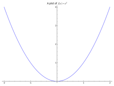
Nonlinear optimization I: Extrema of functions

Discrete Mathematics and Optimization
Bioinformatics

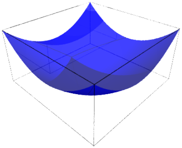
Functions of several variables

How to deal with functions of several variables?

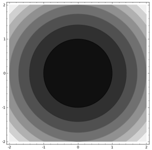
$$f : D \subset \mathbb{R}^n \longrightarrow \mathbb{R}^m$$



- $f : \mathbb{R} \longrightarrow \mathbb{R}$: visualize with plot of f,



- $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$: visualize with plot of f,



visualize level curves of f

- $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$, mmmh!

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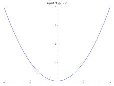

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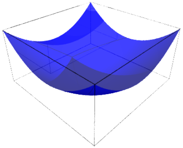

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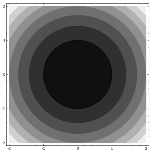

visualize level curves of f

- $f : \mathbb{R}^{300} \longrightarrow \mathbb{R}$, mmmmmmmmmmmmh!

1. Partial derivatives

How to extend the tools of calculus to functions of several variables?

Definition

Let $f : D \subset \mathbb{R}^n \longrightarrow \mathbb{R}$. The partial derivative of f at $\vec{x} \in D$ with respect to the i–th coordinate is

$$\frac{\partial f}{\partial x_i}(\vec{x}) = \lim_{h \to 0} \frac{f(\vec{x} + h\vec{e_i}) - f(\vec{x})}{h}$$

if the limit exists.

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if the limit exists.

- Reduction to one dimensional case: If $g(h) = f(\vec{x} + h\vec{e_i})$ then

$$\frac{\partial f}{\partial x_i}(\vec{x}) = g'(0)$$

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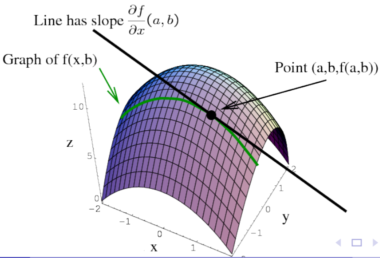
if the limit exists.

- Geometric interpretation: $\frac{\partial f}{\partial x_i}(\vec{x})$ is the slope of the tangent line to the graph of $g(h) = f(\vec{x} + h\vec{e_i})$ at $h = 0$.



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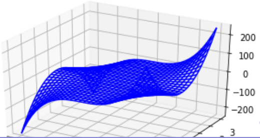
if the limit exists.

- How to compute: Think of all variables but the one we consider and use differentiation rules of one variable.

$$f(x,y) = x^3y^2 : \frac{\partial f}{\partial x}(x,y) = 3x^2y^2$$
$$\frac{\partial f}{\partial y}(x,y) = 2x^3y$$



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- How to compute: Think of all variables but the one we consider and use differentiation rules of one variable.

$$f(x, y, z) = e^{xy} \cos z$$

$$\frac{\partial f}{\partial x}(x, y, z) = ye^{xy} \cos z$$
$$\frac{\partial f}{\partial y}(x, y, z) = xe^{xy} \cos z$$
$$\frac{\partial f}{\partial z}(x, y, z) = -e^{xy} \sin z$$

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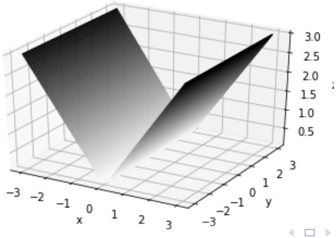
- Why should it fail to exist? The function $g(h) = f(\vec{x} + h\vec{e_i})$ may be not differentiable at 0: not continuous, not smooth,...



2. The gradient

Definition

Let $f : D \subset \mathbb{R}^n \longrightarrow \mathbb{R}$. The gradient of f at $\vec{x} \in D$ is the vector in $\mathbb{R}^n$

$$\nabla f(\vec{x}) = (\frac{\partial f}{\partial x_1}(\vec{x}), \ldots, \frac{\partial f}{\partial x_n}(\vec{x}))$$

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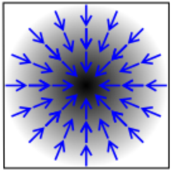
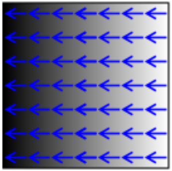
- If the gradient exists and is nonzero, then it is perpendicular to the level sets of f, pointing at the direction of maximum (local) increasing rate of f.





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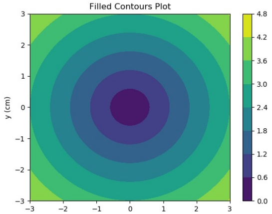
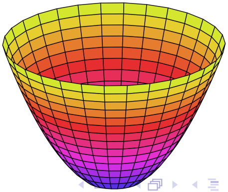
  $f(x, y) = x^2 + y^2$
  $\nabla f(x, y) = (2x, 2y),\ \nabla f(1, 1) = (2, 2)$





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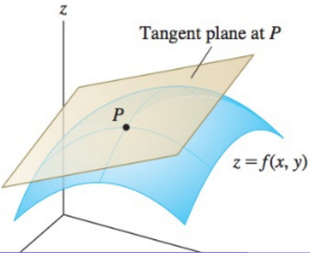
- If the gradient exists at $\vec{x}$ one gets the linear approximation of f at $\vec{x}$

$$f(\vec{x} + \vec{h}) \approx f(\vec{x}) + \nabla f(\vec{x}) \cdot \vec{h}$$



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$$f(\vec{x} + \vec{h}) \approx f(\vec{x}) + \nabla f(\vec{x}) \cdot \vec{h}$$

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

$$\nabla f(1,2) = (2,4)$$

$$f(1+h, 2+k) \approx f(1,2) + \nabla f(1,2) \cdot (h,k) = 5 + 2h + 4k$$

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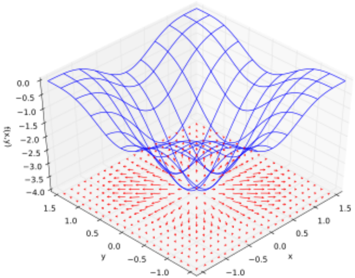
- If the gradient exists and is zero at a point $\vec{x}$ then x is a critical point of f: all curves on the graph of f through $\vec{x}$ have a critical point in $\vec{x}$.



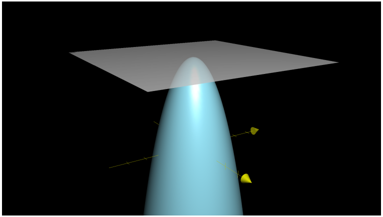
3. Extrema of functions

Theorem

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$. If f has a local extremum at $\vec{x} \in D$ and ∇f exists at $\vec{x}$ then

$$\nabla f(\vec{x}) = 0.$$

- The point $\vec{x}$ is a local maximum of f if $f(\vec{x}) \geq f(\vec{x} + \vec{h})$ for every ' small' $\vec{h} \in \mathbb{R}^n$.
  Then all curves on the graph of f through $\vec{x}$ have a local maximum at $\vec{x}$.



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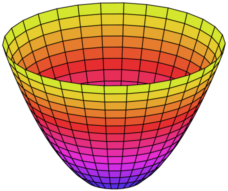
  Then all curves on the graph of f through $\vec{x}$ have a local minimum at $\vec{x}$.

$$f(x, y) = x^2 + y^2,\ \nabla f(x, y) = 0 \ \Rightarrow (x, y) = (0, 0)$$



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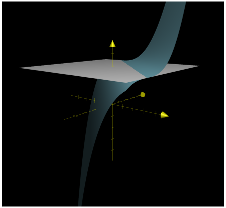
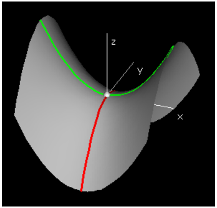
- We may have $\nabla f(\vec{x}) = 0$ in points which are not local extrema.





How to decide the nature of a critical point?

4. The Hessian

Definition

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$. Suppose that all partial derivatives of f exist in all points in a neighborhood of $\vec{x} \in D$. The second derivative of f with respect to x_i and x_j at $\vec{x}$ is

$$\frac{\partial^2 f}{\partial x_j \partial x_i}(\vec{x}) = \frac{\frac{\partial f}{\partial x_i}}{\partial x_j}(\vec{x}) = \lim_{h \to 0} \frac{\frac{\partial f}{\partial x_i}(\vec{x} + h\vec{e_j}) - \frac{\partial f}{\partial x_i}(\vec{x})}{h}$$

if the limit exists.

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

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

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

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if the limit exists.

- If all second partial derivatives of f exist in $\vec{x} \in D$ then the Hessian matrix of f at $\vec{x}$ is

$$Hf(\vec{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2}(\vec{x}) & \frac{\partial^2 f}{\partial x_1 x_2}(\vec{x}) & \cdots & \frac{\partial^2 f}{\partial x_1 x_n}(\vec{x}) \\ \frac{\partial^2 f}{\partial x_2 x_1}(\vec{x}) & \frac{\partial^2 f}{\partial x_2^2}(\vec{x}) & \cdots & \frac{\partial^2 f}{\partial x_2 x_n}(\vec{x}) \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 f}{\partial x_n x_1}(\vec{x}) & \frac{\partial^2 f}{\partial x_n x_2}(\vec{x}) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(\vec{x}) \end{pmatrix}$$

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

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

$$Hf(x,y) = \begin{pmatrix} 2y & 2x+2y \\ 2x+2y & 2x \end{pmatrix}, \ Hf(1,-1) = \begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix}$$

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if the limit exists.

- If the second partial derivatives are continuous functions in a neighborhood of x then

$$\frac{\partial^2 f}{\partial x_j \partial x_i}(\vec{x}) = \frac{\partial^2 f}{\partial x_i \partial x_j}(\vec{x})$$

  The Hessian matrix in this case is symmetric.
- We denote by $\mathcal{C}^2(D)$ the class of functions $f : D \subset \mathbb{R}^n \to \mathbb{R}$ which have all second derivatives in D and are continuous functions.

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Theorem

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be of class $\mathcal{C}^2(D)$. Then

$$f(\vec{x} + \vec{h}) \approx f(\vec{x}) + \nabla f(\vec{x}) \cdot \vec{h} + \frac{1}{2}\vec{h}^T \cdot Hf(\vec{x}) \cdot \vec{h}$$

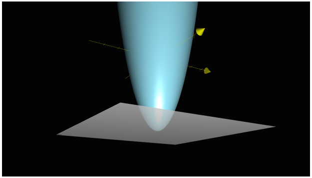
- The second order approximation in the theorem allows us to determine the nature of extrema of f at critical points.

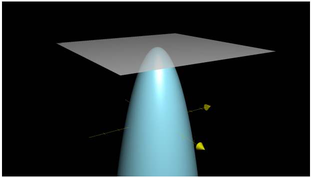
5. The nature of critical points

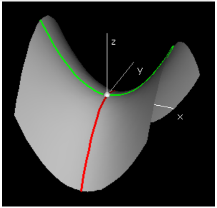
Theorem

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be of class $\mathcal{C}^2(D)$. Let $\vec{x}$ be a critical point of f. Assume that $H \neq 0$.

- *If H is positive definite at $\vec{x}$ then $\vec{x}$ is a (strict) local minimum of f.*
- *If H is negative definite at $\vec{x}$ then $\vec{x}$ is a (strict) local maximum of f.*
- *if H is not definite at $\vec{x}$ then $\vec{x}$ is a saddle point of f.*







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- A simple criteria to decide if H is definite: Let Δ_k denote the determinant of the $k \times k$ principal submatrix of H, $k = 1, \ldots, n$.
  - H is positive definite if and only if $\Delta_k > 0$ for $k = 1, \ldots, n$.
  - H is negative definite if and only if $(-1)^k \Delta_k > 0$ for $k = 1, \ldots, n$.

6. Global extrema

When local extrema can be ensured to be global?

Theorem

Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be of class $\mathcal{C}^2(D)$. Then

$$f(\vec{x}+\vec{h}) = f(\vec{x}) + \nabla f(\vec{x}) \cdot \vec{h} + \frac{1}{2} h^T \cdot H(\vec{x}+\theta\vec{h}) \cdot \vec{h},\ 0 \leq \theta \leq 1.$$

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- If $H(\vec{x})$ is positive definite for all $\vec{x} \in \mathbb{R}^n$ then x is a (strict) global minimum of f.
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Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be a continous function on D. If D is a closed and bounded then f has a global maximum and a global minimum.

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Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continous function. If

$$\lim_{\|x\| \to \infty} f(x) = \infty,$$

then f has a global minimum.

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- If $H(y)$ is positive definite for all $y \in D$ then x is a (strict) global minimum of f.
- If $H(y)$ is negative definite for all $y \in D$ then x is a (strict) global maximum of f.

Summary

- The tools of calculus are useful for nonlinear optimization: methods for locating extreme values of functions.
- Partial derivatives, gradient and Hessian are the several variable analogous to derivatives in one variable.
- The linear (local) approximation of a function in $\mathcal{C}^2$ is

$$f(\vec{y}) = f(\vec{x}) + \nabla f(\vec{x}) \cdot (\vec{y} - \vec{x}) + o(\|\vec{y} - \vec{x}\|)$$

- The quadratic (local) approximation of a function in $\mathcal{C}^3$ is

$$f(\vec{y}) = f(\vec{x}) + \nabla f(\vec{x}) \cdot (\vec{y} - \vec{x}) + (\vec{y} - \vec{x})^T Hf(\vec{x})(\vec{y} - \vec{x}) + o(\|\vec{y} - \vec{x}\|^2).$$

- Local extrema of a function are to be found among its critical points: $\nabla f(\vec{x}) = \mathbf{0}$.
- The nature of critical points can be elucidated by the Hessian.