

*∂y∂x* .

To develop a multivariable Taylor series, we introduce the standard subscript notation for partial derivatives,

*f ∂ f ∂ f*

*∂*2 *f*

*∂*2 *f*

*∂*2 *f*

*x* = *∂x* , *fy* = *∂y* , *fxx* = *∂x*2 , *fxy* = *∂x∂y* , *fyy* = *∂y*2 , etc.

The Taylor series of *f* (*x*, *y*) is then written as

*f* (*x*, *y*) = *f* + *fx x* + *fyy* + 1 . *fxx x*2 + 2 *fxyxy* + *fyyy*2Σ + . . . ,

2!

where the function and all its partial derivatives on the right-hand side are evaluated at the origin.

**The method of least squares**

Local maxima and minima of a multivariable function can be found by computing the zeros of the partial derivatives. These zeros are called the critical points of the function. A critical point need not be a maximum or minimum, for example it might be a minimum in one direction and a maximum in another (called a saddle point), but in many problems maxima or minima may be assumed to exist. Here, we illustrate the procedure for minimizing a function by solving the least-squares problem.

Suppose there is some experimental data that you want to fit by a straight line (illustrated on the right). In general, let the data consist of a set of *n* points given by (*x*1, *y*1), . . . , (*xn*, *yn*). Here, we assume that the *x* values are exact, and the *y* values are noisy. We further assume that the best fit line to the data takes the form *y* = *β*0 + *β*1*x*. Although we know that the line can not go through all the data points, we can try to find

y

the line that minimizes the sum of the squares of the vertical x

distances between the line and the points.

Define this function of the sum of the squares to be

*n*

*f* (*β*0, *β*1) = ∑ (*β*0 + *β*1*xi yi*)2 .

*−*

*i*=1

Here, the data is assumed given and the unknowns are the fitting parameters *β*0 and *β*1. It should be clear from the problem specification, that there must be values of *β*0 and *β*1 that minimize the function *f* = *f* (*β*0, *β*1). To determine, these values, we set *∂ f* /*∂β*0 = *∂ f* /*∂β*1 = 0. This results in the equations

*n*

∑(*β*0 + *β*1*xi yi*) = 0,

*−*

*i*=1

*n*

∑ *xi* (*β*0 + *β*1*xi yi*) = 0.

*−*

*i*=1

We can write these equations as a linear system for *β*0 and *β*1 as

*n n n n n*

*β*0*n* + *β*1 ∑ *xi* = ∑ *yi*, *β*0 ∑ *xi* + *β*1 ∑ *x*2 = ∑ *xiyi*.

*i*

*i*=1

*i*=1

*i*=1

*i*=1

*i*=1

The solution for *β*0 and *β*1 in terms of the data is given by

∑ *x*2 ∑ *yi −* ∑ *xiyi* ∑ *xi n* ∑ *xiyi −* (∑ *xi*)(∑ *yi*)

*β*0 = *i* 2

2 , *β*1 =

2 2 ,

*n* ∑ *xi −* (∑ *xi*)

where the summations are from *i* = 1 to *n*.

*n* ∑ *xi −* (∑ *xi*)

**Chain rule**

Partial derivatives are used in applying the chain rule to a function of several variables. Consider a two-dimensional scalar field *f* = *f* (*x*, *y*), and define the total differential of *f* to be

*d f* = *f* (*x* + *dx*, *y* + *dy*) *− f* (*x*, *y*).

We can write *d f* as

*d f* = [ *f* (*x* + *dx*, *y* + *dy*) *− f* (*x*, *y* + *dy*)] + [ *f* (*x*, *y* + *dy*) *− f* (*x*, *y*)]

*∂ f*

= *∂x*

*dx* +

*∂ f dy*.

*∂y*

If one has *f* = *f* (*x*(*t*), *y*(*t*)), say, then division of *d f* by *dt* results in

*d f ∂ f dx ∂ f dy*

*dt* = *∂x dt* + *∂y dt* .

And if one has *f* = *f* (*x*(*r*, *θ*), *y*(*r*, *θ*)), say, then the corresponding chain rule is given by

*∂ f* =

*∂r*

*∂ f ∂x*

*∂x ∂r*

*∂ f ∂y*

+ *∂y ∂r* ,

*∂ f* =

*∂θ*

*∂ f ∂x*

*∂x ∂θ*

*∂ f ∂y*

+ *∂y ∂θ* .

*Example: Consider the differential equation dx*

*u t*, *x t*

*. Determine a formula for d*2 *x in terms of u and its*

*partial derivatives.*

*dt* = (

( ))

*dt*2

Applying the chain rule, we have at time *t*,

*d*2 *x*

*∂u ∂u dx*

*dt*2 = *∂t* + *∂x dt*

*∂u*

= *∂t*

*∂u*

+ *u ∂x* .

The above formula is called the material derivative and in three dimensions forms a part of the Navier- Stokes equation for fluid flow.

**Triple product rule**

Suppose that three variables *x*, *y* and *z* are related by the equation *f* (*x*, *y*, *z*) = 0, and it that is possible to write *x* = *x*(*y*, *z*) and *z* = *z*(*x*, *y*). Taking differentials of *x* and *y*, we have

*dx* = *∂x dy* + *∂x dz*, *dz* = *∂z dx* + *∂z dy*.

*∂y ∂z ∂x ∂y*

We can make use of the second equation to eliminate *dz* in the first equation to obtain

*dx* = *∂x dy* + *∂x* . *∂z dx* + *∂z dy*Σ ;

*∂y ∂z ∂x ∂y*

or collecting terms,

.1 *− ∂x ∂z* Σ *dx* = . *∂x* + *∂x ∂z* Σ *dy*.

*∂z ∂x*

*∂y*

*∂z ∂y*

Since *dx* and *dy* are independent variations, the terms in parenthesis must be zero. The left-hand-side results in the reciprocity relation

*∂x ∂z*

*∂z ∂x*

= 1,

which states the intuitive result that *∂z*/*∂x* and *∂x*/*∂z* are multiplicative inverses of each other. The right-hand-side results in

*∂x ∂x ∂z*

*∂y* = *− ∂z ∂y* ,

which, when making use of the reciprocity relation, yields the counterintuitive triple product rule,

*∂x ∂y ∂z*

*∂y ∂z ∂x* = *−*1.

**Triple product rule: example**

*Example: Demonstrate the triple product rule using the ideal gas law.*

The ideal gas law states that

*PV* = *nRT*,

where *P* is the pressure, *V* is the volume, *T* is the absolute temperature, *n* is the number of moles of the gas, and *R* is the ideal gas constant. We say *P*, *V* and *T* are the state variables, and the ideal gas law is a relation of the form

*f* (*P*, *V*, *T*) = *PV − nRT* = 0.

We can write *P* = *P*(*V*, *T*), *V* = *V*(*P*, *T*), and *T* = *T*(*P*, *V*), that is,

*P* = *nRT* , *V* = *nRT* , *T* = *PV* ;

*V*

and the partial derivatives are given by

*P nR*

*∂P nRT*

*∂V nR*

*∂T V*

The triple product results in

*∂V* = *− V*2 ,

*∂T* = *P* ,

= .

*∂P nR*

*∂P ∂V ∂T* = *−* . *nRT* Σ . *nR* Σ . *V* Σ = *−nRT* = *−*1,

*∂V ∂T ∂P*

*V*2

*P*

*nR*

*PV*

where we make use of the ideal gas law in the last equality.

**Gradient**

Consider the three-dimensional scalar field *f* = *f* (*x*, *y*, *z*), and the differential *d f* , given by

*d f* = *∂ f dx* + *∂ f dy* + *∂ f dz*.

*∂x ∂y ∂z*

Using the dot product, we can write this in vector form as

*d f* = . *∂ f* ***�*** + *∂ f* ***�*** + *∂ f* ***�***Σ *·* (*dx****�*** + *dy****�*** + *dz****�***) = **∇** *f · d****�***,

*∂x ∂y*

where in Cartesian coordinates,

*∂z*

*∂ f ∂ f ∂ f*

**∇** *f* = *∂x* ***�*** + *∂y* ***�*** + *∂z* ***�***

is called the gradient of *f* . The nabla symbol **∇** is pronounced “del” and **∇** *f* is pronounced “del- *f* ”. Another useful way to view the gradient is to consider **∇** as a vector differential operator which has the form

*∂ ∂ ∂*

**∇** = ***�*** *∂x* + ***�*** *∂y* + ***�*** *∂z* .

Because of the properties of the dot product, the differential *d f* is maximum when the infinitesimal displacement vector *d****�*** is along the direction of the gradient **∇** *f* . We then say that **∇** *f* points in the direction of maximally increasing *f* , and whose magnitude gives the slope (or gradient) of *f* in that direction.

*Example: Compute the gradient of f* (*x*, *y*, *z*) = *xyz.*

The partial derivatives are easily calculated, and we have

**∇** *f* = *yz* ***�*** + *xz* ***�*** + *xy* ***�***.

**Divergence**

Consider in Cartesian coordinates the three-dimensional vector field, ***�*** = *u*1(*x*, *y*, *z*)***�*** + *u*2(*x*, *y*, *z*)***�*** + *u*3(*x*, *y*, *z*)***�***. The divergence of ***�***, denoted as **∇** *·* ***�*** and pronounced “del-dot-u”, is defined as the scalar field given by

**∇** *·* ***�*** = .***�***  *∂* + ***�***  *∂* + ***�***  *∂* Σ *·* (*u*1***�*** + *u*2***�*** + *u*3***�***)

*∂x*

*∂y*

*∂z*

= *∂u*1 + *∂u*2 + *∂u*3 .

*∂x ∂y ∂z*

Here, the dot product is used between a vector differential operator **∇** and a vector field ***�***. The diver- gence measures how much a vector field spreads out, or diverges, from a point. A more math-based description will be given later.

*Example: Let the position vector be given by* ***�*** = *x****�*** + *y****�*** + *z****�****. Find* **∇** *·* ***�****.*

A direct calculation gives

*∂ ∂ ∂*

*Example: Let* ***𝐹*** = ***�***

*|****�****|*3

**∇** *·* ***�*** = *∂x x* + *∂y y* + *∂z z* = 3.

*for all* ***�*** *ƒ*= 0*. Find* **∇** *·* ***𝐹*** *.*

Writing out the components of ***𝐹*** , we have

*x y z*

***𝐹*** = *F*1***�*** + *F*2***�*** + *F*3***�*** = (*x*2 + *y*2 + *z*2)3/2 ***�*** + (*x*2 + *y*2 + *z*2)3/2 ***�*** + (*x*2 + *y*2 + *z*2)3/2 ***�***.

Using the quotient rule for the derivative, we have

*∂F*1 (*x*2 + *y*2 + *z*2)3/2 *−* 3*x*2(*x*2 + *y*2 + *z*2)1/2 1 3*x*2

*∂x* = (*x*2 + *y*2 + *z*2)3 = *|****�****|*3 *− |****�****|*5 ,

and analogous results for *∂F*2/*∂y* and *∂F*3/*∂z*. Adding the three derivatives results in

3 3(*x*2 + *y*2 + *z*2) 3 3

**∇** *·* ***𝐹*** = *|****�****|*3 *−*

*|****�****|*5 = *|****�****|*3 *− |****�****|*3 = 0,

valid as long as *|****�****| ƒ*= 0, where ***𝐹*** diverges. In the study of electrostatics, ***𝐹*** is proportional to the electric field of a point charge located at the origin.

**Curl**

Consider in Cartesian coordinates the three-dimensional vector field ***�*** = *u*1(*x*, *y*, *z*)***�*** + *u*2(*x*, *y*, *z*)***�*** + *u*3(*x*, *y*, *z*)***�***. The curl of ***�***, denoted as **∇** *×* ***�*** and pronounced “del-cross-u”, is defined as the vector field given by

***� � �***

. .

**∇** *×*

. *∂u*3 *∂u*2 Σ

. *∂u*1 *∂u*3 Σ

. *∂u*2 *∂u*1 Σ

***�*** = *∂*/*∂x ∂*/*∂y ∂*/*∂z* =

. .

*∂y − ∂z* ***�*** +

*∂z − ∂x* ***�*** +

*∂x − ∂y* ***�***.

. *u*1 *u*2 *u*3 .

Here, the cross product is used between a vector differential operator and a vector field. The curl measures how much a vector field rotates, or curls, around a point. A more math-based description will be given later.

*Example: Show that the curl of a gradient is zero, that is,* **∇** *×* (**∇** *f* ) = 0*.*

We have

 ***� � �*** 

 

**∇** *×* (**∇** *f* ) = *∂*/*∂x ∂*/*∂y ∂*/*∂z*

*∂ f* /*∂x ∂ f* /*∂y ∂ f* /*∂z*

. *∂*2 *f ∂*2 *f* Σ . *∂*2 *f*

=

*∂y∂z − ∂z∂y*

***�*** +

*∂z∂x − ∂x∂z*

***�*** +

*∂x∂y − ∂y∂x*

***�*** = 0,

*∂*2 *f* Σ

. *∂*2 *f*

*∂*2 *f* Σ

using the equality of mixed partials.

*Example: Show that the divergence of a curl is zero, that is,* **∇** *·* (**∇** *×* ***�***) = 0*.* We have

**∇** *·* (**∇** *×* ***�***) = *∂* . *∂u*3 *− ∂u*2 Σ + *∂* . *∂u*1 *− ∂u*3 Σ + *∂* . *∂u*2 *− ∂u*1 Σ

*∂x*

*∂y*

*∂z*

*∂y*

*∂z*

*∂x*

*∂z*

*∂x*

*∂y*

. *∂*2*u*1 *∂*2*u*1 Σ . *∂*2*u*2 *∂*2*u*2 Σ . *∂*2*u*3 *∂*2*u*3 Σ

=

*∂y∂z − ∂z∂y*

+

*∂z∂x − ∂x∂z*

+

*∂x∂y − ∂y∂x*

= 0,

again using the equality of mixed partials.