Multivariate Calculus & Optimization

Lecture 13

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1

multivariate/multivariable/multidimensional calculus

$$f(x) \quad \text{vs.} \quad f(x, y), f(x, y, z), f(x, y, z, \ldots)$$

Multivariable (or multivariate) calculus extends single-variable calculus to functions of multiple variables. It includes:

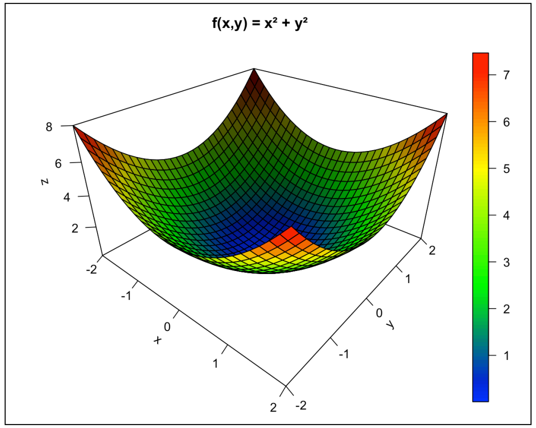
- Partial derivatives: Differentiation with respect to one variable while keeping others constant.
- Multiple integrals: Double and triple integrals for computing areas, volumes, and more.
- Vector calculus: Topics like gradient, line/surface integrals.
- Optimization: Finding local maxima/minima of functions with/without constraints

$$f(x, y) = x^2 + y^2$$

2

surface plot

3D visualization showing how a function behaves



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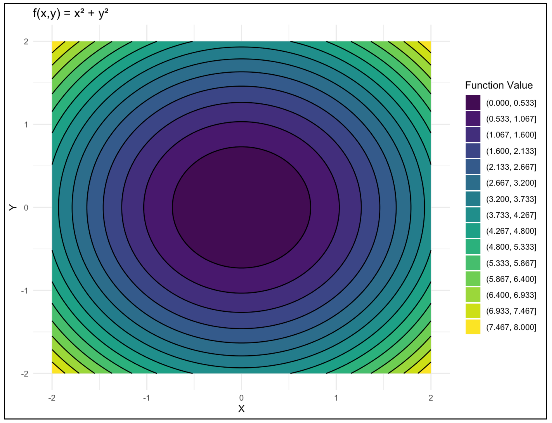
contour plot

2D visualization providing provide a top-down view of function values



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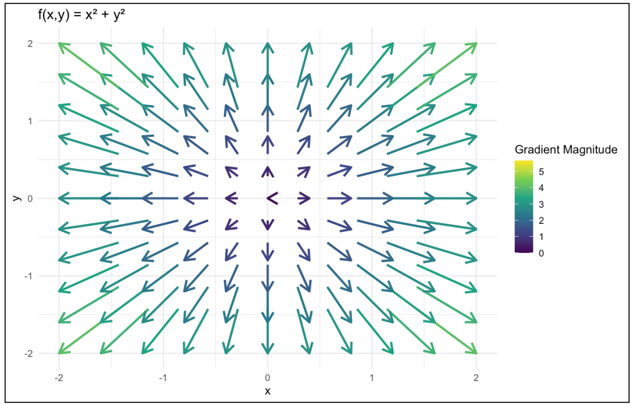
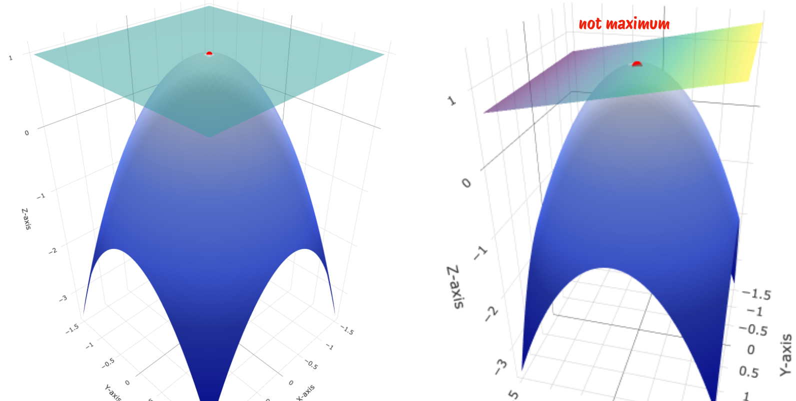
gradient plot

The gradient $\nabla f = (2x, 2y)$ shows the direction of steepest ascent



optimization



$f(x, y) = 1 - x^2 - y^2$

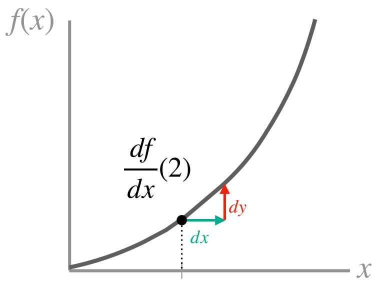
partial derivatives

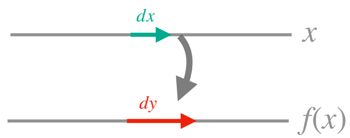
A partial derivative is the derivative of a multivariable function with respect to one variable while treating all other variables as constants.

derivatives recap

Before: assume $f(x)$ with derivative $\dfrac{df}{dx}$. What does this mean?

$$\boxed{\frac{df}{dx} = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}}$$





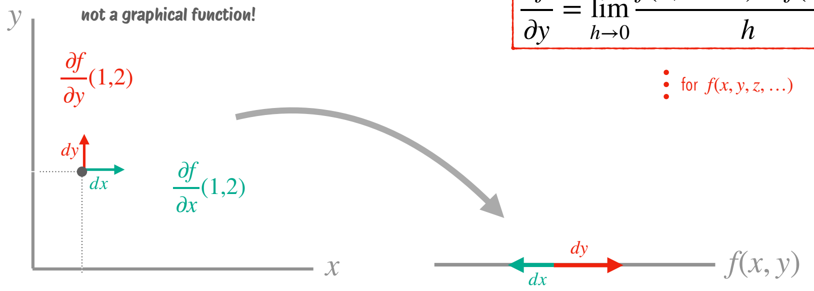
partial derivatives

Now: assume $f(x,y)$ with $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$

$$\boxed{\frac{\partial f}{\partial x} = \lim_{h\to 0} \frac{f(a+h,b)-f(a,b)}{h}}$$

$$\boxed{\frac{\partial f}{\partial y} = \lim_{h\to 0} \frac{f(a,b+h)-f(a,b)}{h}}$$

$\vdots$ for $f(x,y,z,\dots)$



partial derivatives

A partial derivative is the derivative of a multivariable function with respect to one variable while treating all other variables as constants.

example

Assume following function: $f(x,y) = x^2y + 3xy^3$

Partial Derivative with Respect to x: $\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}(x^2y + 3xy^3) \implies \frac{\partial f}{\partial x} = 2xy + 3y^3$

Partial Derivative with Respect to y: $\frac{\partial f}{\partial y} = \frac{\partial}{\partial y}(x^2y + 3xy^3) \implies \frac{\partial f}{\partial y} = x^2 + 9xy^2$

the symmetry of second partial derivatives

example

$f(x,y) = x^2y + 3xy^3$

$\frac{\partial f}{\partial x} = 2xy + 3y^3$

$\frac{\partial f}{\partial y} = x^2 + 9xy^2$

the symmetry of second partial derivatives

example

$f(x,y) = x^2y + 3xy^3$

$\frac{\partial f}{\partial x} = 2xy + 3y^3$

$\frac{\partial f}{\partial y} = x^2 + 9xy^2$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = 2y$$

$$\frac{\partial^2 f}{\partial xy} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = 2x + 9y^2$$

the symmetry of second partial derivatives

example

$$f(x,y) = x^2y + 3xy^3$$

$$\frac{\partial f}{\partial x} = 2xy + 3y^3 \qquad \frac{\partial f}{\partial y} = x^2 + 9xy^2$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = 2y$$

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$$\frac{\partial^2 f}{\partial yx} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = 2x + 9y^2$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) = 18xy$$

the symmetry of second partial derivatives

example

$$f(x,y) = x^2y + 3xy^3$$

$$\frac{\partial f}{\partial x} = 2xy + 3y^3 \qquad \frac{\partial f}{\partial y} = x^2 + 9xy^2$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = 2y$$

$$\frac{\partial^2 f}{\partial xy} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = 2x + 9y^2$$

$$\frac{\partial^2 f}{\partial yx} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = 2x + 9y^2$$

$$\frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) = 18xy$$

the symmetry of second partial derivatives

Schwarz's theorem

If the second partial derivatives are continuous, the order of differentiation is not important and we therefore have:

$$\frac{\partial^2 f}{\partial xy} = \frac{\partial^2 f}{\partial yx}$$

gradient

The gradient of a scalar function $f(x_1, x_2, \ldots, x_n)$ is a vector field that points in the direction of the greatest rate of increase of f.

For a function $f : \mathbb{R}^n \to \mathbb{R}$, the gradient is denoted as:

$$\nabla f = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right)$$

where each component is a partial derivative of f with respect to one of the variables.

Direction: The gradient points in the direction of the steepest ascent of f

Magnitude: The magnitude $\|\nabla f\|$ represents the rate of the steepest increase.

Zero Gradient: If $\nabla f = 0$, the point is a critical point (possible max, min, or saddle point).

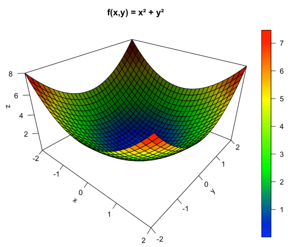
gradient

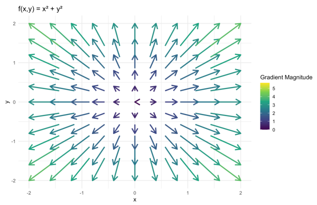
The gradient captures all the partial derivative information of a multivariable function.

example

For $f(x, y) = x^2 + y^2$, the gradient is:

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (2x, 2y)$$





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gradient

$$f(x, y) = x^2 + y^2 \implies \nabla f = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

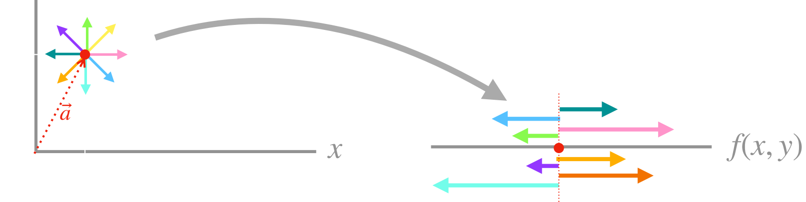
directional derivatives

$$\boxed{\nabla_{\vec{v}} f(\vec{a}) = \lim_{h \to \infty} \frac{f(\vec{a} + h \cdot \vec{v}) - f(\vec{a})}{h}}$$

not a graphical function!

$$\nabla_{\vec{v}} f = v_1 \frac{\partial f}{\partial x} + v_2 \frac{\partial f}{\partial y} \quad \text{where} \quad \vec{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$\boxed{\max_{\|\vec{v}=1\|} \nabla f(a, b) \cdot \vec{v}}$$



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gradient

Zero Gradient:

If $\nabla f = 0$, the point is a critical point (max, min, or saddle point)

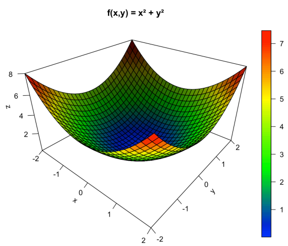
example

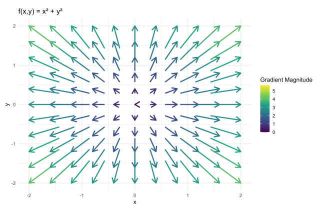
For $f(x, y) = x^2 + y^2$, the gradient is:

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (2x, 2y)$$

Find minimum (we see from image):

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \vec{0}$$





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gradient: saddle point

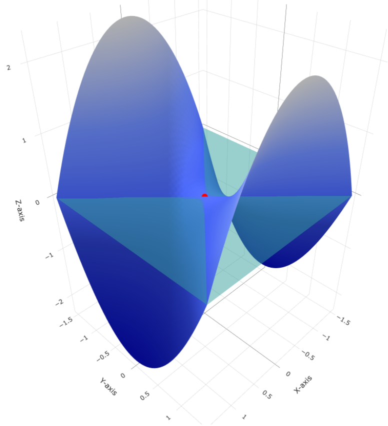
example

For $f(x, y) = x^2 - y^2$, the gradient is:

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (2x, -2y)$$

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \vec{0}$$

What's the solution? Is it max or min?



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Second Partial Derivative Test

$$H = \left(\frac{\partial^2 f}{\partial x^2}\right) \cdot \left(\frac{\partial^2 f}{\partial y^2}\right) - \left(\frac{\partial^2 f}{\partial y \partial x}\right)^2 = \underbrace{\overbrace{f_{xx}(x_0, y_0)}^{\text{Concavity in x-direction}}\overbrace{f_{yy}(x_0, y_0)}^{\text{Concavity in y-direction}}}_{\text{Positive only when x and y directions agree on concavity direction}} - \underbrace{f_{xy}(x_0, y_0)^2}_{\text{How much } f \text{ looks like } g(x,y)=xy}$$

for each critical point (x_0, y_0)

if $H > 0 \implies$ max or min

$H < 0 \implies$ saddle

$H = 0 \implies$ unknown

$f_{xx}(x_0, y_0) < 0 \implies (x_0, y_0)$ is a local maximum point

$f_{xx}(x_0, y_0) > 0 \implies (x_0, y_0)$ is a local minimum point

the Hessian

The Hessian matrix is a square matrix of second-order partial derivatives of a scalar-valued function $f(x_1, x_2, \ldots, x_n)$ is

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

- The Hessian matrix is a square matrix of second-order partial derivatives of a scalar-valued function
- The Hessian provides a way to classify critical points (where the gradient is zero):
  - If the Hessian is positive definite ($H > 0$), the critical point is a local minimum.
  - If the Hessian is negative definite ($H < 0$), the critical point is a local maximum.
  - If the Hessian has both positive and negative eigenvalues, the critical point is a saddle point.

Definiteness

For quadratic symmetrical matrix A with eigenvalues λ:

- $\lambda > 0 \rightarrow$ positive definite
- $\lambda < 0 \rightarrow$ negative definite
- $\lambda \geq 0 \rightarrow$ positive semidefinite
- $\lambda \leq 0 \rightarrow$ negative semidefinite
- indefinite $\rightarrow$ both positive and negative eigenvalues

global min/max

example

For Function: $f(x, y) = 4 - x^2 - y^2$ the Hessian is given by

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix}$$

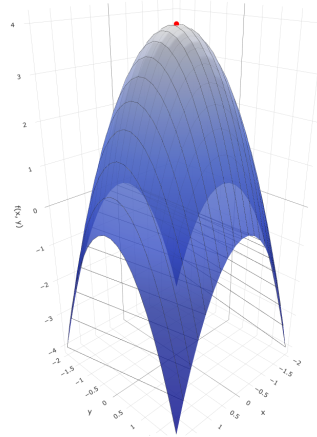
Both eigenvalues are negative (-2, -2), so H is negative definite

$\implies$ Local max at (0,0)

Is it global?

Since $f(x, y) \rightarrow -\infty$ as $|x|, |y| \rightarrow \infty$, the function is unbounded and has only one maximum, which must be global

$\implies$ (0,0) is the global maximum, and f(0,0) = 4



Hessian

The Hessian provides a way to classify critical points (where the gradient is zero).

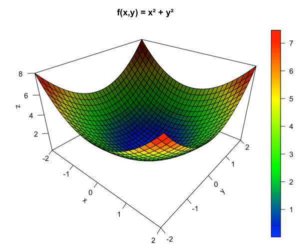
example

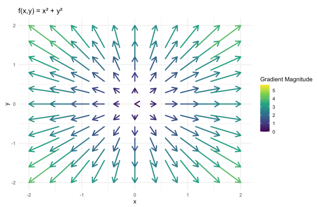
For $f(x, y) = x^2 + y^2$, the Hessian is:

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

Diagonal matrix with positive values indicating function is convex

Eigenvalues?





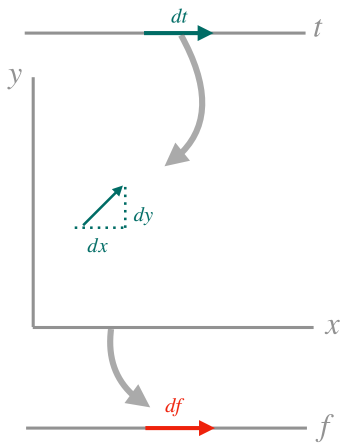
chain rule: multivariable functions

If $f(x(t), y(t))$, and both x and y are functions of a single variable t, then:

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

chain rule: multivariable functions

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



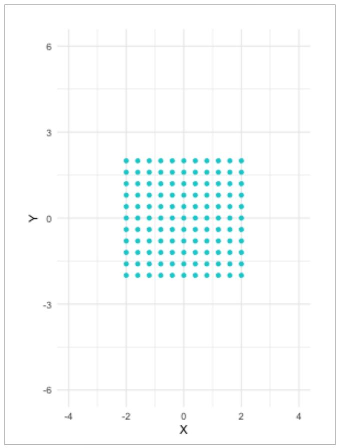
1 $dx = \frac{dx}{dt}dt \qquad dy = \frac{dy}{dt}dt$

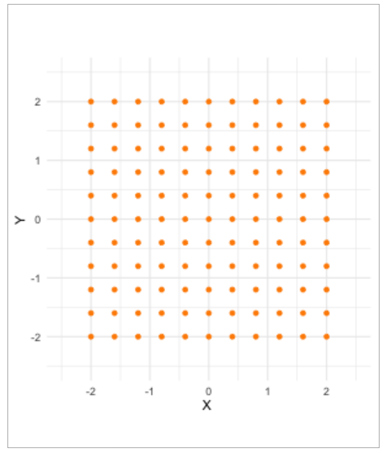
2 $df_{dx} = \frac{\partial f}{\partial x}dx \qquad df_{dy} = \frac{\partial f}{\partial y}dy$

$$df = \frac{\partial f}{\partial x}\frac{dx}{dt}dt + \frac{\partial f}{\partial y}\frac{dy}{dt}dt$$

$$\frac{df}{dt} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt}$$

linear and non-linear transformation





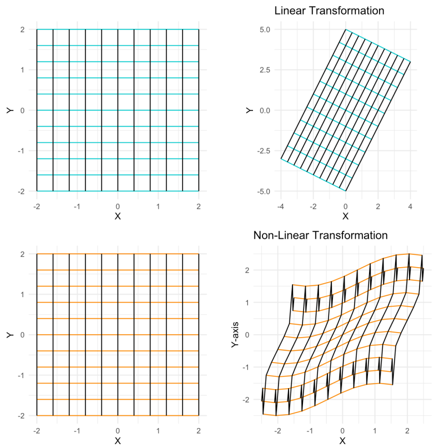
linear and non-linear transformation

Linear:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = A \cdot \begin{bmatrix} x \\ y \end{bmatrix} \text{ where } A = \begin{bmatrix} 1 & 1 \\ -1 & 2 \end{bmatrix}$$

Non-Linear:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} f(x,y) \\ g(x,y) \end{bmatrix} = \begin{bmatrix} x + 0.5\sin(y) \\ y + 0.5\sin(x) \end{bmatrix}$$



linear and non-linear transformation

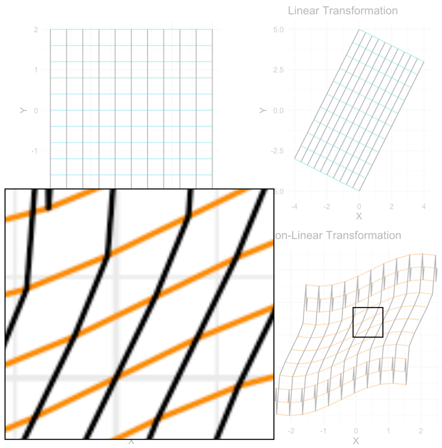
Linear:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = A \cdot \begin{bmatrix} x \\ y \end{bmatrix} \text{ where } A = \begin{bmatrix} 1 & 1 \\ -1 & 2 \end{bmatrix}$$

Non-Linear:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} f(x,y) \\ g(x,y) \end{bmatrix} = \begin{bmatrix} x + 0.5\sin(y) \\ y + 0.5\sin(x) \end{bmatrix}$$

but locally linear when we zoom in!



the Jacobian

If we have a function $f: \mathbb{R}^n \to \mathbb{R}^m$ mapping an $n-$dimensional input to an $m-$dimensional output,

$$f(x_1, x_2, \ldots, x_n) = \begin{bmatrix} f_1(x_1, x_2, \ldots, x_n) \\ f_2(x_1, x_2, \ldots, x_n) \\ \vdots \\ f_m(x_1, x_2, \ldots, x_n) \end{bmatrix},$$

then the Jacobian matrix contains all first-order partial derivatives of f: $J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$

the Jacobian

- The Jacobian matrix is a matrix of all first-order partial derivatives of a vector-valued function. It generalizes the concept of a derivative to multiple variables and dimensions.
- Measures how a function transforms space:
  It describes the local scaling, rotation, or shearing of a function.
- Useful in nonlinear transformations
- The Jacobian determinant represents the factor by which the transformation stretches or squishes the $n-$dimensional volumes around a certain input.

the Jacobian

example

Let f be a transformation from $\mathbb{R}^2$ to $\mathbb{R}^2$ with the following Jacobian matrix:

$$J = \begin{bmatrix} 3x^2 - 4 & 0 \\ 0 & 3y^2 - 4 \end{bmatrix}$$

What is the determinant of f? How will f stretch or squish the space around the point $(1, -1)$?

where the Hessian, gradient and Jacobian meet

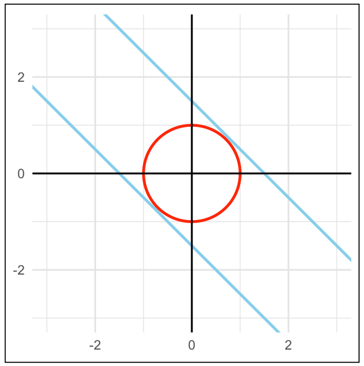
- The gradient points in the direction of steepest ascent.
- The Jacobian describes how the components of a vector function change with respect to changes in input variables
- The Hessian describes the local curvature of a scalar function

Matrix	Purpose	Function Type	Size
Gradient ∇f	First-order derivatives	$f: \mathbb{R}^n \to \mathbb{R}$	$n \times 1$
Jacobian J	First-order derivatives of vector functions	$f: \mathbb{R}^n \to \mathbb{R}^m$	$m \times n$
Hessian H	Second-order derivatives	$f: \mathbb{R}^n \to \mathbb{R}$	$n \times n$

- Gradient is the Jacobian of a scalar function $f: \mathbb{R}^n \to \mathbb{R}$: $\nabla f = J$
- Hessian is the Jacobian of the Gradient ∇f : $H = J_{\nabla f}$

next week: constrained optimization

Optimize $f(x, y)$ subject to $g(x, y) = k$



$$f(x, y) = 2x + y$$
$$g(x, y) = x^2 + y^2 = 1$$