Maths for Computer Science
Calculus

Dr Eleni Akrida

Multivariate Extrema & Hessian Matrix

Contents for this topic

- Recall bivariate extrema:
  - What are they?
  - How do we find them?

- Finding extrema of multivariate functions with more than 2 variables

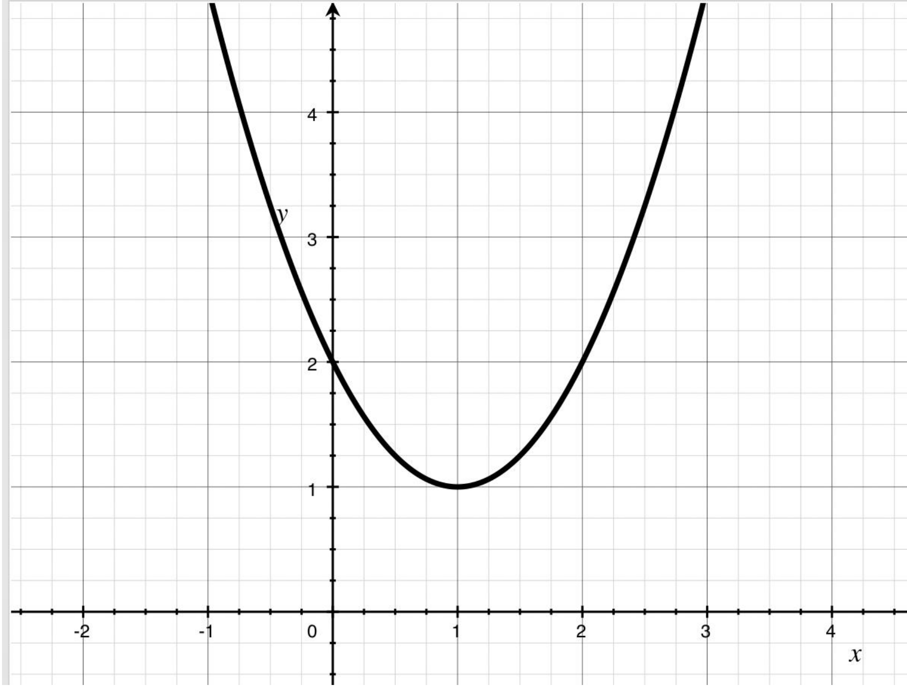
Univariate extrema

Let $f(x)$ be a function defined on an interval $[a, b]$ and differentiable at a point $x_0 \in [a, b]$.

If x_0 is a maximum or minimum of f, **then** $f'(x_0) = 0$.

Example: $y(x) = (x-1)^2 + 1$

$y'(x) = 2(x-1)$ is equal to 0 at $x = 1$.



Durham University

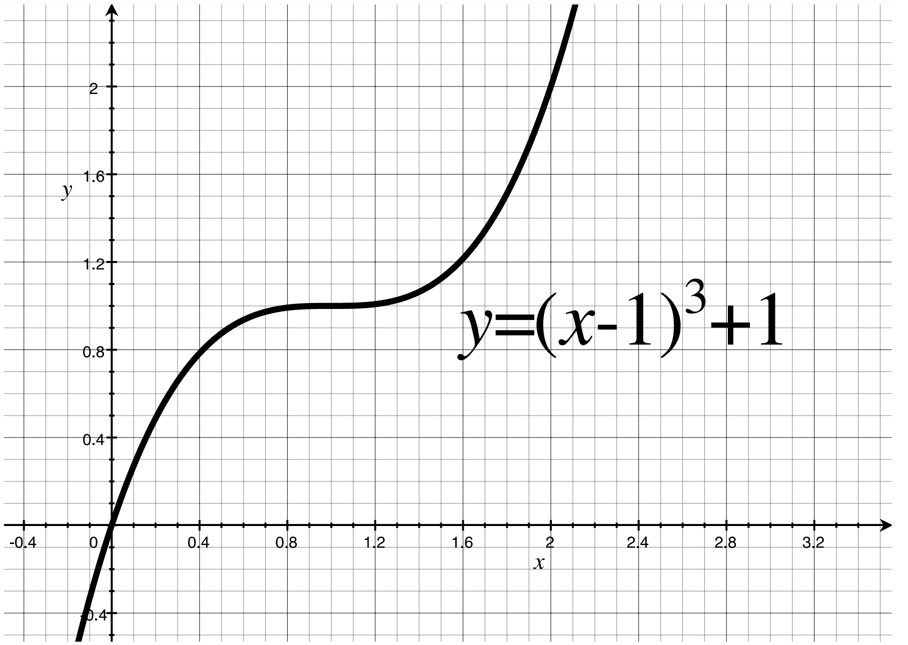
Univariate extrema

Is it enough to find points x_0 where $f'(x_0) = 0$?

Let $f(x)$ be a function defined on an interval $[a, b]$ and differentiable at a point $x_0 \in [a, b]$.

If x_0 is a maximum or minimum of f, **then** $f'(x_0) = 0$.

The derivative being zero is a necessary condition but not a sufficient one for x_0 to be a min or max of f.



Not all stationary points are extrema. We want to work out how to find the extrema, if any.

Univariate extrema

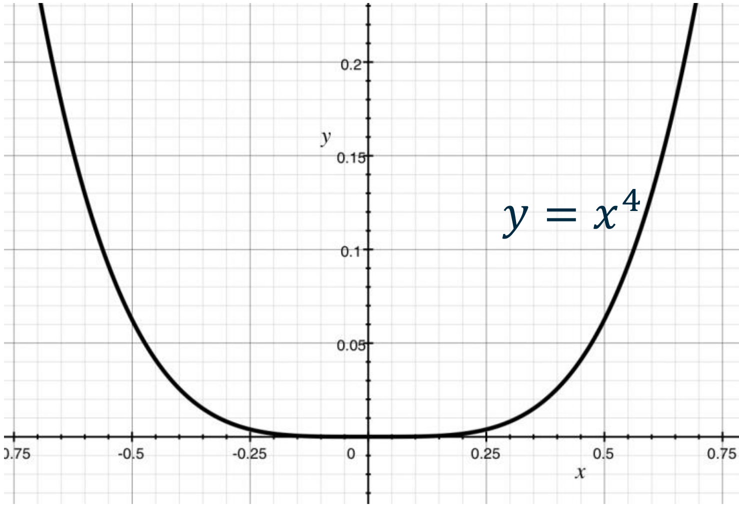
For a twice differentiable univariate function $f(x)$ with continuous derivatives:

- If $f'(x) = 0$ we have a **stationary point**.
- If $f'(x) = 0$ and $f''(x) < 0$ we have a **maximum**.
- If $f'(x) = 0$ and $f''(x) > 0$ we have a **minimum**.
- If $f'(x) = 0$ and $f''(x) = 0$ we **may** have a **stationary inflection point**.
- If $f'(x) \neq 0$ and $f''(x) = 0$ we **may** have a **non-stationary inflection point**.

Why only *may*? Consider $f(x) = x^4$.

At $x = 0$ we have $f(x) = f'(x) = f''(x) = 0$.

In general you need to look at the first non-zero derivative. If it is the k^{th} derivative and k is odd it is an inflection. If k is even, it is an extremum.



Bivariate extrema

For a stationary point, where $\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (0,0)$, is it enough to check that $\frac{\partial^2 f}{\partial x^2}$ and $\frac{\partial^2 f}{\partial y^2}$ are both positive or both negative to say it is a minimum or maximum?

No: Consider $f(x, y) = x^2 + y^2 + axy$.

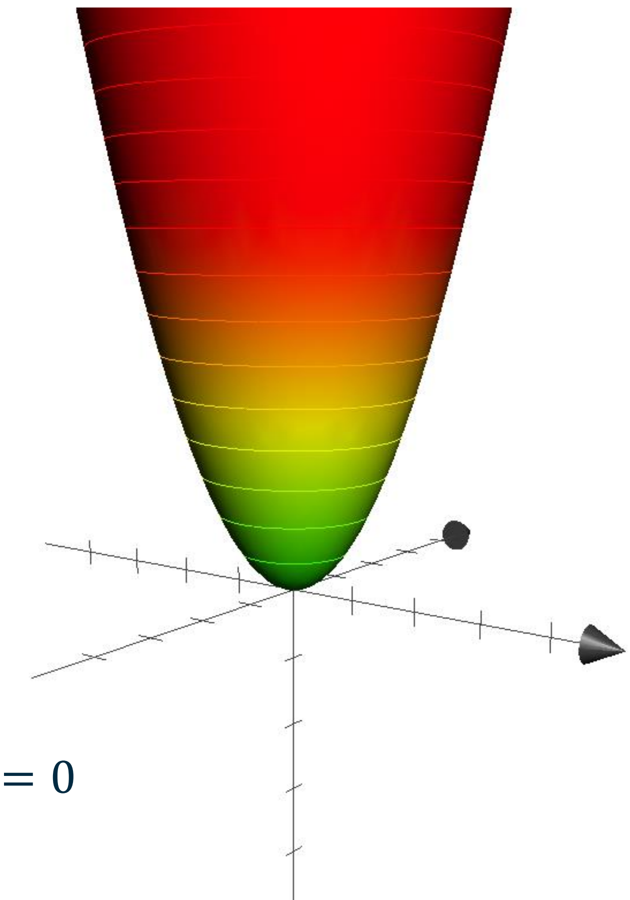
$\frac{\partial f}{\partial x} = 2x + ay$, $\frac{\partial^2 f}{\partial x^2} = 2$, and

$\frac{\partial f}{\partial y} = 2y + ax$, $\frac{\partial^2 f}{\partial y} = 2$.

So positive curvature (concave up) in both the x and y directions.

But as a varies the shape of the surface changes from a minimum to a saddle.

https://www.geogebra.org/m/rvm4dbaw



$a = 0$

Bivariate extrema

For a stationary point, where $\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (0{,}0)$, is it enough to check that $\frac{\partial^2 f}{\partial x^2}$ and $\frac{\partial^2 f}{\partial y^2}$ are both positive or both negative to say it is a minimum or maximum?

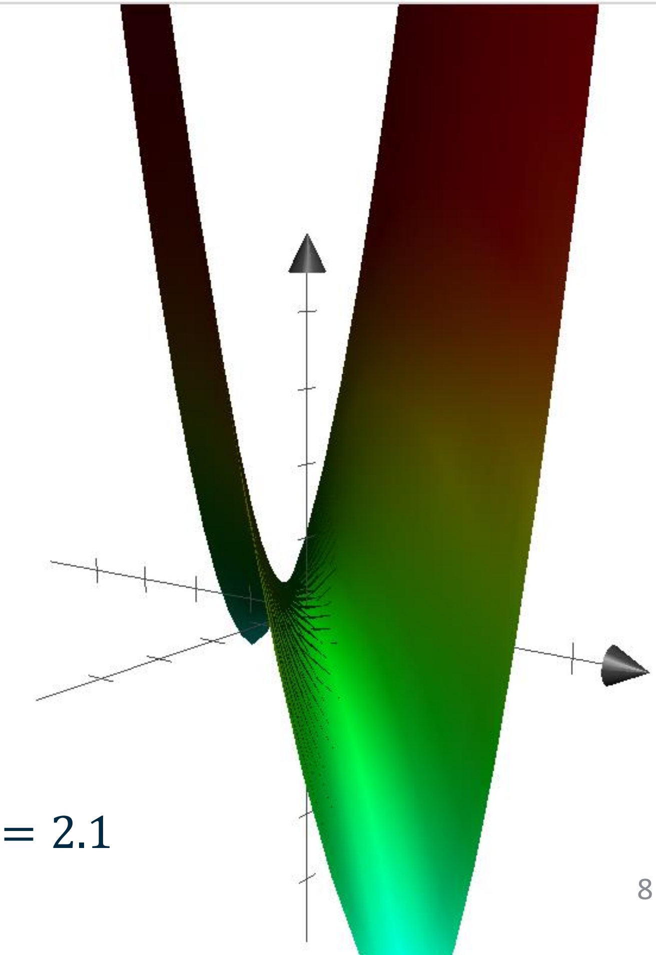
No: Consider $f(x, y) = x^2 + y^2 + axy$.

$\frac{\partial f}{\partial x} = 2x + ay$, $\frac{\partial^2 f}{\partial x^2} = 2$, and

$\frac{\partial f}{\partial y} = 2y + ax$, $\frac{\partial^2 f}{\partial y} = 2$.

So positive curvature (concave up) in both the x and y directions.

But as a varies the shape of the surface changes from a minimum to a saddle.



$a = 2.1$

Bivariate extrema

For a stationary point, where $\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) = (0,0)$, is it enough to check that $\frac{\partial^2 f}{\partial x^2}$ and $\frac{\partial^2 f}{\partial y^2}$ are both positive or both negative to say it is a minimum or maximum?

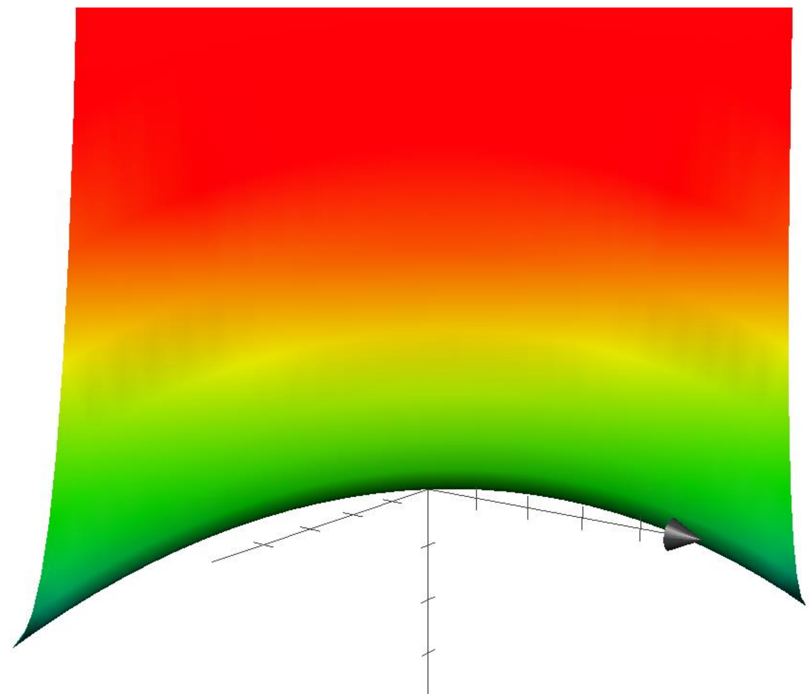
No: Consider $f(x, y) = x^2 + y^2 + axy$.

$\frac{\partial f}{\partial x} = 2x + ay$, $\frac{\partial^2 f}{\partial x^2} = 2$, and

$\frac{\partial f}{\partial y} = 2y + ax$, $\frac{\partial^2 f}{\partial y} = 2$.

So positive curvature (concave up) in both the x and y directions.

But as a varies the shape of the surface changes from a minimum to a saddle.



$a = -2.1$

Bivariate extrema

To identify a minimum or maximum we must also consider:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial y}\right] = f_{xy} \text{ and } \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y}\left[\frac{\partial f}{\partial x}\right] = f_{yx}.$$

We gather all the 2nd order partial derivatives into the **Hessian matrix**:

$$\boldsymbol{H}_f = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x^2} & \dfrac{\partial^2 f}{\partial x \partial y} \\ \dfrac{\partial^2 f}{\partial y \partial x} & \dfrac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{bmatrix}$$

which contains information about curvature in all directions and for $f \in C^2$ is symmetric.

2^{nd} derivative test for bivariate extrema

A well-known test for determining the form of bivariate extrema.

Stationary point

Theorem:

Suppose $f(x, y) \in C^2$ and $f_x(x_0, y_0) = 0 = f_y(x_0, y_0)$, then

- (x_0, y_0) is a local maximum if $f_{xx}f_{yy} - f_{xy}^2 > 0$ and $f_{xx} < 0$ at (x_0, y_0);
- (x_0, y_0) is a local minimum if $f_{xx}f_{yy} - f_{xy}^2 > 0$ and $f_{xx} > 0$ at (x_0, y_0);
- (x_0, y_0) is a saddle point if $f_{xx}f_{yy} - f_{xy}^2 < 0$ at (x_0, y_0);
- If $f_{xx}f_{yy} - f_{xy}^2 = 0$ then the test is inconclusive and higher order derivatives must be analysed.

Note: $f_{xx}f_{yy} - f_{xy}^2 = f_{xx}f_{yy} - f_{xy}f_{yx} = \det\left(H_f\right)$.

2^{nd} derivative test and eigenvalues

Recall that for univariate functions:

$$f(x_0 + x) \approx f(x_0) + f'(x_0)x + \frac{f''(x_0)}{2}x^2$$

For multivariate functions, the linear approximation is:

$$f: \mathbb{R}^n \to \mathbb{R}, \qquad f(\boldsymbol{x_0} + \boldsymbol{v}) \approx \underbrace{f(\boldsymbol{x_0})}_{\textit{Constant}} + \underbrace{\nabla f(\boldsymbol{x_0}).\boldsymbol{v}}_{\textit{Linear term}}$$

Vector we are approximating near

Variable input

The 2^{nd} order partial derivatives again give a quadratic approximation:

$$f(\boldsymbol{x_0} + \boldsymbol{v}) \approx \underbrace{f(\boldsymbol{x_0})}_{\textit{Constant}} + \underbrace{\nabla f(\boldsymbol{x_0}).\boldsymbol{v}}_{\textit{Linear term}} + \underbrace{\frac{1}{2}\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{H_f}(\boldsymbol{x_0})\boldsymbol{v}}_{\textit{Quadratic term}}$$

At a stationary point the second term is zero, so if $\boldsymbol{x_0}$ is stationary then:

$$f(\boldsymbol{x_0} + \boldsymbol{v}) \approx f(\boldsymbol{x_0}) + \frac{1}{2}\boldsymbol{v}^{\boldsymbol{T}}\boldsymbol{H_f}(\boldsymbol{x_0})\boldsymbol{v}$$

2^{nd} derivative test and eigenvalues

At a stationary point $\boldsymbol{x_0}$ the quadratic approximation is:

$$f(\boldsymbol{x_0}+\boldsymbol{v}) \approx f(\boldsymbol{x_0}) + \frac{1}{2}\boldsymbol{v}^T \boldsymbol{H_f}(\boldsymbol{x_0})\boldsymbol{v}$$

But $\boldsymbol{H_f}(\boldsymbol{x_0})$ is real and symmetric

$\Rightarrow \boldsymbol{H_f}(\boldsymbol{x_0})$ has orthogonal eigenvectors $\boldsymbol{e_1}, \dots, \boldsymbol{e_n}$ with eigenvalues $\lambda_1, \dots, \lambda_n \in \mathbb{R}$

$\Rightarrow$ We can write $\boldsymbol{v} = c_1 e_1 + \cdots + c_n e_n$ and (with some simplifying)

$$f(\boldsymbol{x_0}+\boldsymbol{v}) \approx f(\boldsymbol{x_0}) + \frac{1}{2}\boldsymbol{v}^T \boldsymbol{H_f}(\boldsymbol{x_0})\boldsymbol{v}$$

$$= f(\boldsymbol{x_0}) + \frac{1}{2}(c_1\boldsymbol{e_1} + \cdots + c_n\boldsymbol{e_n})^T \boldsymbol{H_f}(\boldsymbol{x_0})(c_1\boldsymbol{e_1} + \cdots + c_n\boldsymbol{e_n})$$

$$= f(\boldsymbol{x_0}) + \frac{\lambda_1}{2}c_1^2 + \cdots + \frac{\lambda_n}{2}c_n^2$$

So this looks

- like a parabolic bowl open up if all $\lambda_i > 0$,
- like a parabolic bowl open down if $\lambda_i < 0$,
- like a saddle if there are λ_i, λ_j with opposite signs.
    - Note that for $n = 2$, $\det\left(H_f\right) = \lambda_1\lambda_2$

2^{nd} derivative test for multivariate extrema

Theorem:

Suppose $f(x, y) \in C^2$ and $f_x(x_0, y_0) = 0 = f_y(x_0, y_0)$, then

- (x_0, y_0) is a local minimum if the eigenvalues of $H_f(x_0, y_0)$ are all positive;
- (x_0, y_0) is a local maximum if the eigenvalues of $H_f(x_0, y_0)$ are all negative;
- (x_0, y_0) is a saddle point if some eigenvalues of $H_f(x_0, y_0)$ are positive, some negative;
- If $H_f(x_0, y_0)$ is singular, i.e. has a 0 eigenvalue, then the test is inconclusive.

Example

Identify the nature of the stationary points of:

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

1. Find the stationary points by solving:

$$\begin{Bmatrix} f_x = 0 \\ f_y = 0 \\ f_z = 0 \end{Bmatrix} \Leftrightarrow \begin{Bmatrix} 2x - y = 0 \\ 2y - x = 0 \\ 2z - 2 = 0 \end{Bmatrix} \Leftrightarrow \begin{Bmatrix} y = 2x \\ 4x - x = 0 \\ z = 1 \end{Bmatrix} \Leftrightarrow \begin{Bmatrix} x = 0 \\ y = 0 \\ z = 1 \end{Bmatrix},$$

   i.e. there is a single stationary point, $\mathbf{x_0} = (0,0,1)$.

2. The Hessian at $\boldsymbol{x_0}$ is:

$$H_f(0,0,1) = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

3. To find the eigenvalues of the above, solve:

$$\left|H_f(0,0,1) - \lambda I\right| = 0 \Leftrightarrow \begin{vmatrix} 2-\lambda & -1 & 0 \\ -1 & 2-\lambda & 0 \\ 0 & 0 & 2-\lambda \end{vmatrix} = 0 \Leftrightarrow (2-\lambda)^3 - (-1)(-1)(2-\lambda) = 0$$

$$\Leftrightarrow (2-\lambda)^3 - (2-\lambda) = 0 \Rightarrow \begin{Bmatrix} 2-\lambda = 0 \\ (2-\lambda)^2 - 1 = 0 \end{Bmatrix} \Rightarrow \begin{Bmatrix} \boldsymbol{\lambda = 2} \\ 2-\lambda = \pm 1 \Rightarrow \begin{Bmatrix} \boldsymbol{\lambda = 1} \\ \boldsymbol{\lambda = 3} \end{Bmatrix} \end{Bmatrix}$$

4. Since all of them are positive, the stationary point is a minimum.

What we learnt

Recap of how to find extrema for univariate and bivariate functions

Finding extrema for multivariate functions

- Stationary points at $f_{x_1} = f_{x_2} = \cdots = f_{x_n} = 0$
  - If also H_f has all eigenvalues positive, then minimum
  - If also H_f has all eigenvalues negative, then maximum
  - If H_f has both pos and neg eigenvalues, then saddle point