Basics of Numerical Optimization: Preliminaries

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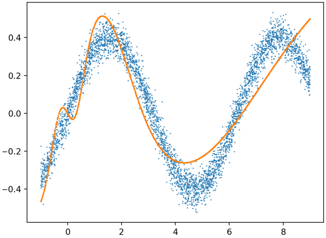
Supervised learning as function approximation



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- Training data: $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$ with $\boldsymbol{y}_i \approx f_0(\boldsymbol{x}_i)$
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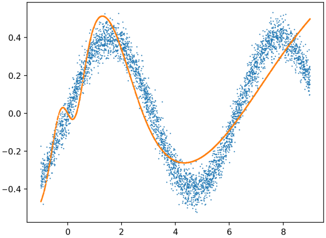

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$$\min_{f \in \mathcal{H}} \sum_i \ell(\boldsymbol{y}_i, f(\boldsymbol{x}_i)) + \Omega(f)$$

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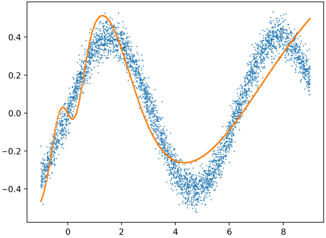

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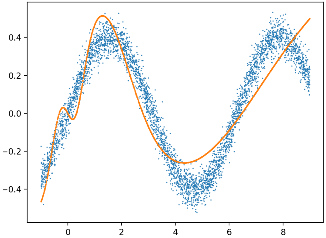

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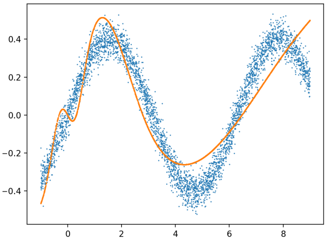

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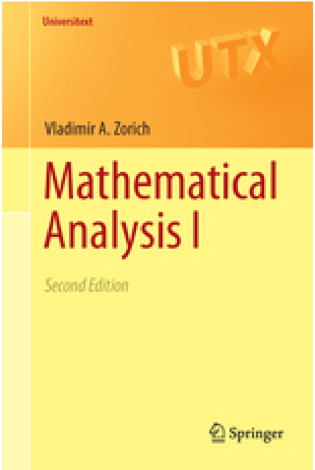
Now we start to focus on **optimization**.

Outline

Elements of multivatiate calculus

Optimality conditions of unconstrained optimization

Recommended references



[Munkres, 1997, Zorich, 2015, Coleman, 2012]

Our notation

- scalars: x, vectors: $\boldsymbol{x}$, matrices: $\boldsymbol{X}$, tensors: $\mathcal{X}$, sets: S

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- $[n] \doteq \{1, \dots, n\}$

Differentiability — first order

Consider $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}^m$

– Definition: **First-order differentiable** at a point $\boldsymbol{x}$ if there exists a matrix $\boldsymbol{B} \in \mathbb{R}^{m \times n}$ such that

$$\frac{f(\boldsymbol{x} + \boldsymbol{\delta}) - f(\boldsymbol{x}) - \boldsymbol{B}\boldsymbol{\delta}}{\|\boldsymbol{\delta}\|_2} \to \mathbf{0} \quad \text{as} \quad \boldsymbol{\delta} \to \mathbf{0}.$$

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- Calculation: $b_{ij} = \frac{\partial f_i}{\partial x_j}(\boldsymbol{x})$
- **Sufficient condition**: if all partial derivatives exist and are **continuous** at $\boldsymbol{x}$, then $f(\boldsymbol{x})$ is differentiable at $\boldsymbol{x}$.

Calculus rules

Assume $f, g : \mathbb{R}^n \to \mathbb{R}^m$ are differentiable at a point $\boldsymbol{x} \in \mathbb{R}^n$.

- **linearity**: $\lambda_1 f + \lambda_2 g$ is differentiable at $\boldsymbol{x}$ and
  $\nabla \left[\lambda_1 f + \lambda_2 g\right](\boldsymbol{x}) = \lambda_1 \nabla f(\boldsymbol{x}) + \lambda_2 \nabla g(\boldsymbol{x})$
- **product**: assume $m = 1$, fg is differentiable at $\boldsymbol{x}$ and
  $\nabla \left[fg\right](\boldsymbol{x}) = f(\boldsymbol{x}) \nabla g(\boldsymbol{x}) + g(\boldsymbol{x}) \nabla f(\boldsymbol{x})$
- **quotient**: assume $m = 1$ and $g(\boldsymbol{x}) \neq 0$, $\frac{f}{g}$ is differentiable at $\boldsymbol{x}$ and
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- **Chain rule**: Let $f : \mathbb{R}^m \to \mathbb{R}^n$ and $h : \mathbb{R}^n \to \mathbb{R}^k$, and f is differentiable at $\boldsymbol{x}$ and $\boldsymbol{y} = f(\boldsymbol{x})$ and h is differentiable at $\boldsymbol{y}$. Then, $h \circ f : \mathbb{R}^n \to \mathbb{R}^k$ is differentiable at $\boldsymbol{x}$, and

$$\boldsymbol{J}_{[h \circ f]}(\boldsymbol{x}) = \boldsymbol{J}_h(f(\boldsymbol{x}))\, \boldsymbol{J}_f(\boldsymbol{x}).$$

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  When $k = 1$**,**

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Differentiability — second order

Consider $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$ and assume f is 1st-order differentiable in a small ball around $\boldsymbol{x}$

- Write $\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x}) \doteq \left[\frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_i}\right)\right](\boldsymbol{x})$ provided the right side well defined

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- **Symmetry**: If both $\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x})$ and $\frac{\partial f^2}{\partial x_i \partial x_j}(\boldsymbol{x})$ exist and both are continuous at $\boldsymbol{x}$, then they are equal.
- **Hessian (matrix)**:

$$\nabla^2 f(\boldsymbol{x}) \doteq \left[\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x})\right]_{j,i}, \tag{1}$$

where $\left[\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x})\right]_{j,i} \in \mathbb{R}^{n \times n}$ has its (j,i)-th element as $\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x})$.

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- $\nabla^2 f$ is symmetric.
- **Sufficient condition**: if all $\frac{\partial f^2}{\partial x_j \partial x_i}(\boldsymbol{x})$ exist and are **continuous**, f is 2nd-order differentiable at $\boldsymbol{x}$ (not converse; we omit the definition due to its technicality).

Taylor's theorem

Vector version: consider $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$

– If f is 1st-order differentiable at $\boldsymbol{x}$, then

$$f(\boldsymbol{x} + \boldsymbol{\delta}) = f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{\delta} \rangle + o(\|\boldsymbol{\delta}\|_2) \text{ as } \boldsymbol{\delta} \to \mathbf{0}.$$

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- If f is 2nd-order differentiable at $\boldsymbol{x}$, then

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Matrix version: consider $f(\boldsymbol{X}) : \mathbb{R}^{m \times n} \to \mathbb{R}$

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$$\text{as } \boldsymbol{\Delta} \to \mathbf{0}.$$

Taylor approximation — asymptotic uniqueness

Let $f : \mathbb{R} \to \mathbb{R}$ be k ($k \geq 1$ integer) times differentiable at a point x. If $P(\delta)$ is a k-th order polynomial satisfying $f\left(x+\delta\right) - P\left(\delta\right) = o(\delta^k)$ as $\delta \to 0$, then $P\left(\delta\right) = P_k(\delta) \doteq f(x) + \sum_{i=1}^{k} \frac{1}{k!} f^{(k)}\left(x\right) \delta^k$.

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Generalization to the vector version

– Assume $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$ is 1-order differentiable at $\boldsymbol{x}$. If $P(\boldsymbol{\delta}) \doteq f(\boldsymbol{x}) + \langle \boldsymbol{v}, \boldsymbol{\delta} \rangle$ satisties that

$$f(\boldsymbol{x} + \boldsymbol{\delta}) - P(\boldsymbol{\delta}) = o(\|\boldsymbol{\delta}\|_2) \quad \text{as } \boldsymbol{\delta} \to \mathbf{0},$$

then $P(\boldsymbol{\delta}) = f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{\delta} \rangle$, i.e., the 1st-order Taylor expansion.

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  then $P(\boldsymbol{\delta}) = f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{\delta} \rangle$, i.e., the 1st-order Taylor expansion.
- Assume $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$ is 2-order differentiable at $\boldsymbol{x}$. If $P(\boldsymbol{\delta}) \doteq f(\boldsymbol{x}) + \langle \boldsymbol{v}, \boldsymbol{\delta} \rangle + \frac{1}{2} \langle \boldsymbol{\delta}, \boldsymbol{H}\boldsymbol{\delta} \rangle$ with $\boldsymbol{H}$ symmetric satisties that

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Taylor approximation — asymptotic uniqueness

Let $f : \mathbb{R} \to \mathbb{R}$ be k ($k \geq 1$ integer) times differentiable at a point x. If $P(\delta)$ is a k-th order polynomial satisfying $f(x+\delta) - P(\delta) = o(\delta^k)$ as $\delta \to 0$, then $P(\delta) = P_k(\delta) \doteq f(x) + \sum_{i=1}^{k} \frac{1}{k!} f^{(k)}(x)\, \delta^k$.

Generalization to the vector version

- Assume $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$ is 1-order differentiable at $\boldsymbol{x}$. If $P(\boldsymbol{\delta}) \doteq f(\boldsymbol{x}) + \langle \boldsymbol{v}, \boldsymbol{\delta} \rangle$ satisties that

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Similarly for the matrix version. See Chap 5 of [Coleman, 2012] for other forms of Taylor theorems and proofs of the asymptotic uniqueness.

Two ways of deriving gradients and Hessians (Recall HW0!)

(a) Derive the gradient and Hessian of the linear least-squares function $f(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2$. Please include your calculation details.

(b) Let $\sigma = \frac{1}{1+e^{-x}}$, i.e., the *logistic function*. Derive the gradient of the matrix-variable function $g(\boldsymbol{W}) = \|\boldsymbol{y} - \sigma(\boldsymbol{W}\boldsymbol{x})\|_2^2$, where σ is applied to the vector $\boldsymbol{W}\boldsymbol{x}$ elementwise. This is regression based on a simplified one-neuron network. Please include your calculation details.

(a) Consider the least-squares objective $f(\boldsymbol{x}) = \|\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\|_2^2$ again. Recall that for any two vectors $\boldsymbol{a}, \boldsymbol{b}$, $\|\boldsymbol{a} - \boldsymbol{b}\|_2^2 = \|\boldsymbol{a}\|_2^2 - 2\boldsymbol{a}^\intercal\boldsymbol{b} + \|\boldsymbol{b}\|_2^2$. Now $f(\boldsymbol{x} + \boldsymbol{\delta}) = \|(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}) - \boldsymbol{A}\boldsymbol{\delta}\|_2^2$. Expand this square by the previous formula, and compare it to the 2nd order Taylor expansion by plugging your results from **Problem 1(a)**. Are they equal or not? Why? (Hint: You may find this fact useful: for any two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$ and any matrix $\boldsymbol{M} \in \mathbb{R}^{n \times n}$, $\langle \boldsymbol{u}, \boldsymbol{M}\boldsymbol{v} \rangle = \langle \boldsymbol{M}^\intercal \boldsymbol{u}, \boldsymbol{v} \rangle$. This can be derived from the trace cyclic property above.)

(b) Consider the one-neuron network regression again: $g(\boldsymbol{W}) = \|\boldsymbol{y} - \sigma(\boldsymbol{W}\boldsymbol{x})\|_2^2$ with $\sigma = \frac{1}{1+e^{-x}}$, i.e., the *logistic function*. Let's try to work out its 1st order Taylor expansion by direct expansion as follows.

- Show that $\sigma((\boldsymbol{W} + \boldsymbol{\Delta})\boldsymbol{x}) = \sigma(\boldsymbol{W}\boldsymbol{x}) + \sigma'(\boldsymbol{W}\boldsymbol{x}) \odot (\boldsymbol{\Delta}\boldsymbol{x}) + o(\|\boldsymbol{\Delta}\|_F)$ when $\boldsymbol{\Delta} \to \mathbf{0}$. Here, both σ and σ' are applied elementwise, and $\odot$ denotes the elementwise (Hadamard) product.
- So $\boldsymbol{y} - \sigma((\boldsymbol{W} + \boldsymbol{\Delta})\boldsymbol{x}) = (\boldsymbol{y} - \sigma(\boldsymbol{W}\boldsymbol{x})) - \sigma'(\boldsymbol{W}\boldsymbol{x}) \odot (\boldsymbol{\Delta}\boldsymbol{x}) - o(\|\boldsymbol{\Delta}\|_F)$ when $\boldsymbol{\Delta} \to \mathbf{0}$. Substitute this back into the square and use the identity $\|\boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c}\|_2^2 = \|\boldsymbol{a}\|_2^2 + \|\boldsymbol{b}\|_2^2 + \|\boldsymbol{c}\|_2^2 + 2\boldsymbol{a}^\intercal\boldsymbol{b} + 2\boldsymbol{a}^\intercal\boldsymbol{c} + 2\boldsymbol{b}^\intercal\boldsymbol{c}$ to obtain the first-order approximation to $g(\boldsymbol{W} + \boldsymbol{\Delta})$. Remember that any terms lower order than $\|\boldsymbol{\Delta}\|_F$ are not interesting and we can always assume $\boldsymbol{\Delta}$ as small as needed.
- Substitute the result from **Problem 1(b)** into the 1st order Taylor expansion formula above and compare it to the result obtained here. Are they equal or not?

Asymptotic uniqueness — why interesting?

Think of neural networks with identity activation functions

$$f\left(\boldsymbol{W}\right) = \sum_i \|\boldsymbol{y}_i - \boldsymbol{W}_k \boldsymbol{W}_{k-1} \dots \boldsymbol{W}_2 \boldsymbol{W}_1 \boldsymbol{x}_i\|_F^2$$

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– Scalar chain rule?

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Why interesting? See e.g.,
[Kawaguchi, 2016, Lampinen and Ganguli, 2018]

Directional derivatives and curvatures

Consider $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$

- **directional derivative**: $D_{\boldsymbol{v}} f(\boldsymbol{x}) \doteq \frac{d}{dt} f(\boldsymbol{x} + t\boldsymbol{v})$

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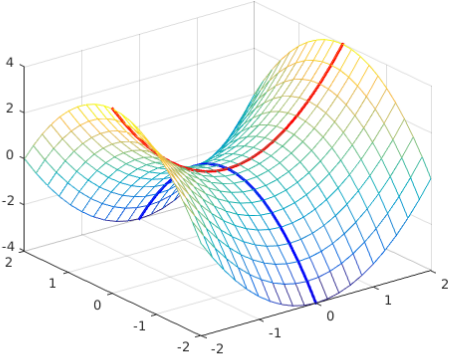
$$f(x, y) = x^2 - y^2$$



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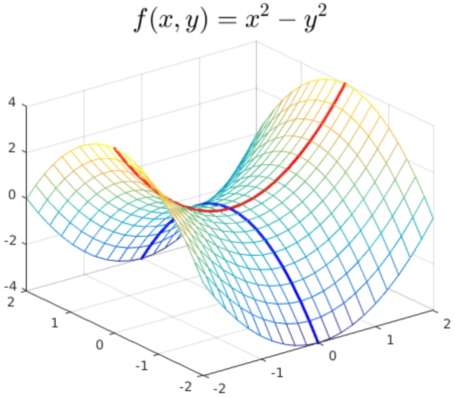


Blue: negative curvature (bending down)

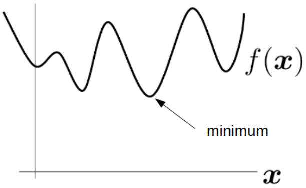
Red: positive curvature (bending up)

Outline

Elements of multivatiate calculus

Optimality conditions of unconstrained optimization

Optimization problems



Nothing takes place in the world whose meaning is not that of some maximum or minimum. – Euler

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \ \text{s. t.} \ \boldsymbol{x} \in C.$$

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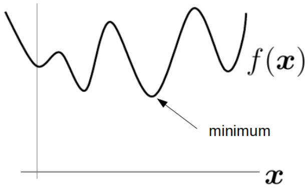

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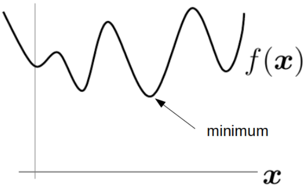

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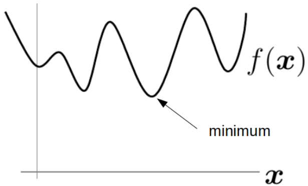

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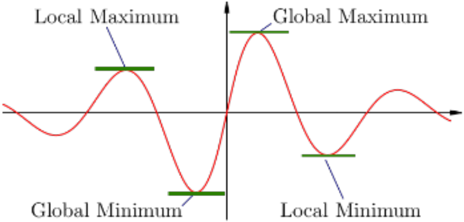
We focus on continuous, unconstrained optimization here.

Global and local mins



Credit: study.com

Let $f(\boldsymbol{x}) : \mathbb{R}^n \to \mathbb{R}$,

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x})$$

- $\boldsymbol{x}_0$ is a **local minimizer** if: $\exists \varepsilon > 0$, so that $f(\boldsymbol{x}_0) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x}$ satisfying $\|\boldsymbol{x} - \boldsymbol{x}_0\|_2 < \varepsilon$. The value $f(\boldsymbol{x}_0)$ is called a **local minimum**.

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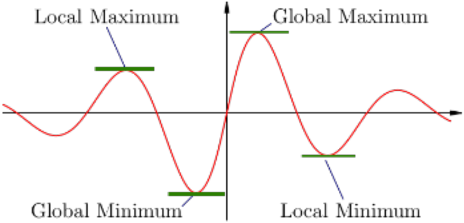

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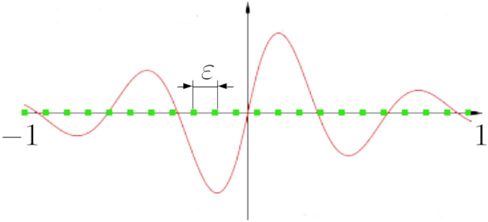
A naive solution

Grid search



– For 1D problem, assume we know the global min lies in $[-1, 1]$

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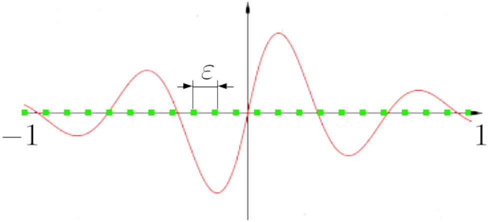

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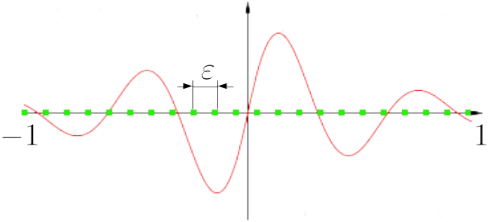

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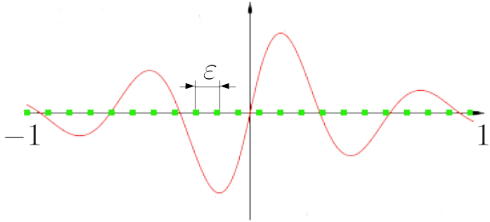

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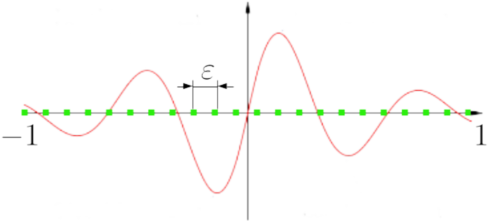

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Better characterization of the local/global mins may help avoid this.

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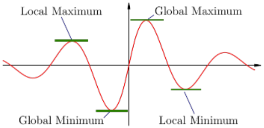

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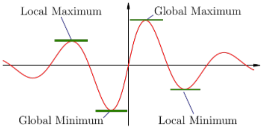

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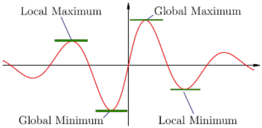

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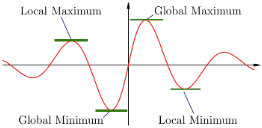

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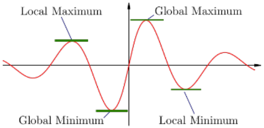

Intuition: ∇f is "rate of change" of function value. If the rate is not zero at $\boldsymbol{x}_0$, possible to decrease f along $-\nabla f(\boldsymbol{x}_0)$

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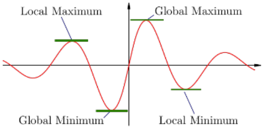

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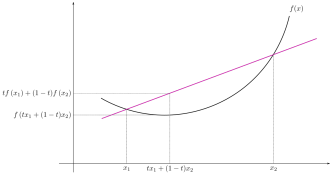

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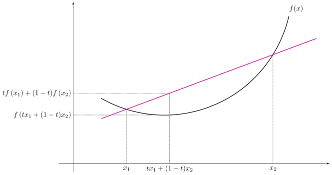

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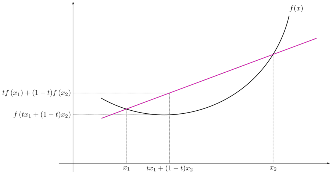

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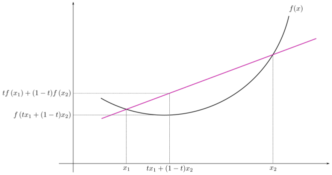

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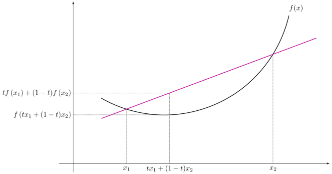

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Proof sketch: if $\boldsymbol{x}, \boldsymbol{z}$ are both local minimizers and $f(\boldsymbol{z}) < f(\boldsymbol{x})$,

$f(\alpha \boldsymbol{z} + (1-\alpha)\boldsymbol{x}) \le \alpha f(\boldsymbol{z}) + (1-\alpha) f(\boldsymbol{x}) < \alpha f(\boldsymbol{x}) + (1-\alpha) f(\boldsymbol{x}) = f(\boldsymbol{x})$.

But $\alpha \boldsymbol{z} + (1-\alpha)\boldsymbol{x} \to \boldsymbol{x}$ as $\alpha \to 0$.

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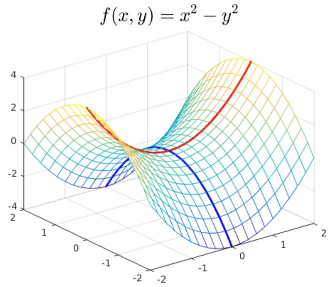
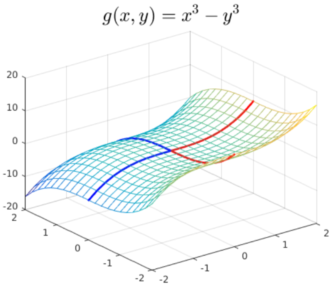
What's in between?

2nd order sufficient: $\nabla f(\boldsymbol{x}_0) = \boldsymbol{0}$ and $\nabla^2 f(\boldsymbol{x}_0) \succ \boldsymbol{0}$
2nd order necessary: $\nabla f(\boldsymbol{x}_0) = \boldsymbol{0}$ and $\nabla^2 f(\boldsymbol{x}_0) \succeq \boldsymbol{0}$





$$\nabla f = \begin{bmatrix} 2x \\ -2y \end{bmatrix}, \nabla^2 f = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} \qquad \nabla g = \begin{bmatrix} 3x^2 \\ -3y^2 \end{bmatrix}, \nabla^2 g = \begin{bmatrix} 6x & 0 \\ 0 & -6y \end{bmatrix}$$

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