

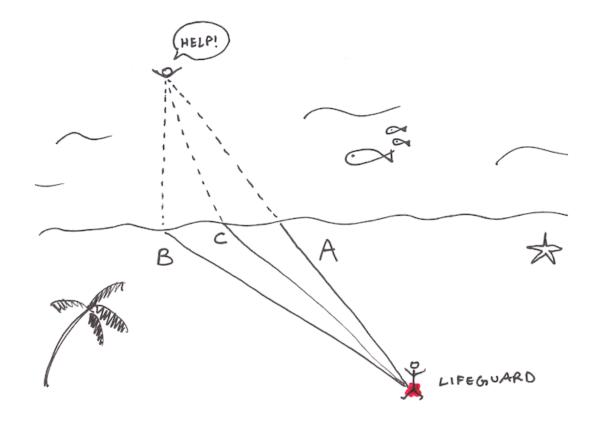
Industrial AI Lab.

**Prof. Seungchul Lee** 

- An important tool in
  - 1) Engineering problem solving and
  - 2) Decision science
- People optimize
- Nature optimizes

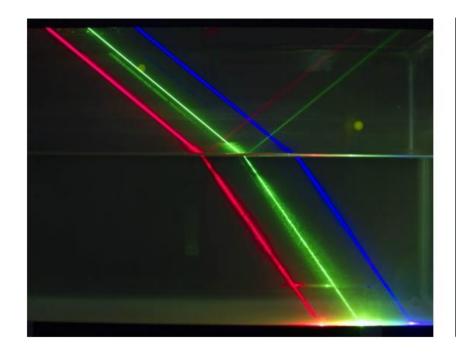


• People optimize





Nature optimizes







- 3 key components
  - 1) Objective function
  - 2) Decision variable or unknown
  - 3) Constraints

#### Procedures

- 1) The process of identifying objective, variables, and constraints for a given problem (known as "modeling")
- 2) Once the model has been formulated, optimization algorithm can be used to find its solutions

# **Optimization: Mathematical Model**

• In mathematical expression

$$\min_{x} f(x)$$
  
subject to  $g_i(x) \le 0$ ,  $i = 1, \dots, m$ 

$$-x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n \text{ is the decision variable}$$

- $-f:\mathbb{R}^n\to\mathbb{R}$  is objective function
- Feasible region:  $C = \{x: g_i(x) \le 0, i = 1, \dots, m\}$
- $-x^* \in \mathbb{R}^n$  is an optimal solution if  $x^* \in C$  and  $f(x^*) \leq f(x)$ ,  $\forall x \in C$

### **Optimization: Mathematical Model**

In mathematical expression

$$\min_{x} f(x)$$
  
subject to  $g_i(x) \le 0$ ,  $i = 1, \dots, m$ 

• Remarks: equivalent

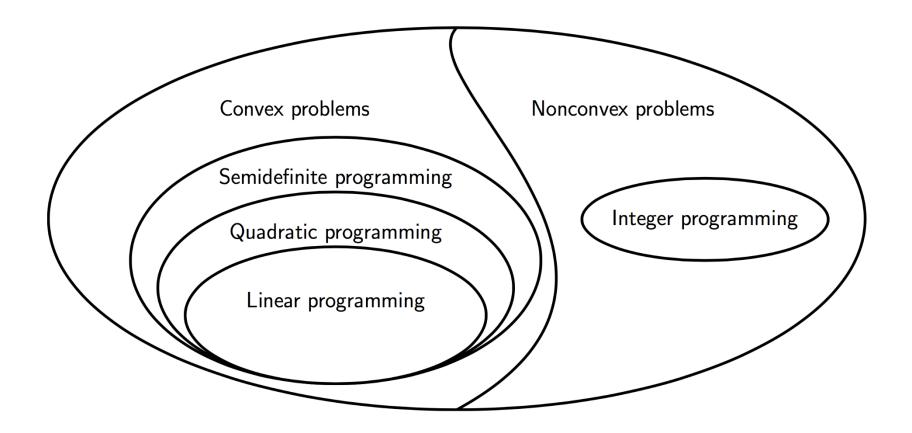
$$\min_{x} f(x) \quad \leftrightarrow \quad \max_{x} -f(x)$$

$$g_{i}(x) \leq 0 \quad \leftrightarrow \quad -g_{i}(x) \geq 0$$

$$h(x) = 0 \quad \leftrightarrow \quad \begin{cases} h(x) \leq 0 & \text{and} \\ h(x) \geq 0 \end{cases}$$

#### **Unconstrained vs. Constrained**

#### Convex vs. Nonconvex





# **Convex Optimization**



### **Convex Optimization**

• An extremely powerful subset of all optimization problems

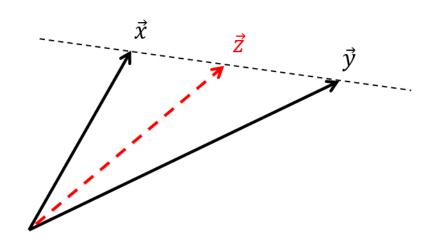
$$\begin{array}{ll}
\text{minimize} & f(x) \\
\text{subject to} & x \in \mathcal{C}
\end{array}$$

- $f: \mathbb{R}^n \to \mathbb{R}$  is a convex function and
- Feasible region *C* is a convex set

- Key property of convex optimization:
  - all local solutions are global solutions

### **Linear Interpolation between Two Points**

•  $\vec{z} = \theta \vec{x} + (1 - \theta) \vec{y}$  and  $\theta \in [0,1]$ 

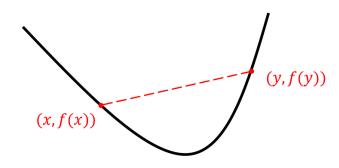


$$ec{z} = ec{y} + heta(ec{x} - ec{y}) = hetaec{x} + (1 - heta)ec{y}, \qquad 0 \leq heta \leq 1$$

$$ext{or} \quad ec{z} = lpha ec{x} + eta ec{y}, \qquad lpha + eta = 1 \ ext{ and } 0 \leq lpha, eta$$

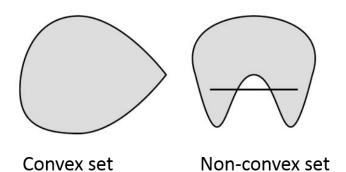
### **Convex Function and Convex Set**

#### convex function



for any  $x,y\in\mathbb{R}^n$  and  $\theta\in[0,1]$   $f(\theta x+(1-\theta)y)\leq\theta f(x)+(1-\theta)f(y)$ 

#### convex set



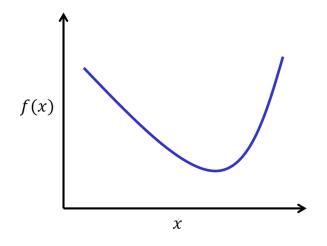
for a 
$$x,y\in\mathcal{C}$$
 and  $\theta\in[0,1]$ , 
$$\theta x+(1-\theta)y\in\mathcal{C}$$

# **Solving Optimization Problems**



### **Solving Optimization Problems**

• Starting with the unconstrained, one dimensional case



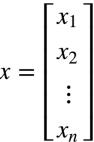
- To find minimum point  $x^*$ , we can look at the derivative of the function f'(x)
- Any location where f'(x) = 0 will be a "flat" point in the function
- For convex problems, this is guaranteed to be a global minimum

### **Solving Optimization Problems**

- Generalization for multivariate function  $f: \mathbb{R}^n \to \mathbb{R}$ 
  - the gradient of f must be zero

$$\mathbb{R}^n \to \mathbb{R}$$

$$\nabla_x f(x) = 0$$



• For defined as above, *gradient* is a *n*-dimensional vector containing partial derivatives with respect to each dimension

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

ullet For continuously differentiable f and unconstrained optimization, optimal point must have

$$\nabla_{x}f(x^{*})=0$$

## How do we Find $\nabla_x f(x) = 0$

- Direct solution
  - In some cases, it is possible to analytically compute  $x^*$  such that  $\nabla_x f(x^*) = 0$

$$f(x) = 2x_1^2 + x_2^2 + x_1x_2 - 6x_1 - 5x_2$$

$$\implies \nabla_x f(x) = \begin{bmatrix} 4x_1 + x_2 - 6 \\ 2x_2 + x_1 - 5 \end{bmatrix}$$

$$\implies x^* = \begin{bmatrix} 4 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

### **Gradients**

Matrix derivatives

у	$\frac{\partial y}{\partial x}$
Ax	$A^T$
$x^T A$	$\boldsymbol{A}$
$x^T x$	2 <i>x</i>
$x^T A x$	$Ax + A^Tx$

### How to Find $\nabla_x f(x) = 0$

#### Direct solution

– In some cases, it is possible to analytically compute  $x^*$  such that  $\nabla_x f(x^*) = 0$ 

у	$\frac{\partial y}{\partial x}$
Ax	$A^T$
$x^T A$	Α
$x^Tx$	2 <i>x</i>
$x^T A x$	$Ax + A^Tx$

$$f(x) = 2x_1^2 + x_2^2 + x_1x_2 - 6x_1 - 5x_2$$

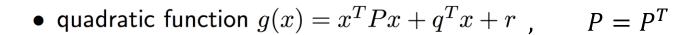
$$\Rightarrow \nabla_x f(x) = \begin{bmatrix} 4x_1 + x_2 - 6 \\ 2x_2 + x_1 - 5 \end{bmatrix}$$

$$\Rightarrow x^* = \begin{bmatrix} 4 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 6 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

### **Examples**

• affine function  $g(x) = a^T x + b$ 

$$\nabla g(x) = a, \qquad \nabla^2 g(x) = 0$$



$$\nabla g(x) = 2Px + q, \qquad \nabla^2 g(x) = 2P$$

• 
$$g(x) = ||Ax - b||^2 = x^T A^T A x - 2b^T A x + b^T b$$

$$\nabla g(x) = 2A^T A x - 2A^T b, \qquad \nabla^2 g(x) = 2A^T A$$

у	$\frac{\partial y}{\partial x}$
Ax	$A^T$
$x^T A$	Α
$x^Tx$	2 <i>x</i>
$x^T A x$	$Ax + A^Tx$

### **Revisit: Least-Square Solution**

• Scalar Objective:  $J = ||Ax - y||^2$ 

$$J(x) = (Ax - y)^{T} (Ax - y)$$

$$= (x^{T}A^{T} - y^{T}) (Ax - y)$$

$$= x^{T}A^{T}Ax - x^{T}A^{T}y - y^{T}Ax + y^{T}y$$

$$\frac{\partial J}{\partial x} = A^{T}Ax + (A^{T}A)^{T}x - A^{T}y - (y^{T}A)^{T}$$

$$= 2A^{T}Ax - 2A^{T}y = 0$$

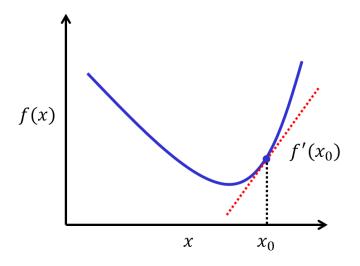
$$\implies (A^{T}A) x = A^{T}y$$

$$\therefore x^{*} = (A^{T}A)^{-1}A^{T}y$$

у	$\frac{\partial y}{\partial x}$
Ax	$A^T$
$x^T A$	Α
$x^Tx$	2 <i>x</i>
$x^T A x$	$Ax + A^Tx$

### How do we Find $\nabla_x f(x) = 0$

- Iterative methods
  - More commonly the condition that the gradient equal zero will not have an analytical solution, require iterative methods



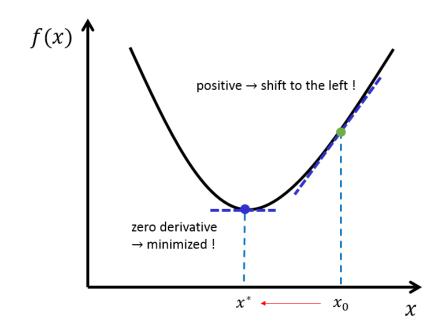
- The gradient points in the direction of "steepest ascent" for function f

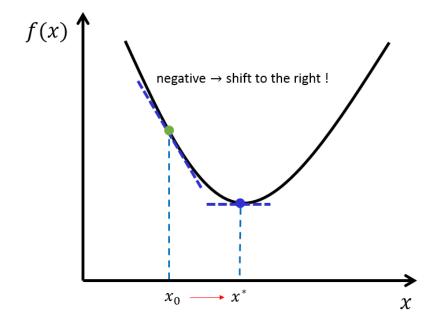
### **Descent Direction (1D)**

• It motivates the *gradient descent* algorithm, which repeatedly takes steps in the direction of the negative gradient

$$x \leftarrow x - \alpha \nabla_x f(x)$$

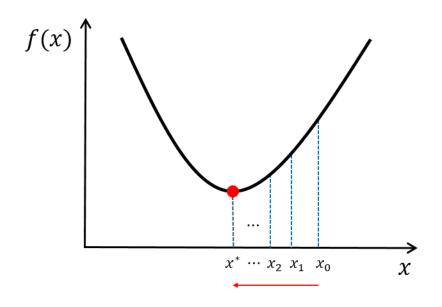
for some step size  $\alpha > 0$ 





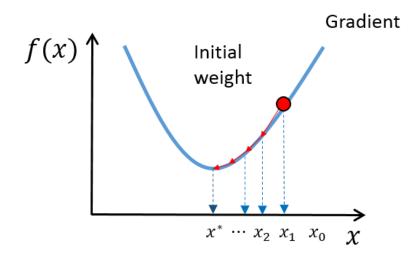
### **Gradient Descent**

Repeat:  $x \leftarrow x - \alpha \nabla_x f(x)$  for some step size  $\alpha > 0$ 

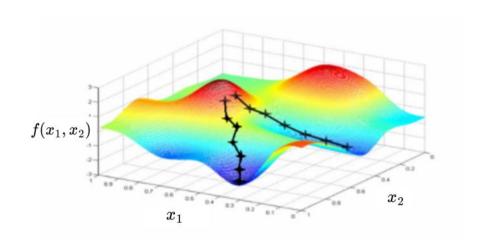


### **Gradient Descent in High Dimension**

Repeat: 
$$x \leftarrow x - \alpha \nabla_x f(x)$$
 for some step size  $\alpha > 0$ 

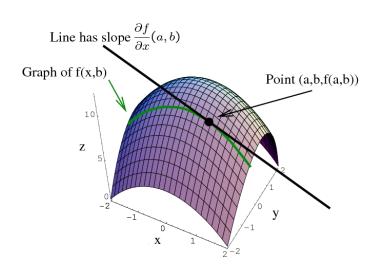


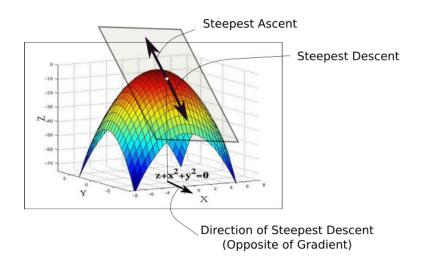
Global cost minimum  $J_{\min}(\omega)$ 

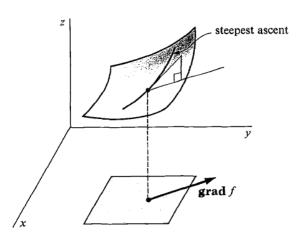


### **Gradient Descent in High Dimension**

Repeat:  $x \leftarrow x - \alpha \nabla_x f(x)$  for some step size  $\alpha > 0$ 







### **Gradient Descent**

$$egin{aligned} &\min & (x_1-3)^2 + (x_2-3)^2 \ &= \min & rac{1}{2}[\,x_1 \quad x_2] \left[egin{aligned} 2 & 0 \ 0 & 2 \end{matrix}
ight] \left[egin{aligned} x_1 \ x_2 \end{matrix}
ight] - \left[\,6 \quad 6\,
ight] \left[egin{aligned} x_1 \ x_2 \end{matrix}
ight] + 18 \end{aligned}$$

• Update rule:  $X_{i+1} = X_i - \alpha_i \nabla f(X_i)$ 

```
H = np.matrix([[2, 0],[0, 2]])
g = -np.matrix([[6],[6]])

x = np.zeros((2,1))
alpha = 0.2

for i in range(25):
    df = H*x + g
    x = x - alpha*df

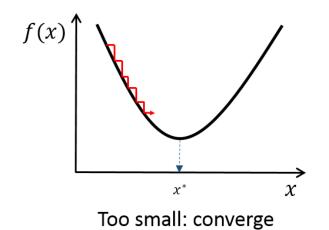
print(x)
```

$f = rac{1}{2} X^T H X + g^T X$
abla f = HX + g

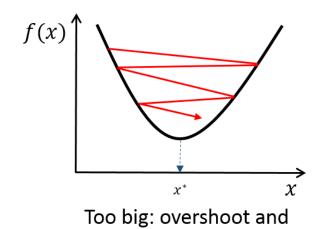
у	$\frac{\partial y}{\partial x}$
Ax	$A^T$
$x^T A$	Α
$x^Tx$	2 <i>x</i>
$x^T A x$	$Ax + A^Tx$

### Choosing Step Size lpha

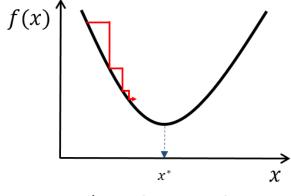
• Learning rate



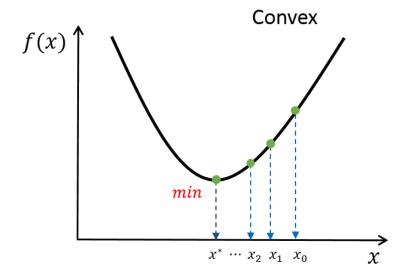
very slowly



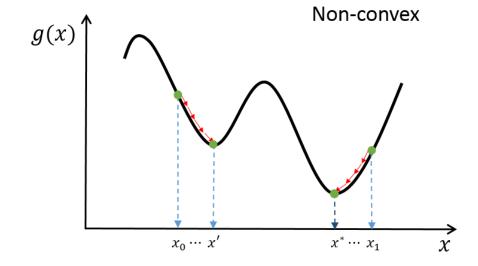
even diverge



### Where will We Converge?



Any local minimum is a global minimum



Multiple local minima may exist

- Random initialization
- Multiple trials



### **Gradient Descent vs. Analytical Solution**

- Analytical solution for MSE
- Gradient descent
  - Easy to implement
  - Very general, can be applied to any differentiable loss functions
  - Requires less memory and computations (for stochastic methods)
- Gradient descent provides a general learning framework
- Can be used both for classification and regression
- Training Neural Networks: Gradient Descent

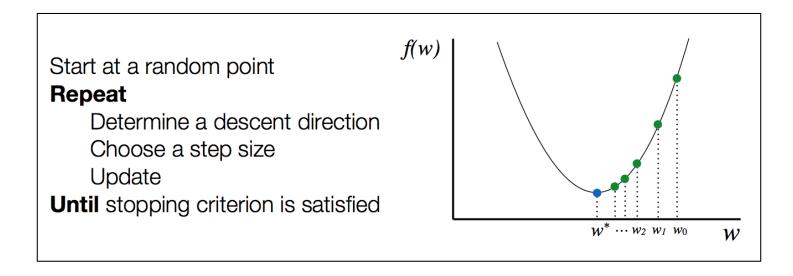
### **Practically Solving Optimization Problems**

- The good news: for many classes of optimization problems, people have already done all the "hard work" of developing numerical algorithms
  - A wide range of tools that can take optimization problems in "natural" forms and compute a solution
- We will use CVX (or CVXPY) as an optimization solver
  - Only for convex problems
  - Download: <a href="https://www.cvxpy.org/">https://www.cvxpy.org/</a>
- Gradient descent
  - Neural networks/deep learning
  - TensorFlow



#### **Summary: Training Neural Networks**

Optimization procedure



- It is not easy to numerically compute gradients in network in general.
  - The good news: people have already done all the "hard work" of developing numerical solvers (or libraries)
  - There are a wide range of tools
    - We will use TensorFlow

# **Examples**



# **Linear Programming**

- Objective function and constraints are both linear
- Convex

$$\max \ 3x_1 + \frac{3}{2}x_2 \qquad \leftarrow \text{ objective function}$$

subject to 
$$-1 \le x_1 \le 2 \leftarrow \text{constraints}$$
  
 $0 \le x_2 \le 3$ 

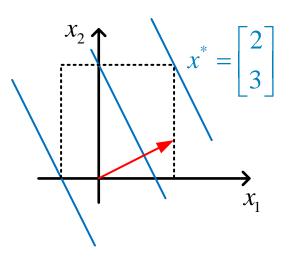
## **Method 1: Geometric Approach**

$$\max \ 3x_1 + \frac{3}{2}x_2 \qquad \leftarrow \text{objective function} \qquad 3x_1 + 1.5x_2 = C \qquad \Rightarrow$$

$$3x_1 + 1.5x_2 = C \qquad \Rightarrow$$

subject to 
$$-1 \le x_1 \le 2 \quad \leftarrow \text{constraints}$$
  $0 \le x_2 \le 3$ 

$$x_2 = -2x_1 + \frac{2}{3}C$$



#### **Method 2: CVXPY**

Many examples will be provided throughout the lecture

#### **Method 2: CVXPY**

```
import numpy as np
import cvxpy as cvx
f = np.array([[3], [3/2]])
1b = np.array([[-1], [0]])
ub = np.array([[2], [3]])
x = cvx.Variable(2,1)
obj = cvx.Minimize(-f.T*x)
constraints = [lb <= x, x <= ub]</pre>
prob = cvx.Problem(obj, constraints)
result = prob.solve()
print(x.value)
print(result)
```

$$\min_x \qquad -igg[ rac{3}{3/2} igg]^T igg[ rac{x_1}{x_2} igg]$$
 subject to  $igg[ rac{-1}{0} igg] \leq igg[ rac{x_1}{x_2} igg] \leq igg[ rac{2}{3} igg]$ 



### **Quadratic Form**

$$q(x_1,\cdots,x_n) = \sum_{i=1}^n \sum_{j=1}^n h_{ij} x_i x_j = x^T H x_i$$



### **Quadratic Programming**

$$egin{array}{lll} & \min & rac{1}{2}x^2 + 3x + 4y & \min_X & X^THX + f^TX \ & ext{subject to} & x + 3y \geq 15 & ext{subject to} & AX \leq b \ & 2x + 5y \leq 100 & A_{eq}X = b_{eq} \ & 3x + 4y \leq 80 & b \leq X \leq ub \ & x,y \geq 0 & b \leq X \leq ub \end{array}$$

#### **Quadratic Programming**

```
f = np.array([[3], [4]])
H = np.array([[1/2, 0], [0, 0]])
A = np.array([[-1, -3], [2, 5], [3, 4]])
b = np.array([[-15], [100], [80]])
1b = np.array([[0], [0]])
x = cvx.Variable(2,1)
obj = cvx.Minimize(cvx.quad form(x, H) + f.T*x)
constraints = [A*x \leftarrow b, lb \leftarrow x]
prob = cvx.Problem(obj, constraints)
result = prob.solve()
print(x.value)
print(result)
```

```
egin{array}{ll} \min_X & X^T H X + f^T X \ & 	ext{subject to} & AX \leq b \ & A_{eq} X = b_{eq} \ & lb \leq X \leq ub \end{array}
```

```
[[ 6.90879937e-10]
[ 5.00000000e+00]]
20.000000000914817
```



### **Example: Shortest Distance**

• Find the best location to listen to singer's voice

$$egin{array}{lll} \min & \sqrt{(x_1-3)^2+(x_2-3)^2} & \Rightarrow & \min & (x_1-3)^2+(x_2-3)^2 \ & & ext{subject to} & x_1+x_2 \leq 3 \ & & x_1 \geq 0 \ & & x_2 \geq 0 \end{array}$$

$$\Rightarrow x_1^2 - 6x_1 + 9 + x_2^2 - 6x_2 + 9$$

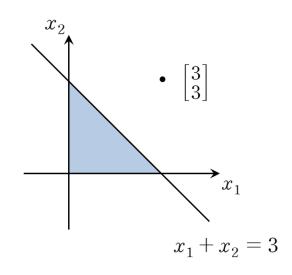
$$= x_1^2 + x_2^2 - 6x_1 - 6x_2 + 18$$

$$= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} 6 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + 18$$

$$\begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le 3$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} \le \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \le \begin{bmatrix} 1 \\ x_2 \end{bmatrix}$$





```
f = np.array([[-6], [-6]])
H = np.array([[1,0], [0,1]])

A = np.array([1,1])
b = 3
lb = np.array([[0], [0]])

x = cvx.Variable(2,1)

obj = cvx.Minimize(cvx.quad_form(x, H) + f.T*x)
constraints = [A*x <= b, lb <= x]

prob = cvx.Problem(obj, constraints)
result = prob.solve()

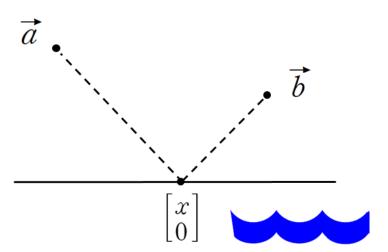
print(x.value)</pre>
```

### **Example: Shortest Distance**

$$\min \ d_1 + d_2 = \min \left\| ec{a} - \left[ egin{array}{c} x \ 0 \end{array} 
ight] 
ight\|_2 + \left\| ec{b} - \left[ egin{array}{c} x \ 0 \end{array} 
ight] 
ight\|_2$$

```
a = np.array([[0], [1]])
b = np.array([[4], [2]])
Aeq = np.array([0,1])
beq = 0
x = cvx.Variable(2,1)
mu = 1
obj = cvx.Minimize(cvx.norm(a-x, 2) + mu*cvx.norm(b-x, 2))
constraints = [Aeq*x == beq]
prob = cvx.Problem(obj, constraints)
result = prob.solve()
print(x.value)
print(result)
```

```
[[ 1.33325114e+00]
 [ 5.33304239e-12]]
4.9999999941398166
```



### **Example: Supply Chain Management**

• Find a point that minimizes the sum of the transportation costs (or distance) from this point to 3 destination points

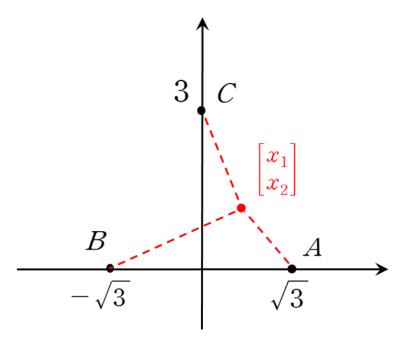
```
a = np.array([[np.sqrt(3)], [0]])
b = np.array([[-np.sqrt(3)], [0]])
c = np.array([[0],[3]])

x = cvx.Variable(2,1)

obj = cvx.Minimize(cvx.norm(a-x, 2) + cvx.norm(b-x, 2) + cvx.norm(c-x, 2))
#obj = cvx.Minimize(cvx.norm(a-x, 1) + cvx.norm(b-x, 1) + cvx.norm(c-x, 1))

prob = cvx.Problem(obj)
result = prob.solve()

print(x.value)
```



```
[[ -1.58674964e-16]
[ 1.00000001e+00]]
```

