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# FUNDAMENTALS OF OPTIMIZATION

## Unconstrained convex optimization

# CONTENT

- Unconstrained optimization problems
- Descent method
- Gradient descent method
- Newton method
- Subgradient method

# Unconstrained convex optimization

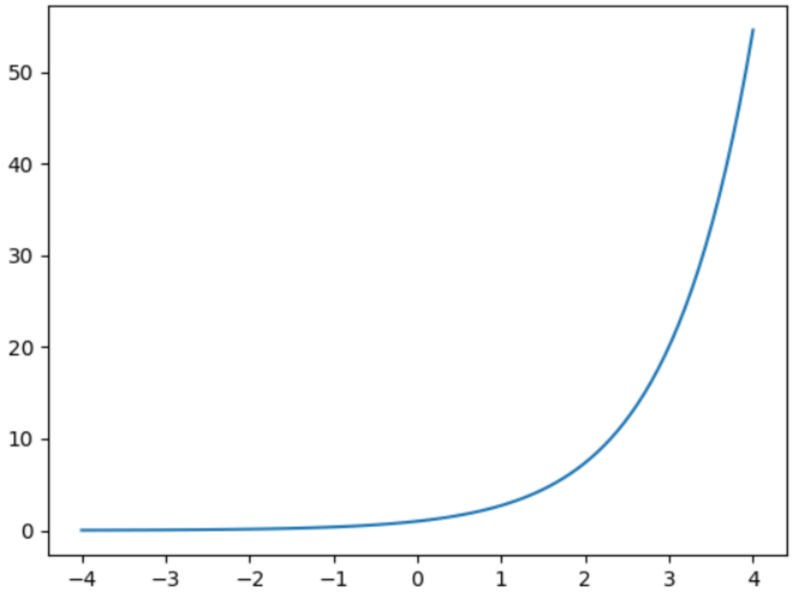
- Unconstrained, smooth convex optimization problem:

$$\min f(x)$$

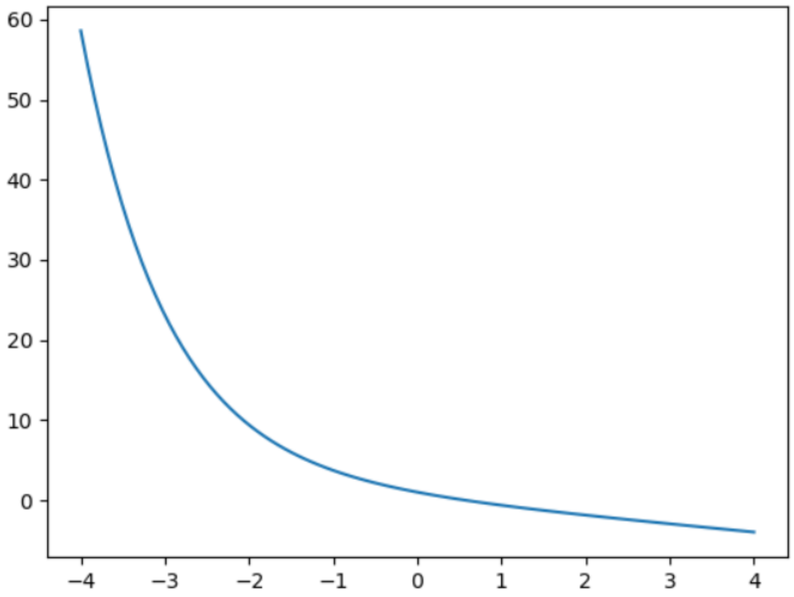
  - $f$: $R^n \rightarrow R$ is convex and twice differentiable
  - ***dom*** $f = R$: no constraint
  - Assumption: the problem is solvable with $f^* = \min_x f(x)$ and $x^* = \text{argMin}_x f(x)$
- To find $x$, solve equation $\nabla f(x^*) = 0$: not easy to solve analytically
- Iterative scheme is preferred: compute minimizing sequence $x^{(0)}, x^{(1)}, \ldots$ s.t. $f(x^{(k)}) \rightarrow f(x^*)$ as $k \rightarrow \infty$
- The algorithm stops at some point $x(k)$ when the error is within acceptable tolerance: $f(x^{(k)}) - f^* \leq \varepsilon$

# Local minimizer

- $x^*$ is a local minimizer for $f$: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for $||x^*-x|| \leq \varepsilon$ ($\varepsilon > 0$ is a constant)
- $x^*$ is a global minimizer for $f$: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for all $x \in R^n$



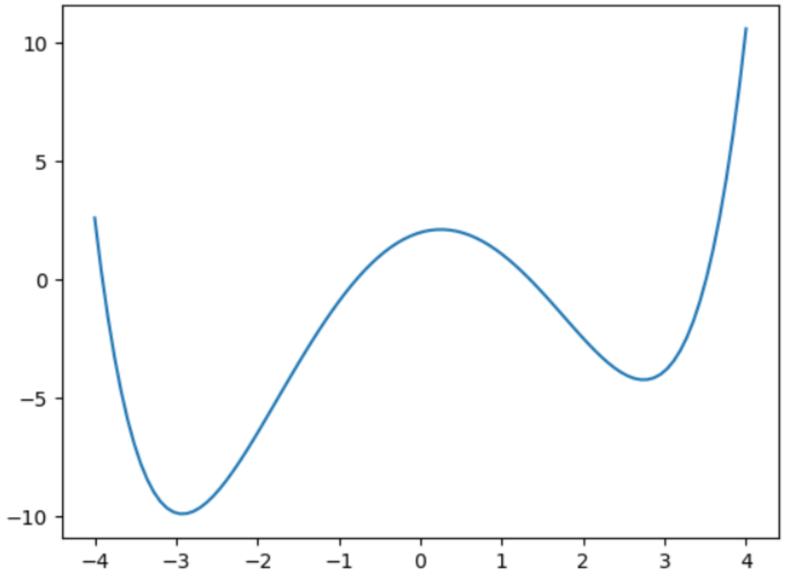

$f(x) = e^x$ has no minimizer



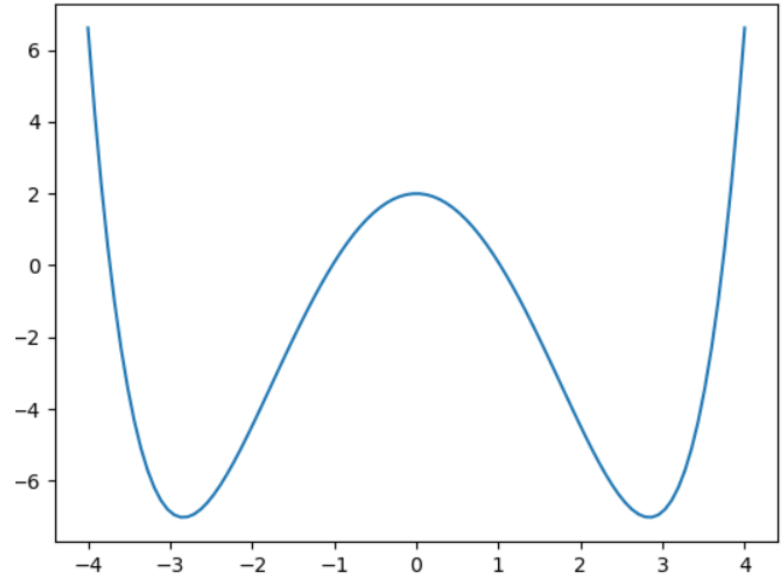

$f(x) = -x + e^{-x}$ has no minimizer

# Local minimizer

- $x^*$ is a local minimizer for $f$: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for $||x^*-x|| \leq \varepsilon$ ($\varepsilon > 0$ is a constant)
- $x^*$ is a global minimizer for $f$: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for all $x \in R^n$




$f(x) = e^x + e^{-x} - 3x^2 + x$ has two local minimizers and one global minimizer




$f(x) = e^x + e^{-x} - 3x^2$ has two global minimizers

# Local minimizer

- **Theorem** (Necessary condition for local minimum) If $x^*$ is a local minimizer for $f$: $R^n \rightarrow R$, then $\nabla f(x^*) = 0$ (x* is also called *stationary point* for *f*)
- **Proof** Suppose that $x^*$ is a local minimizer but $\nabla f(x^*) \neq 0$. We can find a vector $z$ such that $<\nabla f(x^*), z> < 0$ (for instance $z = -\nabla f(x^*)$, $<\nabla f(x^*), z> = -||\nabla f(x^*)||^2 < 0$)
- For a constant $t \geq 0$, consider vector $x(t) = x^* + tz$, and $\varphi(t) = f(x(t))$
- $\frac{d\varphi(t)}{dt}\Big|_{t=0} = \frac{df(x(t))}{dt}\Big|_{t=0} = <\nabla f(x^*), z> < 0 \rightarrow$ with constant $t$ small enough, $\varphi(t) < \varphi(0)$ or $f(x(t)) < f(x^*)$ (conflict with the assumption that $x^*$ is a local minimizer) □

# Local minimizer

**Example**

- $f(x,y) = x^2 + y^2 - 2xy + x$
- $\nabla f(x,y) = \begin{pmatrix} 2x - 2y + 1 \\ 2y - 2x \end{pmatrix} = 0$ has no solution

$\rightarrow$ there is no minimizer of $f(x,y)$

# Local minimizer

- **Theorem** (Sufficient condition for a local minimum) Assume $x^*$ is a stationary point and that $\nabla^2 f(x^*)$ is positive definite, then $x^*$ is a local minimizer

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

# Local minimizer

- Matrix $A_{nxn}$ is called positive definite if

$$A^i = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,i} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,i} \\ & \cdots\cdots & & \\ a_{i,1} \;.\;. & a_{i,2} & \cdots & a_{i,i} \end{pmatrix}, \quad \det(A^i) > 0,\ i = 1,\ldots,n$$

# Local minimizer

- **Example** $f(x,y) = e^{x^2+y^2}$

$$\nabla f(x) = \begin{pmatrix} 2xe^{x^2+y^2} \\ 2ye^{x^2+y^2} \end{pmatrix} = 0 \text{ has unique solution } x^* = (0,0)$$

$$\nabla^2 f(x^*) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} > 0 \rightarrow (0,0) \text{ is a minimizer of f}$$

# Local minimizer

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

$$\nabla f(x) = \begin{pmatrix} -2x + 2y + 1 \\ -2x - 2y \end{pmatrix} = 0$$

has unique solution $x^* = (-1/4, 1/4)$

$$\nabla^2 f(x^*) = \begin{pmatrix} -2 & 2 \\ -2 & -2 \end{pmatrix}$$ is not positive definite

→ cannot conclude $x^*$

# Descent method

Determine starting point $x^{(0)} \in R^n$;

k $\leftarrow$ 0;

while( stop condition not reach){

Determine a search direction $p_k \in R^n$;

Determine a step size $\alpha_k > 0$ s.t. $f(x^{(k)} + \alpha_k p_k) < f(x^{(k)})$;

$x^{(k+1)} \leftarrow x^{(k)} + \alpha_k p_k$;

k $\leftarrow$ k+1;

}

Stop condition may be

- $||\nabla f(x^k)|| \leq \varepsilon$
- $||x^{k+1} - x^k|| \leq \varepsilon$
- k > K (maximum number of iterations)

# Gradient descent method

- Gradient descent schema

$$x^{(k)} = x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)})$$

init $x^{(0)}$;
$k = 1$;
while stop condition not reach{
    specify constant $\alpha_k$;
    $x^{(k)} = x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)})$;
    $k = k + 1$;
}

- $\alpha_k$ might be specified in such a way that $f(x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)}))$ is minimized: $\frac{\partial f}{\partial \alpha_k} = 0$

# Minimize $f(x) = x^4 - 2x^3 - 64x^2 + 2x + 63$

```python
# compute the function value
def f(x):
    return x**4 - 2*x**3 - 64*x**2 + 2*x + 63

# compute the derivative value
def grad(x):
    return 4*x**3 - 6*x**2 - 128 * x + 2

# Gradient descent algorithm with given alpha and initial point
def myGD(alpha, x0):
    x = [x0]
    # loop to evaluate a series of candidate
    for it in range(100000):
        # x[k+1] = x[k] - alpha * f'(x[k])
        x_new = x[-1] - alpha*grad(x[-1])

        # check stop condition (f'(x[k+1]) <= epsilon)
        if abs(grad(x_new)) < 1e-3:
            break

        # append x[k+1] into list
        x.append(x_new)

    # return a list of evaluated candidates and the iteration at which the algorithm stops
    return (x, it)
```

# Minimize $f(x) = x^4 + 3x^2 - 10x + 4$

```
def grad(x):
    return 4*x**3+ 6*x - 10

def f(x):
    return x**4 + 3* x**2  - 10 * x + 4

def myGD(alpha, x0):
    x = [x0]
    for it in range(1000):
        x_new = x[-1] - alpha*grad(x[-1])
#           if abs(grad(x_new)) < 1e-3:
#               break

        if(abs(x[-1] - x_new) < 1e-3):
            break

        x.append(x_new)
    return (x, it)
```

# Minimize $f(x) = x^2 + 5sin(x)$

```
def grad(x):
    return 2*x+ 5*np.cos(x)

def f(x):
    return x**2 + 5*np.sin(x)

def myGD(delta, x0):
    x = [x0]
    for it in range(100):
        x_new = x[-1] - delta*grad(x[-1])
        if abs(grad(x_new)) < 1e-3:
            break
        x.append(x_new)
    return (x, it)
```

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

```
def grad(x, y):
    return (2*x + y - 1, 2*y + x - 1)

def f(x, y):
    return x**2 + y**2 + x*y - x - y

def myGD(delta, x0, y0):
    X = [(x0, y0)]
    for it in range(1000):
        x_new = X[-1][0] - delta*grad(X[-1][0], X[-1][1])[0]
        y_new = X[-1][1] - delta*grad(X[-1][0], X[-1][1])[1]
        if abs(grad(x_new, y_new)[0]) < 1e-6 and abs(grad(x_new, y_new)[1]) < 1e-6:
            break
        X.append((x_new, y_new))
    return (X, it)
```

# Minimize $f(x) = x_1^2 + x_2^2 + x_3^2 - x_1x_2 - x_2x_3 + x_1 + x_3$

- $\alpha_k$ might be specified in such a way that $f(x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)}))$ is minimized: $\frac{\partial f}{\partial \alpha_k} = 0$

```
def grad(x1, x2, x3):
    return [2*x1 + 1 - x2, -x1 + 2*x2 - x3, -x2 + 2*x3 + 1]

def f(x1, x2, x3):
    return x1**2 + x2**2 + x3**2 - x1*x2 - x2*x3 + x1 + x3

def myGD(v1, v2, v3):
    x1 = v1
    x2 = v2
    x3 = v3
    for it in range(1000):
        print(f(x1, x2, x3))
        [D1,D2,D3] = grad(x1,x2,x3)
        A = 2*x1*D1 + 2*x2*D2 + 2*x3*D3 - x1*D2 - x2*D1 - x2*D3 -x3*D2 + D1 + D3
        B = 2*D1*D1 + 2*D2*D2 + 2*D3*D3 -2*D1*D2 - 2*D2*D3
        if B == 0:
            break
        alpha = A/B

        x1 = x1 - alpha*D1
        x2 = x2 - alpha*D2
        x3 = x3 - alpha*D3

        val = grad(x1, x2, x3)
        if (val[0]**2 + val[1]**2 + val[2]**2) < 1e-6:
            break

        X.append([x1, x2, x3])
    return (X, it)
```

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- Newton method
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# Newton method

- Second-order Taylor approximation $g$ of $f$ at $x$ is

$$f(x+h) \approx g(x+h) = f(x) + h\nabla f(x) + \frac{1}{2}h^2 \nabla^2 f(x)$$

- Which is a convex quadratic function of $h$
- g($x$+$h$) is minimized when $\frac{\partial g}{\partial h} = 0 \rightarrow h = -\nabla^2 f(x)^{-1} \nabla f(x)$

# Newton method

Generate $x^{(0)}$; // starting point

$k = 0$;

while stop condition not reach{

$x^{(k+1)} \leftarrow x^{(k)} - \nabla^2 f(x^{(k)})^{-1} \nabla f(x^{(k)})$;

$k = k + 1$;

}

$$f(x) = x_1^2 + x_2^2 + x_3^2 - x_1 x_2 - x_2 x_3 + x_1 + x_3$$

# Newton method

```
import numpy as np


def newton(f,df,Hf,x0):
    x = x0
    for i in range(10):
        iH = np.linalg.inv(Hf(x))
        D = np.array(df(x)).T #transpose matrix: convert from list to
                                    #column vector
        print('df = ',D)
        y = iH.dot(D) #multiply two matrices
        if np.linalg.norm(y) == 0:
            break
        x = x - y
        print('Step ',i,': ',x,' f  = ',f(x))
```

# Newton method

```
def main():
    print('main start....')
    f = lambda x: x[0] ** 2 + x[1] ** 2 + x[2] ** 2 - x[0] * x[1] - x[1] *
                x[2] + x[0] + x[2]  # function f to be minimized
    df = lambda x: [2 * x[0] + 1 - x[1], -x[0] + 2 * x[1] - x[2], -x[1] + 2
                * x[2] + 1]  # gradient
    Hf = lambda x: [[2,-1,0],[-1,2,-1],[0,-1,2]]# Hessian
    x0 = np.array([0,0,0]).T
    newton(f,df,Hf,x0)


if __name__ == '__main__':
    main()
```

# Newton method

| Step | x | y | f |
|---|---|---|---|
| Initialization | [0,0,0] | [1, 1, 1] | 0 |
| Step 1 | [-1., -1., -1.] | [-2.46519033e-32  1.11022302e-16  2.22044605e-16] | -1.0000000000000004 |
| Step 2 | [-1., -1., -1.] | [0.,  0.,  0.] | -1 |

# CONTENT

- Unconstrained optimization problems
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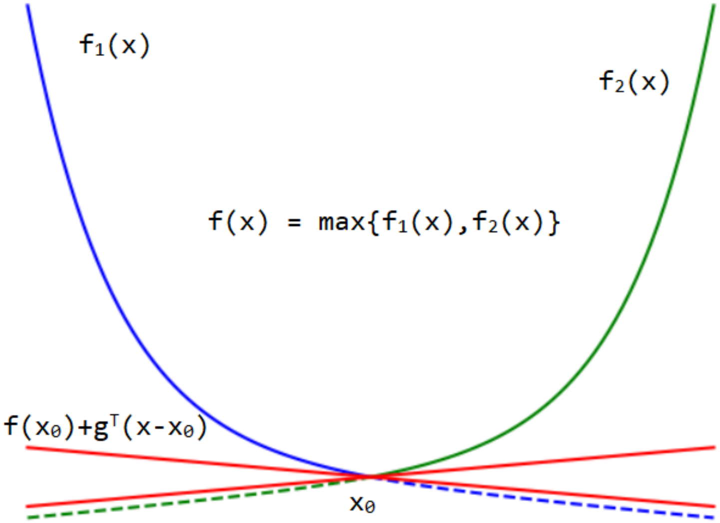
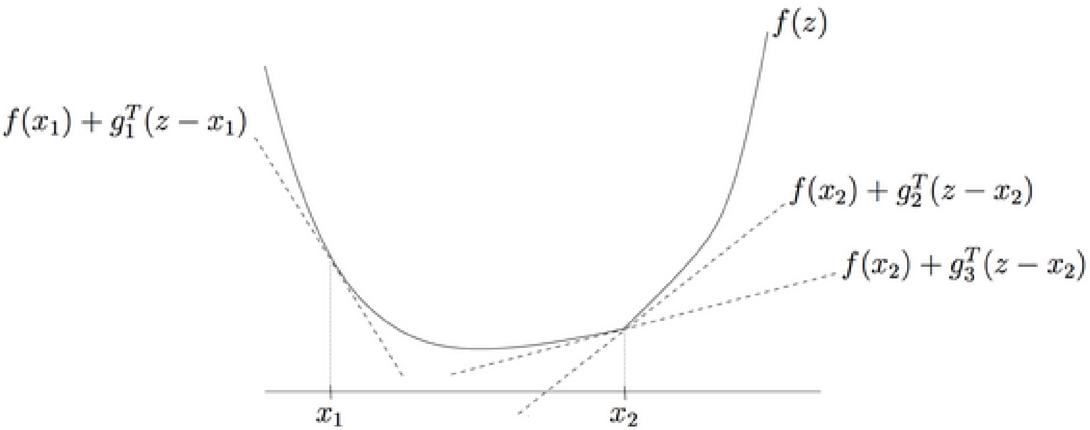
# Subgradient method

- For minimize nondifferentiable convex function
- Subgradient method is not a descent method: the function value can increase

# Subgradient method

- Subgradient of *f* at *x*
  - Any vector *g* such that $f(x') \geq f(x) + g^T(x'-x)$
  - If f is differentiable, only possible choice is $g^{(k)} = \nabla f(x^{(k)})$, → the subgradient method reduces to the gradient method



# Basic subgradient method

$$x^{(k+1)} = x^{(k)} - \alpha_k g^{(k)}$$

- $x^{(k)}$: is at the $k^{\text{th}}$ iteration
- $g^{(k)}$: any subgradient of $f$ at $x^{(k)}$
- $\alpha_k > 0$ is the $k^{\text{th}}$ step size
- Note: subgradient is not a descent method, thus $f_{best}^{(k)} = \min\{f(x^{(1)}), f(x^{(2)}), \ldots, f(x^{(k)})\}$

# Example

$$\text{minimize } f(x) = \max_{i=1,\ldots,m}(a_i^T x + b_i)$$

- Finding subgradient: given $x$, the index $j$ for which

$$a_j^T x + b_j = \max_{i=1,\ldots,m}(a_i^T x + b_i)$$

→ subgradient at $x$ is $g = a_j$

# Example

```
import numpy as np
def solve(A,b):
    f = lambda x: np.max(A.dot(x) + b)
    sg = lambda x: A[np.argmax(A.dot(x) + b)]
    x0 = [0,0,0,0]
    x = np.array(x0).T
    f_best = f(x)
    for i in range(100000):
        alpha = 2
        x = x - alpha*sg(x)
        if f_best > f(x):
            f_best = f(x)
    return f_best
```

# Example

```
def main():
    A = np.array([[1,-2,3,-5],[2,-2,1,1],[-3,2,-2,7]],dtype='double’)
    b = np.array([3,4,5]).T
    rs = solve(A,b)
    print('rs = ',rs)

if __name__ == '__main__':
    main()
```

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# Thank you for your attentions!