# C477: Computational Optimisation Constrained Optimisation – Algorithms

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### **Outline**

#### 1. Projected Methods

- Reminder: Descent Methods
- Projected Gradient Methods
- Projected Gradient with Linear Constraints

#### 2. Lagrangian Methods (Primal/Dual Methods)

- Lagrangian Methods with Equality Constraints
- Lagrangian Methods with Inequality Constraints

#### 3. Penalty Methods

#### Additional material:

- Chapter 22 in An Introduction to Optimization, Chong & Zhak, Third Edition.
- Chapter 12, 13 in Linear and Nonlinear Programming, Luenberger & Ye, Third Edition.

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### 3. Penalty Methods

### **Problem Formulation**

$$\min f(x)$$
s.t.  $h(x) = 0$ 
 $g(x) \le 0$ 

- Where  $f: \mathbb{R}^n \to \mathbb{R}$ ,  $g: \mathbb{R}^n \to \mathbb{R}^p$ ,  $m \le n$  and  $h: \mathbb{R}^n \to \mathbb{R}^m$
- As before  $h_i(x) = 0$ , i = 1, ..., m are equality constraints
- $g_i(\mathbf{x}) \leq 0$ , i = 1, ..., p are inequality constraints
- The feasible region is  $\Omega = \{x \in \mathbb{R}^n \mid h(x) = 0, g(x) \leq 0\}.$

### Reminder: Descent Methods – Unconstrained

- Given a point  $x_k$ .
- Transition to the next point,

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$$

**3** where  $\alpha_k \in \arg\min f(x_k + \alpha_k d_k)$  (if an exact step-size strategy is used)

$$\frac{d_k = -\nabla f(x_k)}{d_k = -\nabla^2 f(x_k)^{-1} \nabla f(x_k)}$$
 (Newton Raphson)

But what if x is required to stay within some feasible set  $\Omega$ ?

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$$d_k = -\nabla f(x_k)$$
 (steepest descent)  
 $d_k = -\nabla^2 f(x_k)^{-1} \nabla f(x_k)$  (Newton Raphson)

But what if x is required to stay within some feasible set  $\Omega$ ?

**Basic idea:** Project point back into feasible set.

$$m{x}_{k+1} = egin{cases} m{x}_{k+1} & ext{if } m{x}_{k+1} \in \Omega \ \Pi[m{x}_{k+1}] & ext{otherwise} \end{cases}$$



**Basic idea:** Project point back into feasible set.

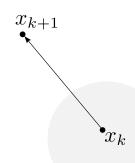
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$$^{\bullet}x_k$$

 $\Omega$ 

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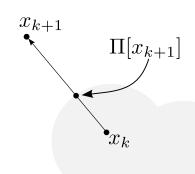
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 $\Omega$ 

#### **Example: Box constraints**

Suppose that the constraint set is,  $\Omega = \{x \in \mathbb{R}^n \mid l_i \leq x_i \leq u_i\}$  Define  $y = \Pi[x]$  as follows,

$$y_i = \begin{cases} u_i & \text{if } x_i > u_i \\ x_i & \text{if } l_i \le x_i \le u_i \\ l_i & \text{if } x_i < l_i \end{cases}$$

A concise way to write the above is  $y_i = \min\{u_i, \max\{l_i, x_i\}\}\$ 

The point  $\Pi[x]$  is called the projection of x into y.

In general the projection operator is defined as,

$$\Pi[x] = \arg\min_{z \in \Omega} \frac{1}{2} ||z - x||_2^2$$

**Interpretation:**  $\Pi[x]$  is the closest point in  $\Omega$  to x

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# **Practical Remarks on Projection Methods**

$$\Pi[x] = \arg\min_{z \in \Omega} \frac{1}{2} ||z - x||_2^2$$

### Projection problem can be as hard as the original problem

Suppose the original problem is:

$$\min \frac{1}{2} ||x||^2$$
  
s.t.  $x \in \Omega$ .

If  $\mathbf{0} \notin \Omega$ ,  $\Pi[\mathbf{0}]$  is as difficult as the original problem.

### Projection not always well defined

If  $\boldsymbol{\Omega}$  is convex then projection is well defined.

But for some  $\Omega$  the  $\arg\min$  may not be well defined.

# **Projected Gradient Methods**

- Given a point  $x_k$ .
- Transition to the next point,

$$\mathbf{x}_{k+1} = \mathbf{\Pi}[\mathbf{x}_k - \alpha_k \mathbf{\nabla} f(\mathbf{x}_k)]$$

■ Where  $\alpha_k \in \arg\min f(\prod [x_k - \alpha_k \nabla f(x_k)])$  (if an exact step-size strategy is used)

# **Example: Projected Gradient Methods**

#### Consider the problem

$$\min \frac{1}{2} \mathbf{x}^{\top} \mathbf{Q} \mathbf{x}$$
  
s.t.  $\|\mathbf{x}\|_2^2 = 1$ 

where  $Q \in \mathbb{R}^{n \times n}$  is a symmetric positive definite matrix. Suppose that a projected gradient method with fixed step size strategy is applied to this problem.

a. Derive a formula for the update equation for the algorithm (i.e. write an explicit formula for  $x_{k+1}$  as a function of  $x_k$ , Q, and fixed step size  $\alpha$ ). You may assume that the argument in the projection operator is never zero.

### **Example: Projected Gradient Methods**

a. Derive a formula for the update equation for the algorithm (i.e. write an explicit formula for  $x_{k+1}$  as a function of  $x_k$ , Q, and fixed step size  $\alpha$ ). You may assume that the argument in the projection operator is never zero.

# **Example: Projected Gradient Methods**

a. The projection problem is

$$\Pi^* = \min_{z} \frac{1}{2} ||x - z||_2^2$$
s.t.  $||z||_2^2 = 1$ 

Note that for any feasible z (i.e.  $||z||_2^2 = 1$ ).

$$\begin{split} \frac{1}{2}\|\pmb{x} - \pmb{z}\|_2^2 &= \frac{1}{2}\|\pmb{z}\|_2^2 + \frac{1}{2}\|\pmb{x}\|_2^2 - \pmb{x}^\top \pmb{z} \\ &\geq \frac{1}{2} + \frac{1}{2}\|\pmb{x}\|_2^2 - \|\pmb{x}\|_2\|\pmb{z}\|_2 \text{ (from Cauchy-Schwarz inequality)} \\ &= \frac{1}{2} + \frac{1}{2}\|\pmb{x}\|_2^2 - \|\pmb{x}\|_2 \end{split}$$

Therefore  $\Pi^* \geq \frac{1}{2} + \frac{1}{2}\|x\|^2 - \|x\|$ . If we choose  $z = x/\|x\|$  the objective function is equal to  $\frac{1}{2} + \frac{1}{2}\|x\|^2 - \|x\|$ . Therefore  $z = x/\|x\|_2$  is the optimal solution of the projected problem. We now have,

$$\mathbf{x}_{k+1} = \beta_k(\mathbf{x}_k - \alpha \mathbf{Q} \mathbf{x}_k) = \beta_k(\mathbf{I} - \alpha \mathbf{Q}) \mathbf{x}_k$$

# **Projected Gradient with Linear Constraints**

$$\min f(x)$$
 s.t.  $Ax = b$ 

#### Where

- $\bullet$   $f: \mathbb{R}^n \to \mathbb{R}$
- $ullet A \in \mathbb{R}^{m \times n}, m < n \text{ and } \operatorname{rank}(A) = m, b \in \mathbb{R}^m.$

# **Derivation of the projection matrix**

#### Suppose that

- $x_k$  is feasible i.e.  $Ax_k = b$
- $d_k$  is a descent but not a feasible direction.

Direction will be feasible if,

$$Ax_{x+1} = A(x_k + \alpha_k d_k) = b$$
  
 $Ax_k + \alpha_k Ad_k = b$ 

So if,

$$Ad_k = 0$$

then  $Ax_{x+1} = b$ .

# **Derivation of the projection matrix**

The projection problem is,

$$\min \frac{1}{2} \|\boldsymbol{d} - \boldsymbol{d}_k\|_2^2$$
  
s.t.  $A\boldsymbol{d} = 0$ 

The projection operator is the matrix  $\mathbf{P} = \mathbf{I} - \mathbf{A}^{\top} (\mathbf{A} \mathbf{A}^{\top})^{-1} \mathbf{A}$ .

# **Derivation of the projection matrix**

The projection problem is,

$$\min \frac{1}{2} \|\boldsymbol{d} - \boldsymbol{d}_k\|_2^2$$
  
s.t.  $A\boldsymbol{d} = 0$ 

The projection operator is the matrix  $P = I - A^{\top} (AA^{\top})^{-1} A$ . To see this note that the first order conditions for this problem are,

$$\boldsymbol{d} - \boldsymbol{d}_k + \boldsymbol{A}^{\top} \boldsymbol{\lambda} = 0$$

Therefore  $\lambda = (AA^{\top})^{-1}Ad_k$ . Substituting this relationship back into the first order condition we obtain that the optimum solution is,

$$\boldsymbol{d} = (\boldsymbol{I} - \boldsymbol{A}^{\top} (\boldsymbol{A} \boldsymbol{A}^{\top})^{-1} \boldsymbol{A}) \boldsymbol{d}_{k}$$

# Properties of the projection matrix

Given a set of linear constraints,

$$Ax = b$$

with  $A \in \mathbb{R}^{m \times n}$ , m < n and  $\operatorname{rank}(A) = m$ ,  $b \in \mathbb{R}^m$ . Then,

$$\boldsymbol{P} = \boldsymbol{I} - \boldsymbol{A}^{\top} (\boldsymbol{A} \boldsymbol{A}^{\top})^{-1} \boldsymbol{A}$$

is called the projection matrix.

**Exercise:** Show that the following statements are true for the projection matrix defined above.

- $\mathbf{2} \mathbf{P}^{\top} = \mathbf{P}$

# Properties of the projection matrix

1. 
$$P^{\top}P = P$$

$$P^{\top} = (I - A^{\top}(AA^{\top})^{-1}A)^{\top} = I - A^{\top}((AA^{\top})^{-1})^{\top}A$$

(where we used the property that for two matrices B C the following holds:  $(BC)^{\top} = C^{\top}B^{\top}$ ). The result follows by direct calculation,

$$P^{\top}P = (I - A^{\top}((AA^{\top})^{-1})^{\top}A)(I - A^{\top}(AA^{\top})^{-1}A)$$

$$= P - A^{\top}((AA^{\top})^{-1})^{\top}A + A^{\top}((AA^{\top})^{-1})^{\top}AA^{\top}(AA^{\top})^{-1}A$$

$$= P - A^{\top}((AA^{\top})^{-1})^{\top}A + A^{\top}((AA^{\top})^{-1})^{\top}A$$

$$= P$$

# Properties of the projection matrix

2.  $\mathbf{P}^{\top} = \mathbf{P}$ . Note that,

$$P^{\top}(I - P) = (I - A^{\top}((AA^{\top})^{-1})^{\top}A)(A^{\top}(AA^{\top})^{-1}A)$$

$$= A^{\top}(AA^{\top})^{-1}A - A^{\top}((AA^{\top})^{-1})^{\top}AA^{\top}(AA^{\top})^{-1}A$$

$$= A^{\top}(AA^{\top})^{-1}A - A^{\top}((AA^{\top})^{-1})^{\top}A$$

$$= A^{\top}(AA^{\top})^{-1}A - A^{\top}(AA^{\top})^{-1}A = 0$$

Therefore using the property of the projection matrix in the previous slide we obtain  $P^\top = P^\top P = P$  (In the derivation of 2. we used the property that for an invertible matrix B then  $(B^\top)^{-1} = (B^{-1})^\top$ ).

# **Projected Gradient with Linear Constraints**

General Iterative algorithm:

$$\mathbf{x}_{k+1} = \Pi[\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k)]$$

If projection is on the set  $\Omega = \{x \in \mathbb{R}^n \mid Ax = b\}$  then,

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha_k \boldsymbol{P} \boldsymbol{\nabla} f(\boldsymbol{x}_k)$$

where  $P = I - A^{\top} (AA^{\top})^{-1} A$ , and  $x_0$  was assumed to be in  $\Omega$ .

# **Projected Gradient with Linear Constraints**

#### Theorem (Feasibility)

In the projected gradient algorithm with linear constraints, if  $x_0$  is feasible, then  $Ax_k = b$ ,  $k \ge 0$ .

#### Proof.

Proof is by induction. Assume that  $Ax_k = b$  we show that  $Ax_{k+1} = b$ . First note that,

$$AP\nabla f(x_k) = A(I - A^{\top}(AA^{\top})^{-1}A)\nabla f(x_k) = (A - A)\nabla f(x_k) = 0.$$

Therefore,

$$Ax_{k+1} = A(x_k - \alpha_k P \nabla f(x_k))) = Ax_k - \alpha_k A P \nabla f(x_k) = b,$$

as required.

# **Projected Gradient and Descent Property**

$$x_{k+1} = x_k - \alpha_k P \nabla f(x_k)$$

where  $P = I - A^{\top} (AA^{\top})^{-1} A$ , and  $x_0$  was assumed to be in  $\Omega$ .

So far we know that if  $x_0$  is feasible then all the iterates  $x_k$  will also be feasible.

But is this a descent algorithm?

# **Projected Gradient and Descent Property**

#### **Theorem**

If  $\{x_k\}$  is the sequence of points generated by the projected gradient algorithm (with the exact step-size strategy). If  $P\nabla f(x_k) \neq 0$  then  $f(x_{k+1}) < f(x_k)$ .

#### Proof.

# **Projected Gradient and Descent Property**

#### **Theorem**

If  $\{x_k\}$  is the sequence of points generated by the projected gradient algorithm (with the exact step-size strategy). If  $P\nabla f(x_k) \neq 0$  then  $f(x_{k+1}) < f(x_k)$ .

#### Proof.

We first recall that,

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha_k \boldsymbol{P} \boldsymbol{\nabla} f(\boldsymbol{x}_k),$$

Let  $\phi_k(\alpha) = f(\mathbf{x}_k - \alpha P \nabla f(\mathbf{x}_k))$  and the step-size is chosen such that  $\alpha_k \in \arg\min_{\alpha > 0} \phi_k(\alpha)$ . We therefore have,

$$\phi_k(\alpha_k) \le \phi_k(\alpha), \forall \alpha \ge 0.$$

Using the chain rule we obtain,

$$\frac{d\phi_k}{d\alpha}(0) = -\nabla f(\mathbf{x}_k)^{\top} \mathbf{P} \nabla f(\mathbf{x}_k)$$

But since  $P = P^{T}P$  we get,

$$\frac{d\phi_k}{d\alpha}(0) = -\nabla f(\mathbf{x}_k)^{\top} \mathbf{P}^{\top} \mathbf{P} \nabla f(\mathbf{x}_k) = -\|\mathbf{P} \nabla f(\mathbf{x}_k)\|^2 < 0,$$

since  $P\nabla f(x_k) \neq 0$  by assumption. Thus there exists  $\bar{\alpha} > 0$  such that  $\phi_k(0) > \phi_k(\alpha)$  for all  $\alpha \in (0, \bar{\alpha}]$ .

# **Projected Gradient and Convergence**

The convergence of the algorithm is based on the previous Theorem and the following result.

#### **Theorem**

Let  $x^*$  be a feasible point then  $P\nabla f(x^*) = 0$  if and only if  $x^*$  satisfies the Lagrange condition.

#### Proof.

# **Projected Gradient and Convergence**

The convergence of the algorithm is based on the previous Theorem and the following result.

#### **Theorem**

Let  $x^*$  be a feasible point then  $P\nabla f(x^*) = 0$  if and only if  $x^*$  satisfies the Lagrange condition.

#### Proof.

We need to show that  $P\nabla f(x^*)=\mathbf{0}$  if and only if  $\nabla f(x^*)=A^{\top}\lambda^*$  for some  $\lambda^*\in\mathbb{R}^m$ . If  $P\nabla f(x^*)=0$  then let  $\lambda^*=(AA^{\top})^{-1}A\nabla f(x^*)$  we then have,

$$0 = P\nabla f(x^*) = \nabla f(x^*) - A^{\top} (AA^{\top})^{-1} A \nabla f(x^*) = \nabla f(x^*) - A^{\top} \lambda^*$$

therefore  $\nabla f(x^*) = A^{\top} \lambda^*$ .

For the other direction, suppose that  $\nabla f(x^*) = A^{\top} \lambda^*$  then,

$$P\nabla f(x^*) = PA^{\top}\lambda^* = (I - A^{\top}(AA^{\top})^{-1}A)A^{\top}\lambda^* = A^{\top}\lambda^* - A^{\top}\lambda^* = 0.$$

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# **Summary Projected Gradient Methods**

- Fast and easy algorithm to implement.
- All the algorithms (including Newton method) can be used in conjunction with projection.

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# **Lagrangian Algorithms**

#### **Equality Constrained Problem**

$$\min f(\mathbf{x})$$
 s.t.  $\mathbf{h}(\mathbf{x}) = 0$ 

Where  $f: \mathbb{R}^n \to \mathbb{R}$ ,  $h: \mathbb{R}^n \to \mathbb{R}^m$  and  $m \le n$ .

#### **First Order Conditions**

$$L(x,\lambda) = f(x) + \lambda^{\top} h(x)$$
 (Lagrangian)  $\nabla f(x) + \nabla h(x) \lambda = \mathbf{0}$  (First Order Conditions)  $h(x) = \mathbf{0}$ 

# **Lagrangian Algorithms**

#### Lagrangian Algorithm

$$x_{k+1} = x_k - \alpha_k(\nabla f(x_k) + \nabla h(x_k)\lambda_k)$$
  
$$\lambda_{k+1} = \lambda_k + \beta_k h(x_k)$$

- **Update equation for** x: same as applying the steepest descent method for minimising  $L(x, \lambda)$  over x with no constraints
- Update equation for  $\lambda$ : same as applying the steepest descent method for maximising  $L(x, \lambda)$  over  $\lambda$
- Only gradients are used so method is called first order method.

### **The General Case**

### **Equality Constrained Problem**

$$\min f(x)$$
s.t.  $h(x) = 0$ 
 $g(x) \leq 0$ 

#### **First Order Conditions**

$$L(x,\lambda)=f(x)+\lambda^{\top}h(x)+\mu^{\top}g(x)$$
 (Lagrangian)  $\nabla f(x)+\nabla h(x)\lambda+\nabla g(x)\mu=0$  (First Order Conditions)  $\mu_ig_i(x)=0$   $\mu\geq 0$   $h(x)=0$   $g(x)\leq 0$ 

## **Lagrangian Algorithm – Inequality constraints**

#### Lagrangian Algorithm

$$x_{k+1} = x_k - \alpha_k (\nabla f(x_k) + \nabla h(x_k) \lambda_k + \nabla g(x_k) \mu_k)$$
  

$$\lambda_{k+1} = \lambda_k + \beta_k h(x_k)$$
  

$$\mu_{k+1} = P_+ [\mu_k + \gamma_k g(x_k)]$$

- $P_+$  is the projection to the positive part of  $\mathbb{R}^p$  applied component wise.
- **Update equation for** x: same as applying the steepest descent method for minimising  $L(x, \lambda, \mu)$  with no constraints
- Update equation for  $\lambda$ : same as applying the steepest descent method for maximising  $L(x, \lambda, \mu)$  over  $\lambda$
- Update equation for  $\mu$ : same as applying the projected steepest descent method for maximising  $L(x, \lambda, \mu)$  over  $\mu$
- Only gradients are used so method is called *first order method*.

## **Lagrangian Algorithm Theory**

- Can be shown that method converges to a KKT point.
- Complementarity condition also satisfied.
- Rate of convergence is linear (since it is based on steepest descent method)
- No guarantees it will converge to the global minimum or that second order conditions will be satisfied.

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# **Basic Idea:** Convert the constrained optimisation problem to an unconstrained problem

Original constrained problem:

$$\min_{x} f(x)$$
$$x \in \Omega$$

#### Modified unconstrained problem:

$$\min_{x} f(x) + \gamma P(x)$$

#### Where:

- ullet  $\gamma$  is a positive scalar called the **penalty parameter.**
- $P: \mathbb{R}^n \to \mathbb{R}$  is called the penalty function. The aim of this function is to penalise points outside  $\Omega$

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#### Original constrained problem:

$$\min_{x} f(x)$$
s.t.  $g_i(x) \le 0$   $i = 1, ..., p$ .

Penalty Function:

$$P(\mathbf{x}) = \sum_{i=1}^{p} g_i^+(\mathbf{x})$$

where

$$g_i^+(\mathbf{x}) = \max\{0, g_i(\mathbf{x})\} = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) \leq 0 \\ g_i(\mathbf{x}) & \text{if } g_i(\mathbf{x}) > 0 \end{cases}$$

The penalty function defined above is also called the <u>absolute value</u> penalty function since it is equal to  $\sum_{i=1}^{p} |g_i(x)|$ 

#### **Example**

Suppose the feasible region is given by,

$$g_1(x) = x - 2 \le 0.$$
  
 $g_2(x) = -(x+1)^3 \le 0$ 

The penalty function is defined as follows,

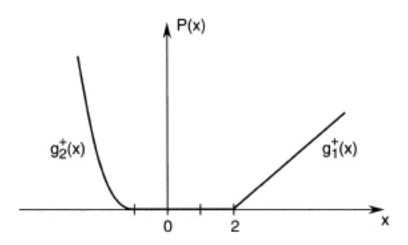
$$g_1^+(x) = \max\{0, g_1(x)\} = \begin{cases} 0 & \text{if } x \le 2\\ x - 2 & \text{otherwise} \end{cases}$$

$$g_2^+(x) = \max\{0, g_2(x)\} = \begin{cases} 0 & \text{if } x \ge -1 \\ -(x+1)^3 & \text{otherwise} \end{cases}$$

So,

$$P(x) = g_1^+(x) + g_2^+(x) = \begin{cases} x - 2 & \text{if } x > 2\\ 0 & \text{if } -1 \le x \le 2\\ -(x + 1)^3 & \text{if } x < -1 \end{cases}$$

# **Example**



The absolute value penalty function may not be differentiable everywhere (e.g. last example P(x) is not differentiable at x=2). Some differentiable & widely used alternatives are:

The Courant-Beltrami penalty function

$$P(x) = \sum_{i=1}^{p} (g_i^+(x))^2$$

Logarithmic Barrier function

$$P(\mathbf{x}) = -\sum_{i=1}^{p} \log(-g_i(\mathbf{x}))$$

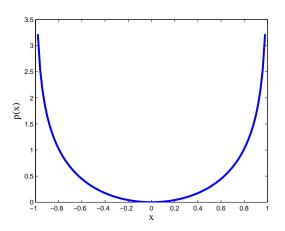
Inverse Barrier function

$$P(\mathbf{x}) = -\sum_{i=1}^{p} \frac{1}{g_i(\mathbf{x})}$$

For the two barrier functions the convention is to let the penalty parameter  $\gamma$  go to zero

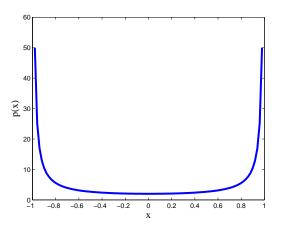
The Logarithmic Barrier Function associated with the constraint,

$$-1 \le x \le 1$$



The Inverse Barrier Function associated with the constraint,

$$-1 \le x \le 1$$



# **Penalty Methods Summary**

- Penalty methods convert the problem into an unconstrained problem and use unconstrained algorithms (e.g. Steepest Descent, Newton Method etc..)
- Logarithmic Barrier Methods are very popular for solving convex optimisation problems (these are polynomial time algorithms)
- Convergence results exists that guarantee that these methods will converge to a KKT point as  $\gamma \to \infty$  (or zero in the case of barrier penalty functions)
- Because of the penalty parameter problem becomes ill conditioned