Machine Learning

CMPT 726

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Linear Algebra and Calculus Review (cont’d)

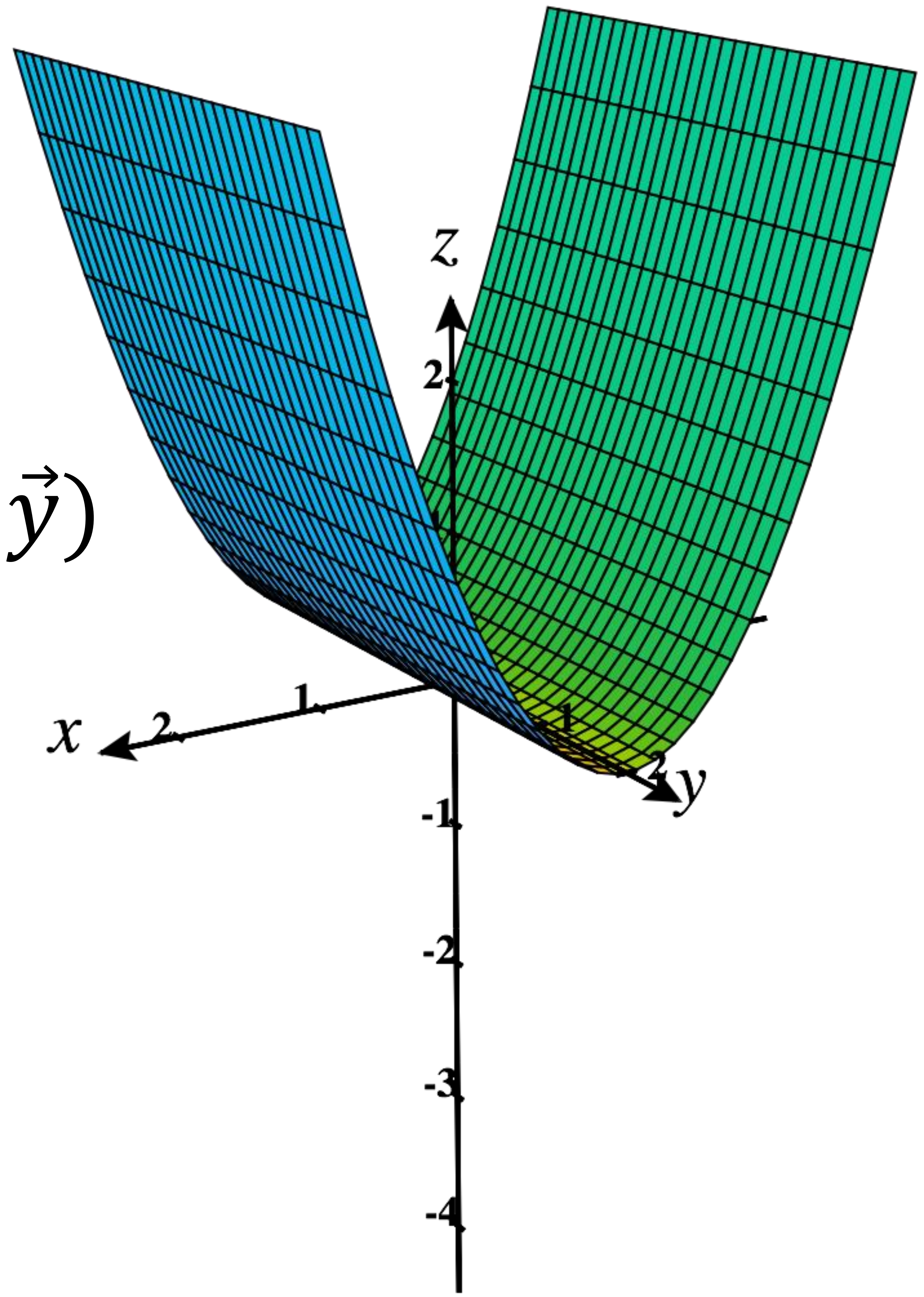
Convexity/Concavity

Convex function:

A line segment between **any** two points on the surface lies **on or above** the surface:

$$\alpha f(\vec{x}) + (1-\alpha) f(\vec{y}) \geq f(\alpha \vec{x} + (1-\alpha)\vec{y})$$

where $0 \leq \alpha \leq 1$



Or equivalently: Hessian of function is **positive semi-definite** everywhere, e.g.:

$$f(\vec{x}) = \vec{x}^{\top} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \vec{x} = x_1^2$$

Convexity/Concavity

Strictly convex function:

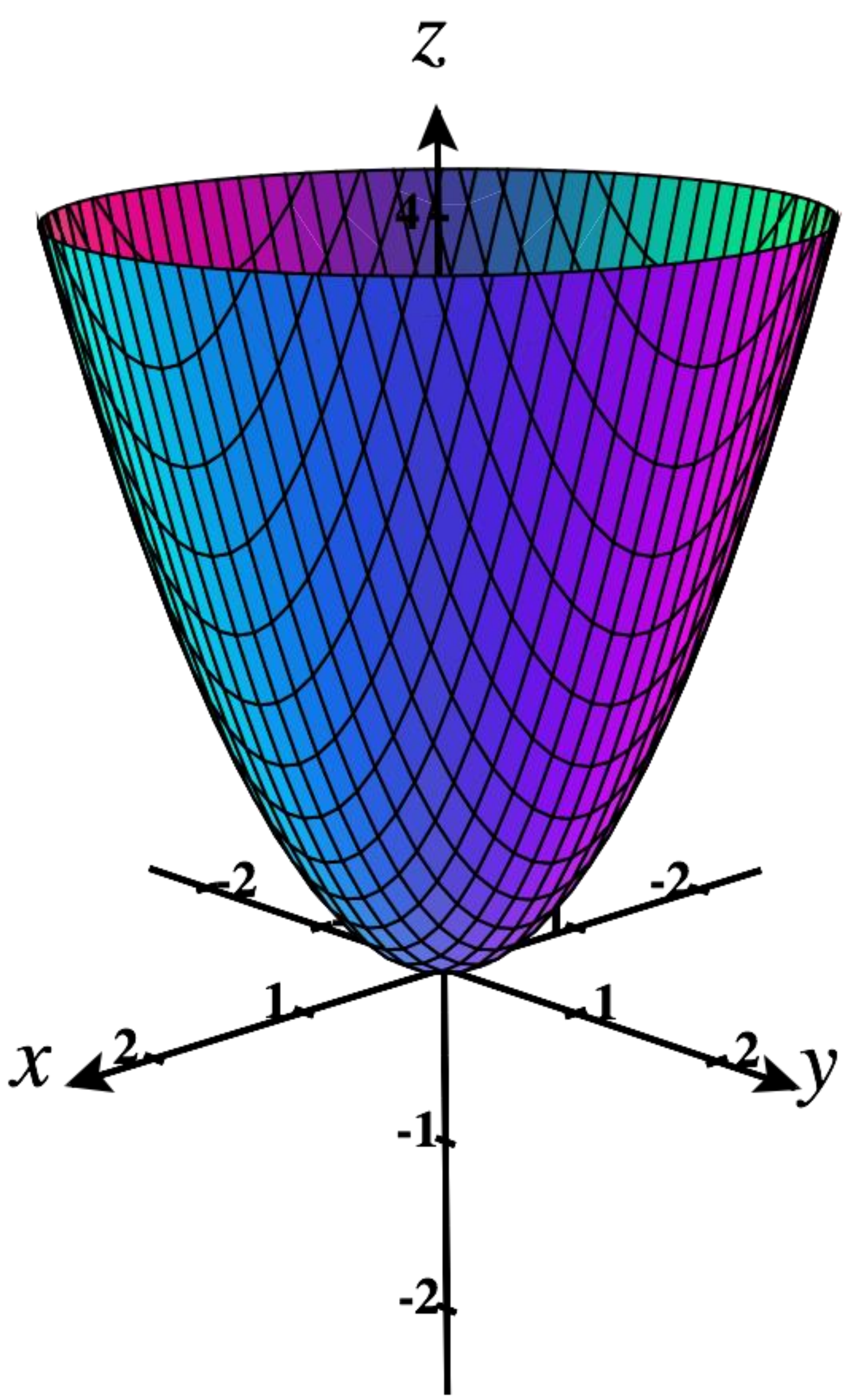
A line segment between **any** two points
on the surface lies **above** the surface:

$$\alpha f(\vec{x}) + (1-\alpha)f(\vec{y}) > f(\alpha\vec{x} + (1-\alpha)\vec{y})$$

where $0 < \alpha < 1$

If the Hessian is **positive definite** everywhere, e.g.:

$$f(\vec{x}) = \vec{x}^{\mathsf{T}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \vec{x} = x_1^2 + x_2^2$$



Then the function is strictly convex (but not the other way around!)

Convexity/Concavity

Concave function:

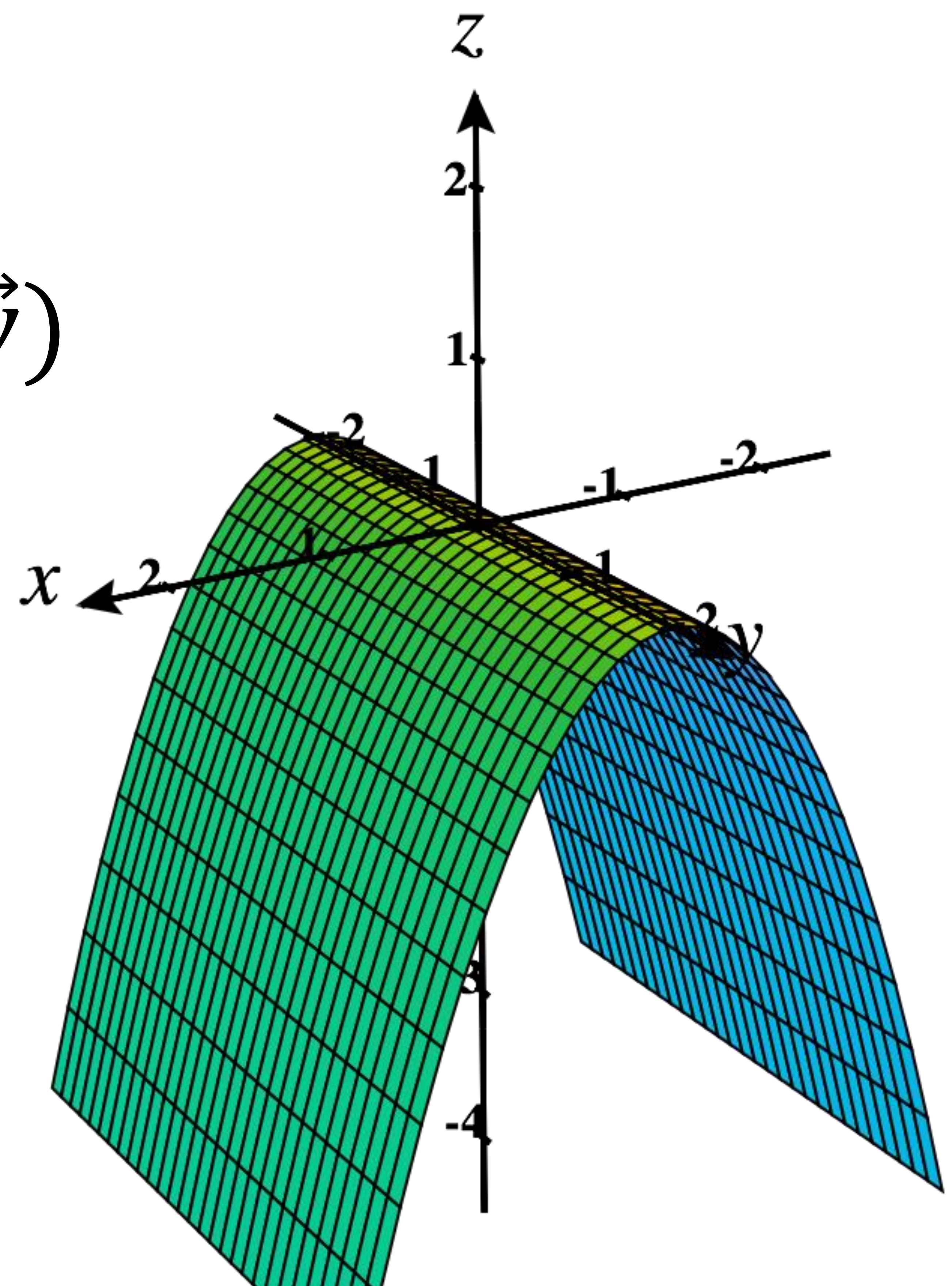
A line segment between **any** two points on the surface lies **on or below** the surface:

$$\alpha f(\vec{x}) + (1-\alpha) f(\vec{y}) \leq f(\alpha \vec{x} + (1-\alpha)\vec{y})$$

where $0 \leq \alpha \leq 1$

Or equivalently: Hessian of function is **negative semi-definite** everywhere, e.g.:

$$f(\vec{x}) = \vec{x}^\top \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix} \vec{x} = -x_1^2$$



Convexity/Concavity

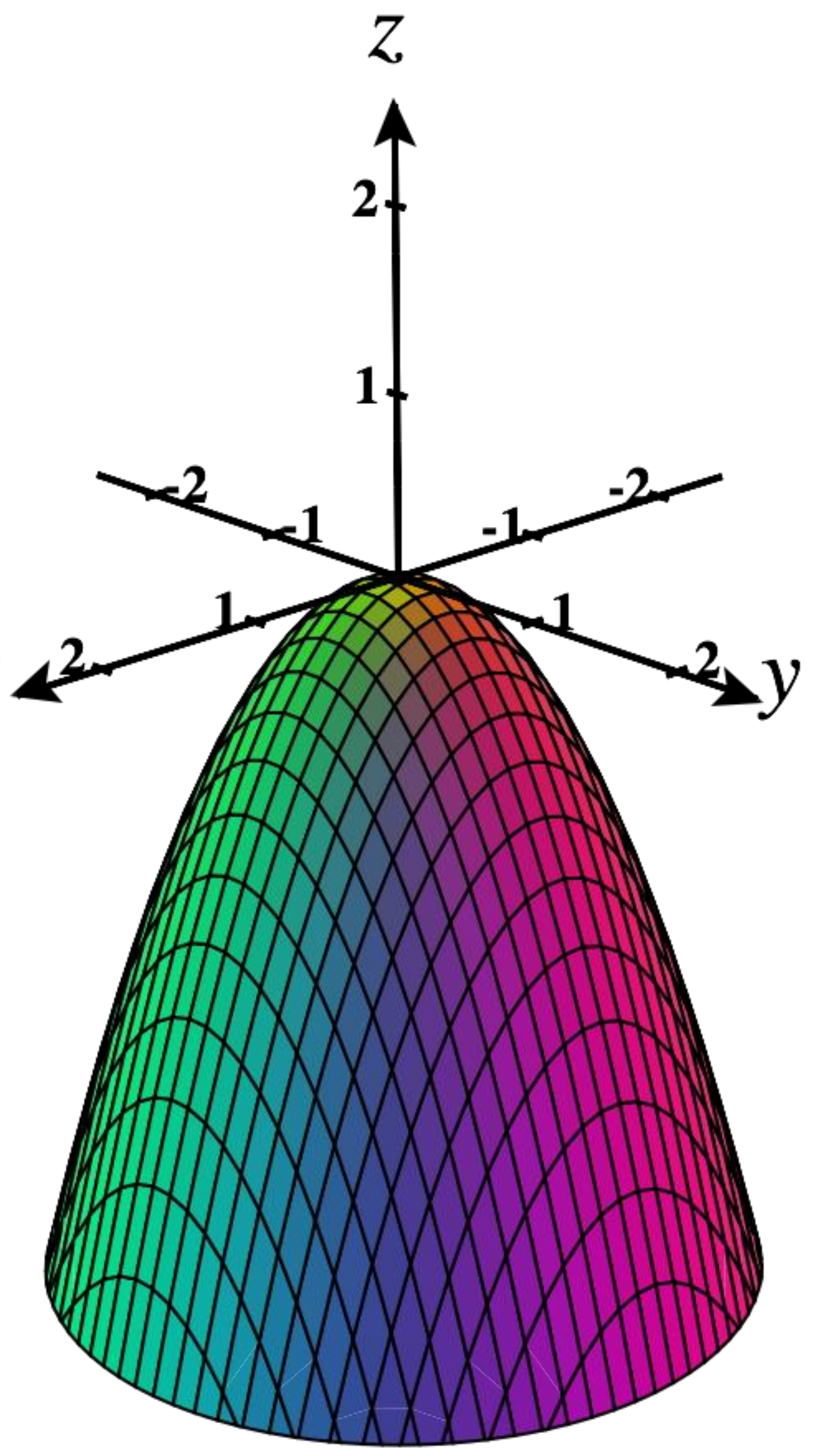
Strictly concave function:

A line segment between **any** two points
on the surface lies **below** the surface:
$$\alpha f(\vec{x}) + (1-\alpha) f(\vec{y}) < f(\alpha\vec{x} + (1-\alpha)\vec{y})$$

where $0 < \alpha < 1$

If the Hessian is **negative definite** everywhere, e.g.:
$$f(\vec{x}) = \vec{x}^{\mathsf{T}} \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \vec{x} = -x_1^2 - x_2^2$$

Then the function is strictly concave (but not the other way around!)



Jensen's Inequality

Definition of convex functions:

$$\alpha f(\vec{x}) + (1-\alpha) f(\vec{y}) \geq f(\alpha \vec{x} + (1-\alpha)\vec{y}), \text{ where } 0 \leq \alpha \leq 1$$

Jensen's inequality generalizes this to convex combinations of many points:

$$\sum_{i=1}^{n} \alpha_i f(\vec{x}_i) \geq f\left(\sum_{i=1}^{n} \alpha_i \vec{x}_i\right), \text{where } \alpha_i \geq 0 \ \forall i, \text{and } \sum_{i=1}^{n} \alpha_i = 1$$

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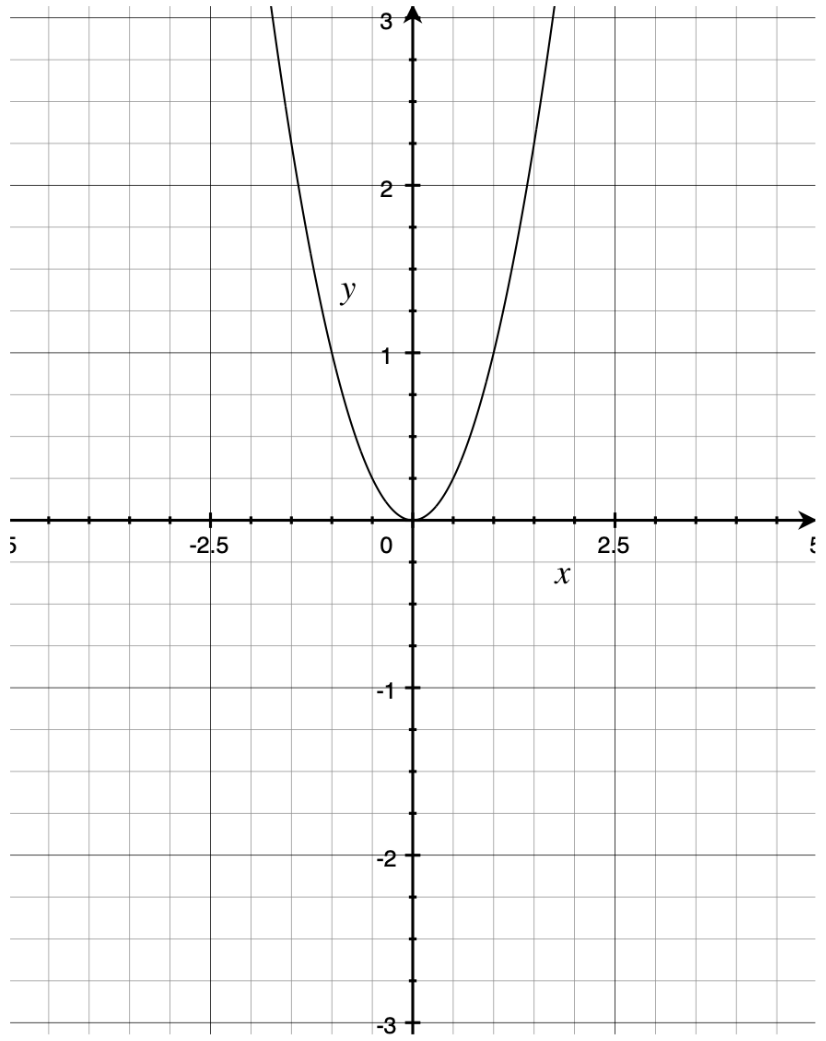
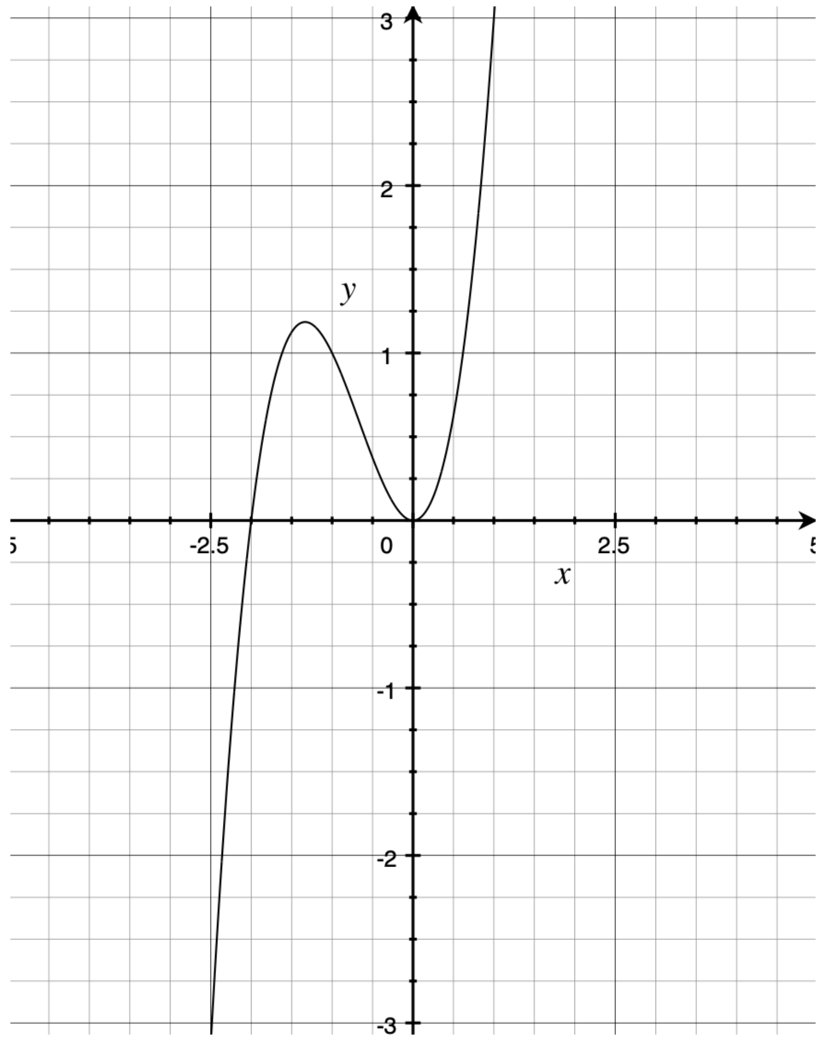
Optimality Conditions

Consider a univariate function $f\colon \mathbb{R} \to \mathbb{R}$ that is everywhere twice differentiable.
How can we find the points where f is minimized or maximized?

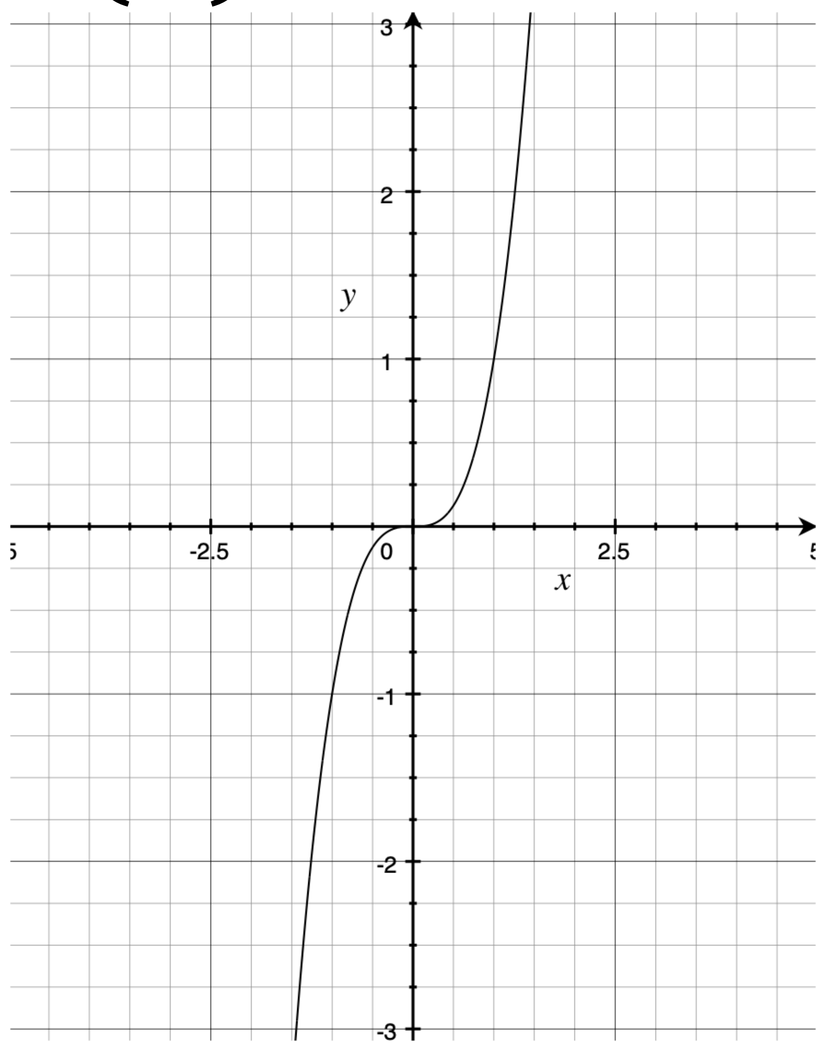
Critical points: All points x where $f'(x) = 0$.



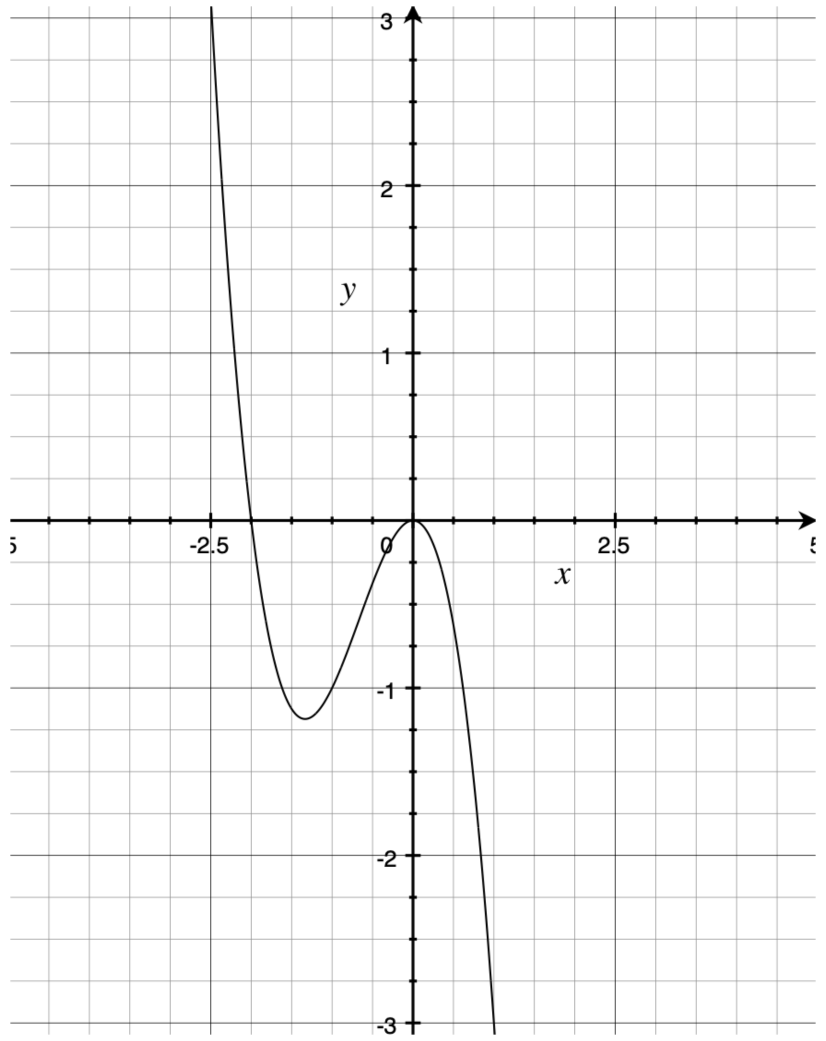
Global minimum



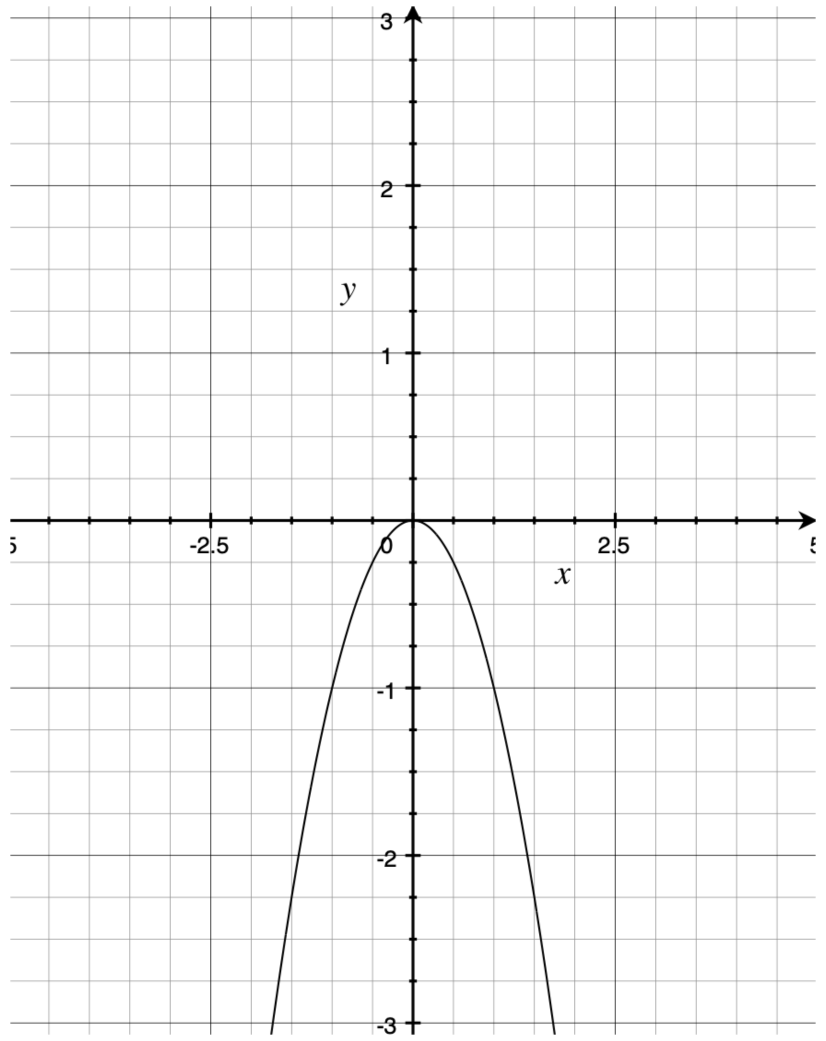
Local minimum



Saddle point



Local maximum



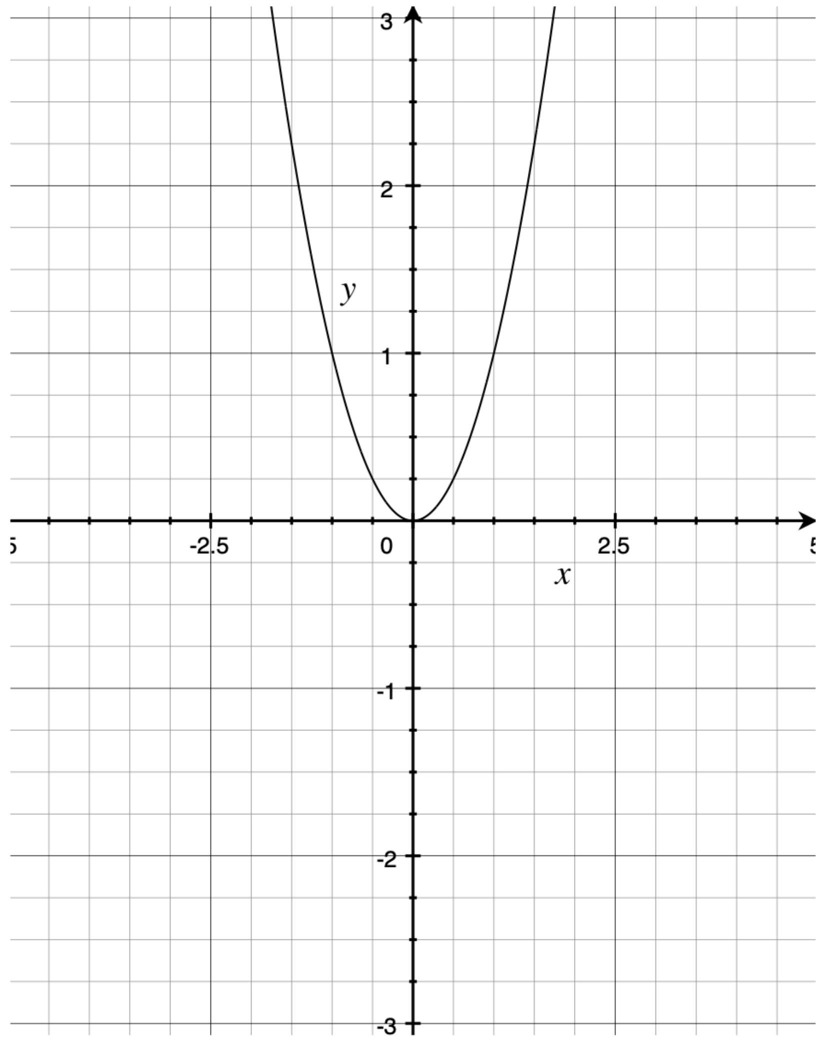
Global maximum

Optimality Conditions

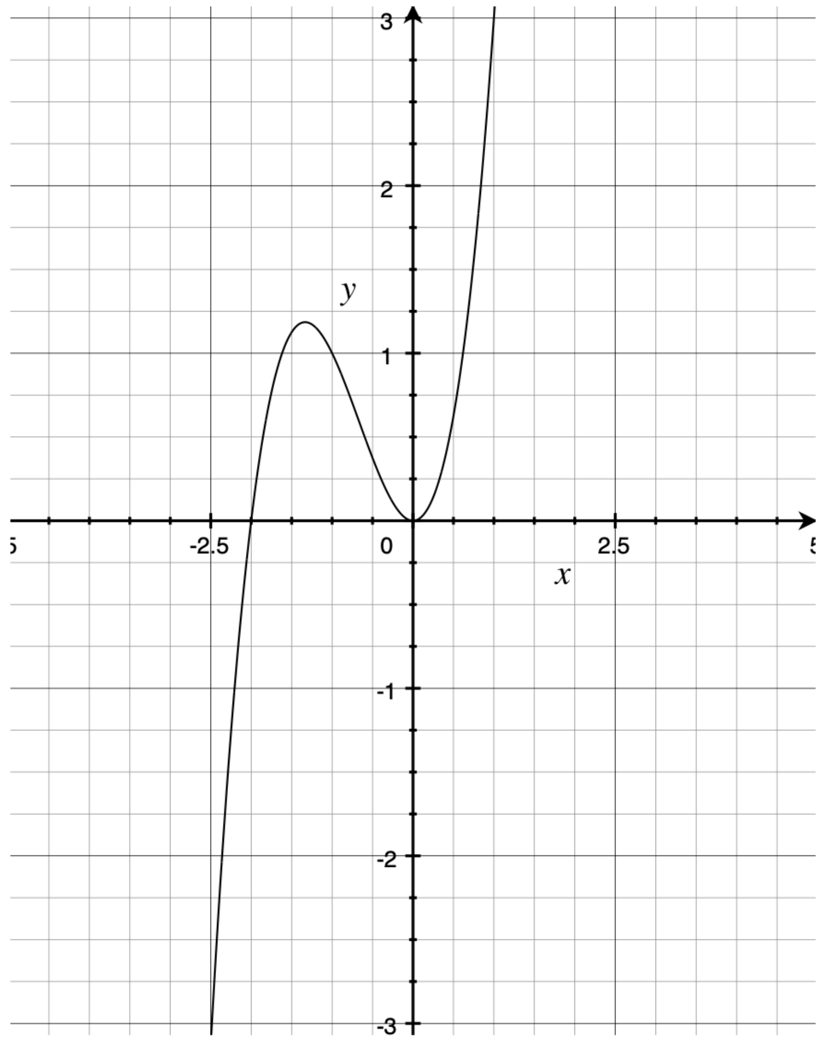
To differentiate these cases, we can check the second derivative at the critical points.

If $f''(x) > 0$, local/global minimum
If $f''(x) < 0$, local/global maximum
If $f''(x) = 0$, could be a local/global minimum, a local/global maximum, or a saddle point

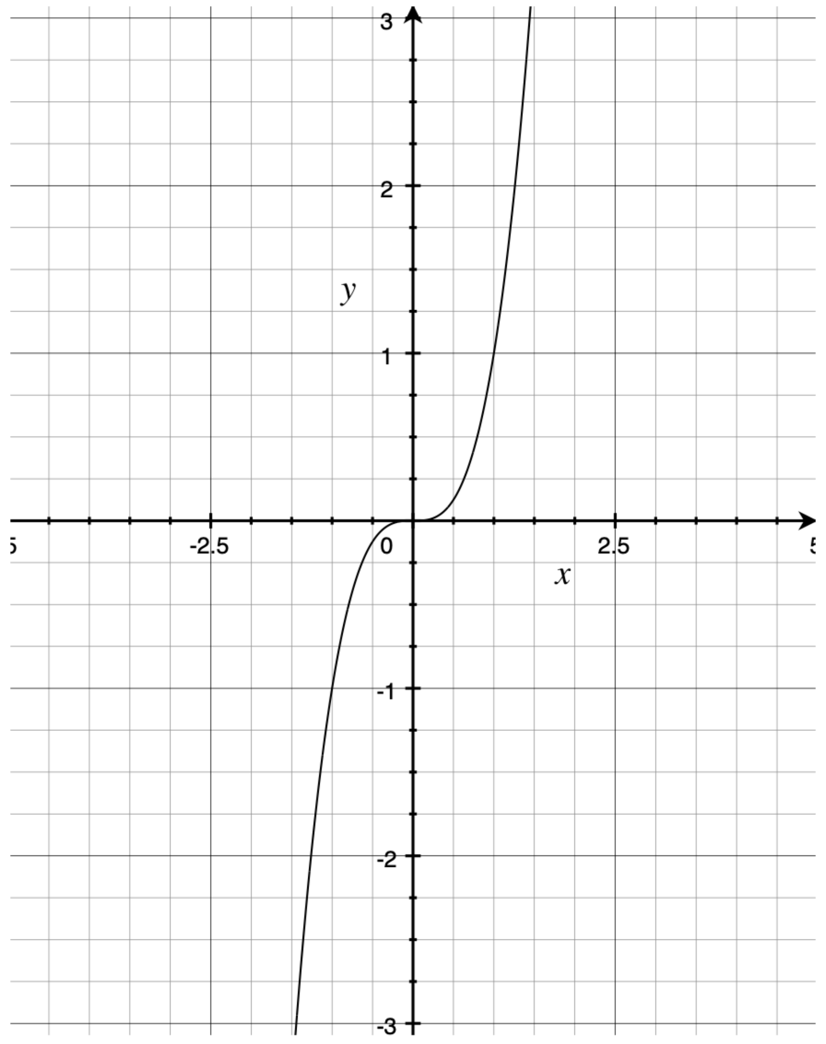
Hard to distinguish local and global minima/maxima in general



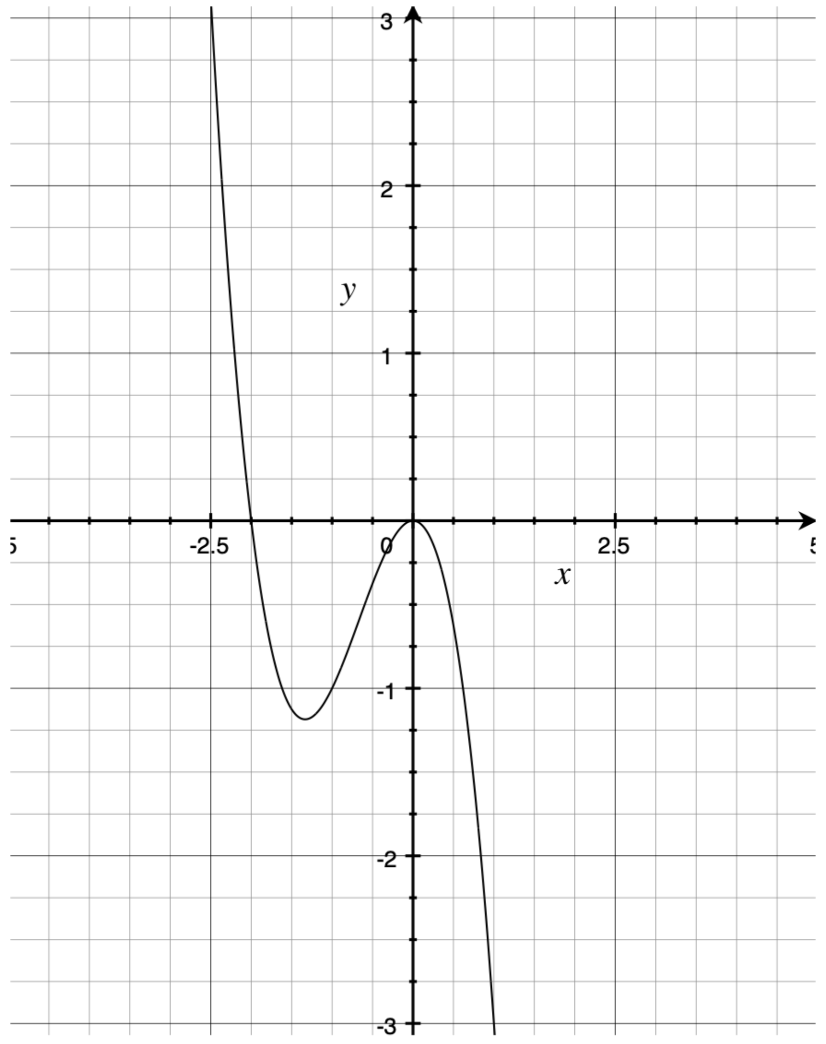
Global minimum



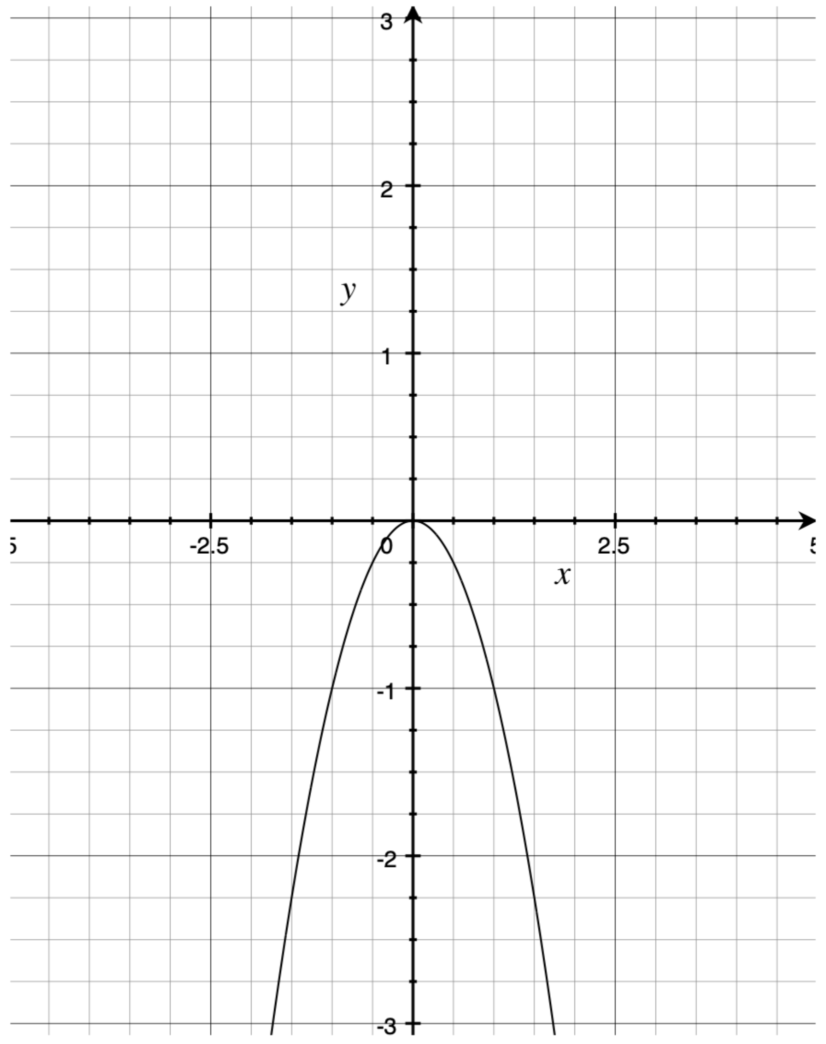
Local minimum



Saddle point



Local maximum

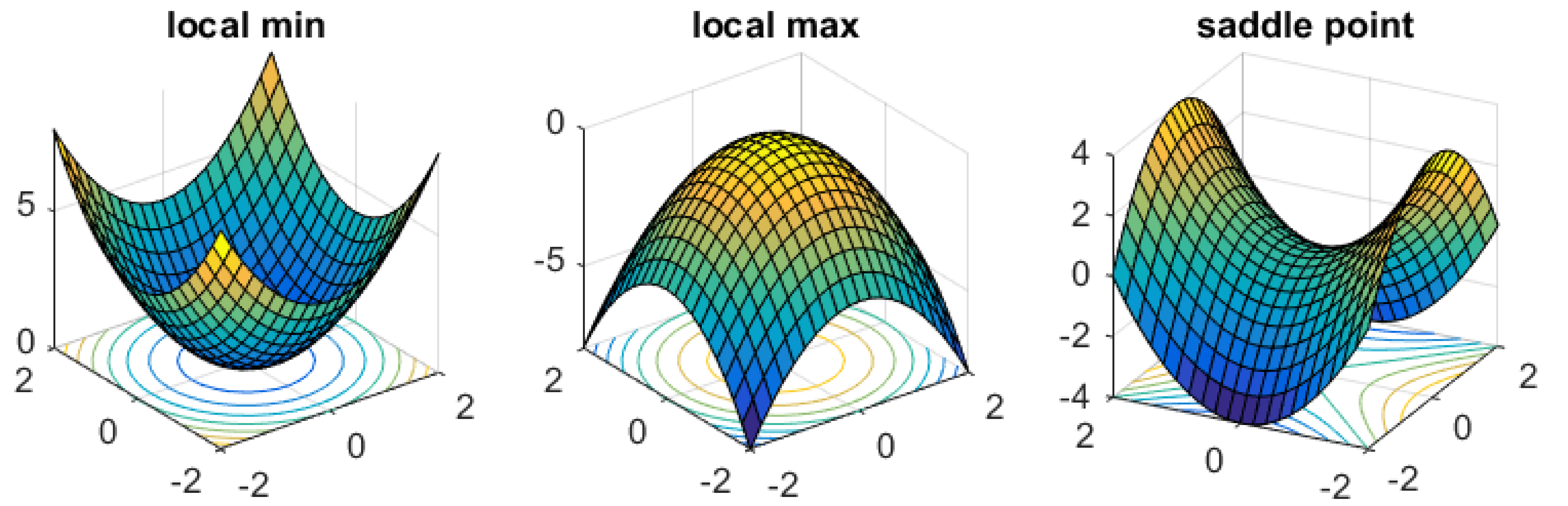


Global maximum

Optimality Conditions

Consider a multivariate function $f\colon \mathbb{R}^n \to \mathbb{R}$ that is everywhere twice differentiable. How can we find the points where f is minimized or maximized?

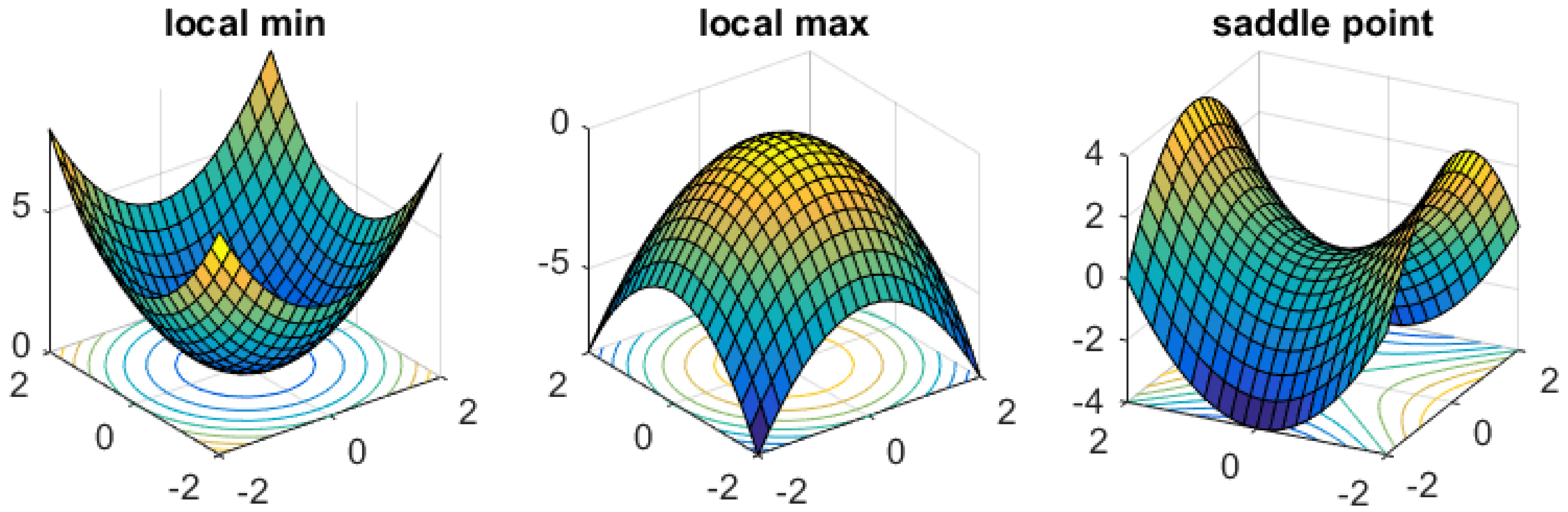
Critical points: All points $\vec{x}$ where $\frac{\partial f}{\partial \vec{x}}(\vec{x}) = \vec{0}$.



Optimality Conditions

To differentiate these cases, we can check the Hessian evaluated at the critical points.

If $\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top}(\vec{x}) \succ 0$ (positive definite), local/global minimum
If $\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top}(\vec{x}) \prec 0$ (negative definite), local/global maximum
If $\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top}(\vec{x})$ is indefinite, saddle point
If $\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top}(\vec{x}) \succcurlyeq 0$ (positive semi-definite) or $\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} f(\vec{x}) \preccurlyeq 0$ (negative semi-definite), could be a local/global minimum, a local/global maximum, or a saddle point



Global Optimality and Convexity/Concavity

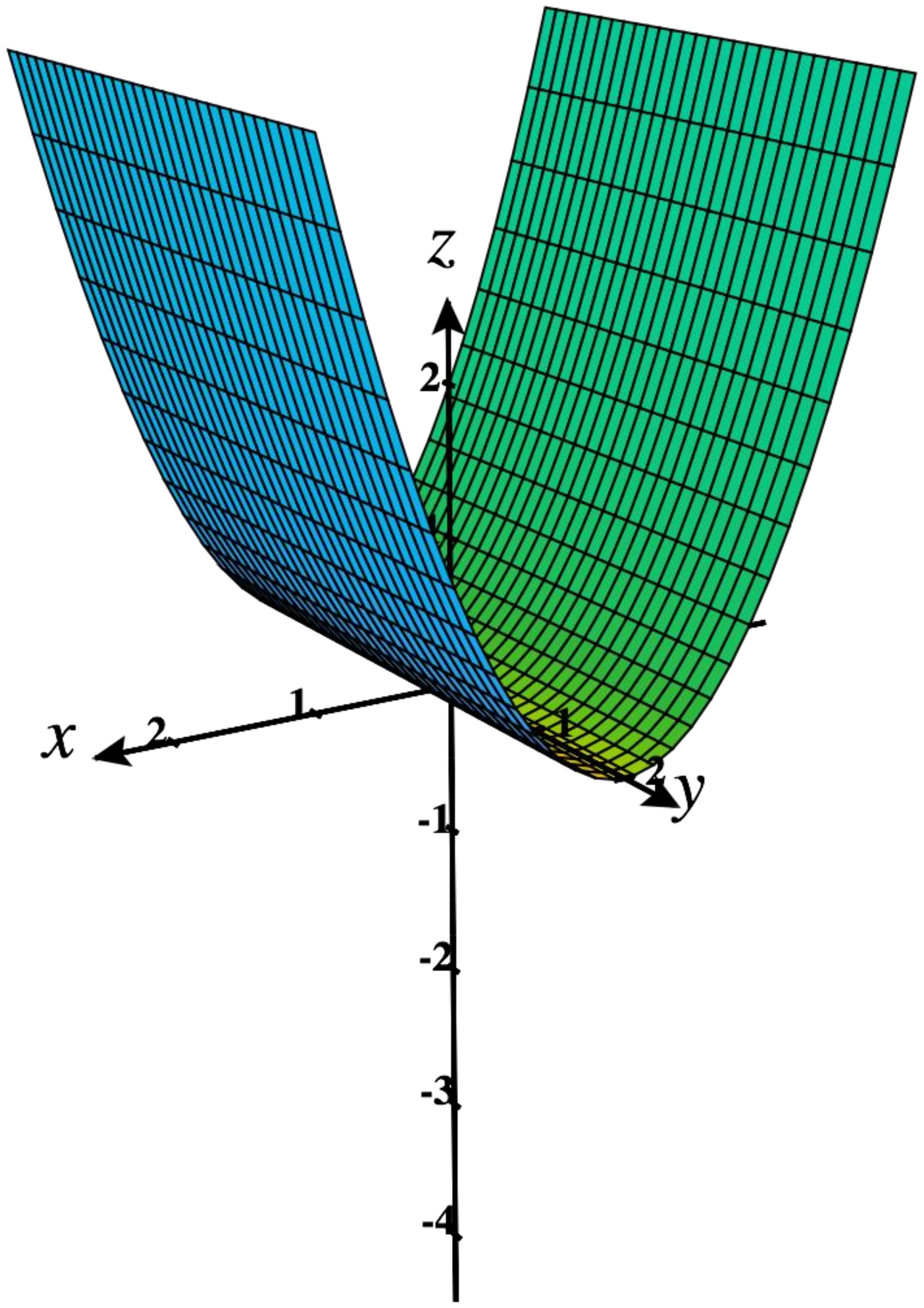
Recall: it is hard to distinguish local optima (that are not global optima) from global optima.

Convexity/concavity is a sufficient (but not necessary) condition for every local optimum to be a global optimum.

In a **convex** function:

Every **critical point** is a **local minimum**.

Every **local minimum** is a **global minimum**.



Global Optimality and Convexity/Concavity

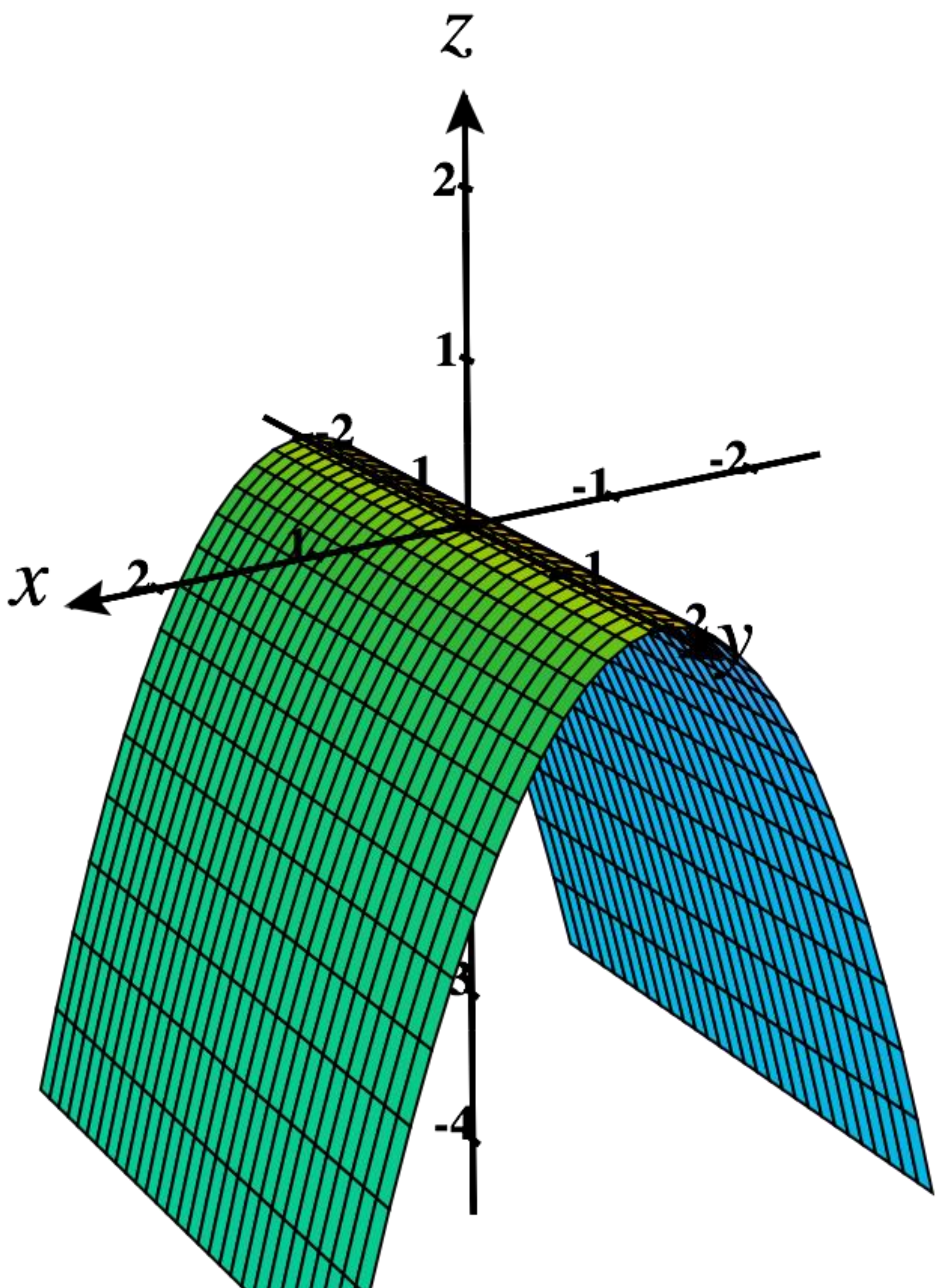
Recall: it is hard to distinguish local optima (that are not global optima) from global optima.

Convexity/concavity is a sufficient (but not necessary) condition for every local optimum to be a global optimum.

In a **concave** function:

Every **critical point** is a **local maximum**.

Every **local maximum** is a **global maximum**.

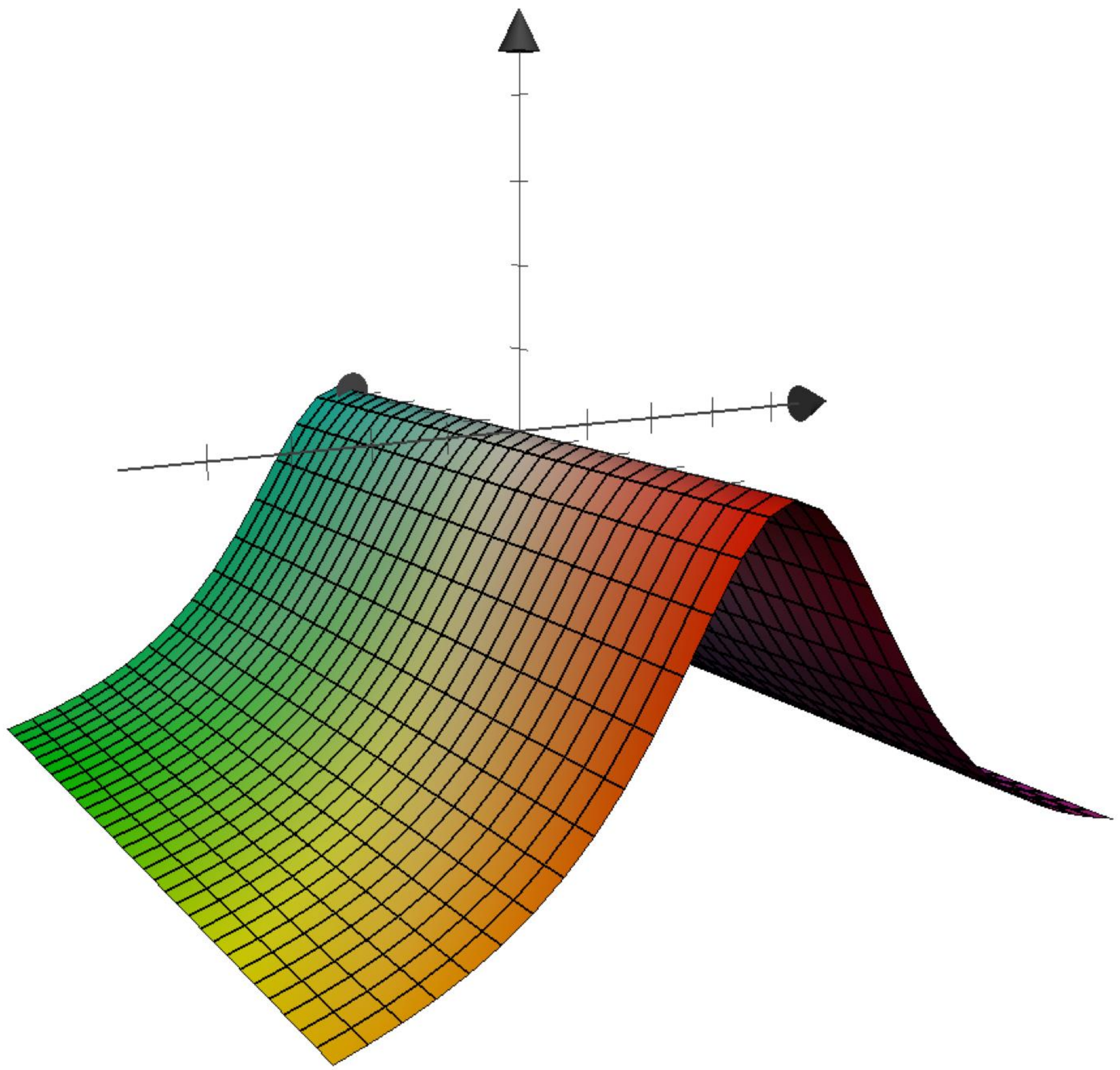


Global Optimality and Convexity/Concavity

Recall: it is hard to distinguish local optima (that are not global optima) from global optima.

Convexity/concavity is a sufficient (but not necessary) condition for every local optimum to be a global optimum.

Note: There are **non-concave** functions where every **local maximum** is a **global maximum**.



Example

- $f(x) = x^4$: $f''(0) = 0 \Rightarrow$ positive semidefinite Hessian
  - 0 is a local minimum
  - (Hessian is also negative semidefinite)
- $f(x) = -x^4$: $f''(0) = 0 \Rightarrow$ negative semidefinite Hessian
  - 0 is a local maximum
  - (Hessian is also positive semidefinite)

Lipschitz Continuity

A function $f: \mathbb{R}^n \to \mathbb{R}$ is L-Lipschitz if for all $\vec{x}_1, \vec{x}_2$,

$$|f(\vec{x}_1) - f(\vec{x}_2)| \leq L\|\vec{x}_1 - \vec{x}_2\|_2$$

Intuitively, an L-Lipschitz function cannot grow too quickly.

An everywhere differentiable function is L-Lipschitz if and only if $\|\partial f/\partial\vec{x}(\vec{x})\| \leq L$