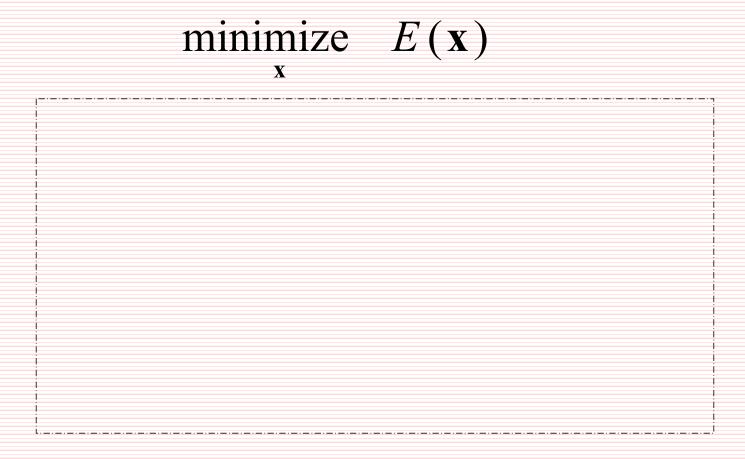
## Intelligent Signal Processing and Control

## Mathematical Foundations IV

Aurobinda Routray

# Optimization

## Optimization: an Overview



## **Unconstrained Optimization**

#### **Steepest Descent Method**

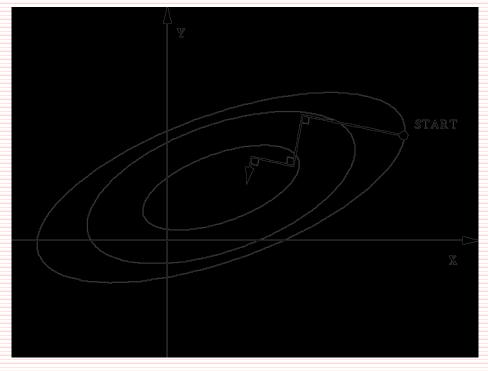
 $E(\mathbf{x})$  to be minimized

 $\mathbf{g}_k$  is the gradient at  $k^{th}$  step

$$\mathbf{g}_k = \nabla E(\mathbf{x}_k)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \mathbf{g}_k$$

 $\alpha$  is an **unknown** non-negative constant that minimizes E(x)



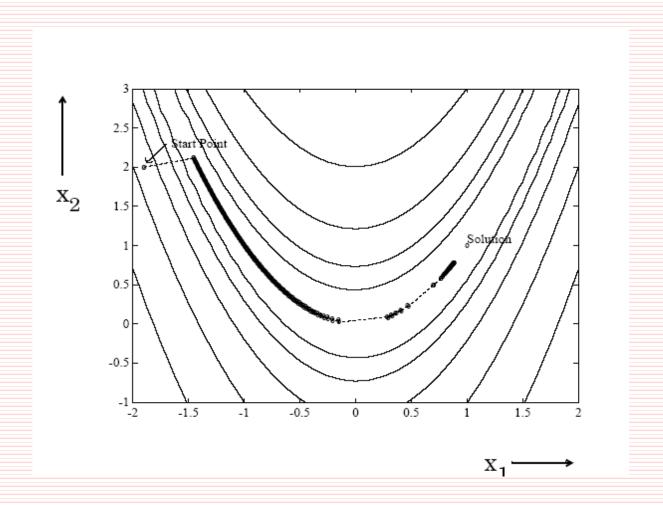
## **Stability**

$$\frac{d\mathbf{x}(t)}{dt} = -\mathbf{\mu}(\mathbf{x}, t) \nabla_x E(\mathbf{x})$$

$$\frac{dE(t)}{dt} = \frac{dE(t)}{d\mathbf{x}} \frac{d\mathbf{x}}{dt} = -\nabla_x^T E(\mathbf{x}) \mathbf{\mu}(\mathbf{x}, t) \nabla_x E(\mathbf{x}) < 0$$
only when  $\mathbf{\mu}(\mathbf{x}, t)$  is positive definite
$$\mathbf{\mu}(\mathbf{x}, t)$$
 is known as the learning matrix
can be assumed to be  $\mu$ . I
where  $\mu$  is a scalar and I is an identity matrix
$$\mu$$
 can be adaptively adjusted within  $[\mu_{\min}, \mu_{\max}]$ 

#### Pit falls

#### **Rosenbrock's Function**



#### Newton's Methods

Newton's method does local approximation of the

Function & to be minimized in the form of a quadratic function

$$q(x) = \varepsilon(x_k) + \varepsilon'(x_k)(x - x_k) + \frac{1}{2}\varepsilon''(x_k)(x - x_k)^2$$

$$\dot{q}(x) = \frac{dq(x)}{dx} = \varepsilon'(x_k) + \varepsilon''(x_k)(x - x_k) \Big|_{\mathbf{x} = \mathbf{x}} = \varepsilon$$

Which gives

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{\mathbf{\epsilon}'(\mathbf{x}_k)}{\mathbf{\epsilon}''(\mathbf{x}_k)}$$

For multivariable functions of the form  $\mathcal{E}(x_1, x_2, x_3, \dots, x_n)$ 

Near **x**<sub>k</sub> the Taylor's series expansion is given as

$$\varepsilon(\mathbf{x}) \cong \varepsilon(\mathbf{x}_{k}) + \nabla_{\mathbf{x}}^{\mathrm{T}} \varepsilon(\mathbf{x}_{k}) (\mathbf{x} - \mathbf{x}_{k}) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_{k})^{\mathrm{T}} H_{k} (\mathbf{x} - \mathbf{x}_{k})$$

$$\nabla_{\mathbf{x}} \varepsilon(\mathbf{x}) \Big|_{\mathbf{x} = \mathbf{x}_{k+1}} = 0$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k - H^{-1} \nabla_{\mathbf{x}} \mathbf{\varepsilon}(\mathbf{x}_k)$$
or

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{H}^{-1} \mathbf{g}_k$$

at
minimum **H** should
be
positive
definite

#### Quasi Newton's Methods

To maintain the positive definiteness of the matrix modifications of the Hessian is necessary

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{H}^{-1} \mathbf{g}_k$$

$$\alpha_k \text{ is a search parameter to minimize } \mathbf{E}$$

Perturb H to prevent ill conditioning by LDU decomposition

$$\mathbf{H} = \mathbf{L}\mathbf{D}\mathbf{U} = \mathbf{L}\mathbf{D}\mathbf{L}^{T}$$

The smallest diagonal element of **D** should be increased to prevent singularity

## Algorithm Modified Newton's Method

- Step 1. Select an initial solution vector  $\mathbf{x}_0$  and convergence tolerance *epsi*
- Step 2. For k=0,1,2& compute  $\mathbf{g}_{\mathbf{k}} = \nabla \mathbf{E}[\mathbf{x}_{\mathbf{k}}]$  if  $\|\mathbf{g}_{\mathbf{k}}\| < epsi$  stop
- Step 3. Compute  $\mathbf{H} = \mathbf{L}.\mathbf{D}.\mathbf{L}^{\mathrm{T}}$
- Step 4. Modify the diagonal elements  $\mathbf{D} \leftarrow \mathbf{D}_{\mathbf{m}}$
- Step 5. Compute the search direction from  $(\mathbf{L}\mathbf{D}_{\mathbf{m}}\mathbf{L}^{\mathsf{T}})\mathbf{d}_{\mathbf{k}} = -\mathbf{g}_{\mathbf{k}}$
- Step 6. Perform line search to determine
  - $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$  the new solution estimate where  $\alpha_k$  is selected such that  $\min_{\alpha \geq 0} \mathcal{E}(\mathbf{x}_k + \alpha \mathbf{d}_k)$

## Algorithm Broyden-Goldfarb-Shanno (BFGS) algorithm

- Step 1. Select an initial solution vector  $\mathbf{x}_0$  and initial Hessian approximation  $\mathbf{B}_0 = \mathbf{I}$
- Step 2. For k=0,1,2 if  $\mathbf{x}_k$  is optimal in some sense then stop
- Step 3. Else compute the gradient of the objective function that is  $\mathbf{g}_k = \nabla \mathbf{E}[\mathbf{x}_k]$  then solve  $\mathbf{B}_k \mathbf{d}_k = -\mathbf{g}_k$  for  $\mathbf{d}_k$
- Step 4. Perform line search to determine

 $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$  the new solution estimate where  $\alpha_k$  is selected such that  $\min_{\alpha \geq 0} \mathcal{E}(\mathbf{x}_k + \alpha \mathbf{d}_k)$ 

- Step 5. Compute  $\delta_k = \mathbf{x}_{k+1} \mathbf{x}_k$  and  $\mathbf{y}_k = \mathbf{g}_{k+1} \mathbf{g}_k$
- Step 6. Compute

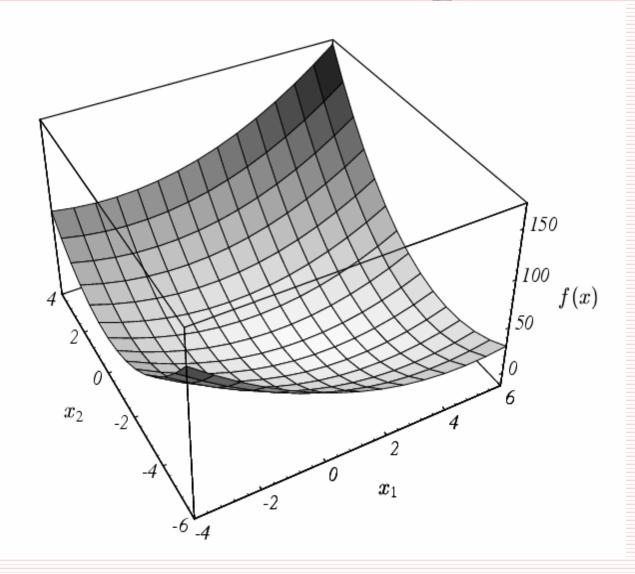
$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\left(\mathbf{B}_k \mathbf{\delta}_k\right) \left(\mathbf{B}_k \mathbf{\delta}_k\right)^T}{\mathbf{\delta}_k^T \mathbf{B}_k \mathbf{\delta}_k} + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{\delta}_k}$$

where  $\mathbf{B}_k$  is the current estimate of the Hessian  $\nabla_{\mathbf{x}}^2 \mathcal{E}(\mathbf{x}_k)$ 

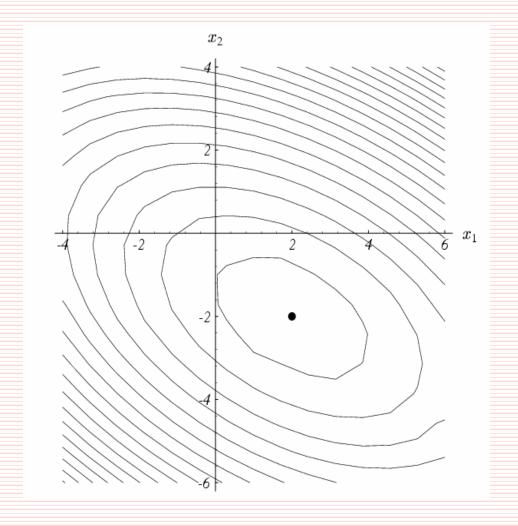
Step 7. Go to Step 2.

## Conjugate Gradient Algorithm

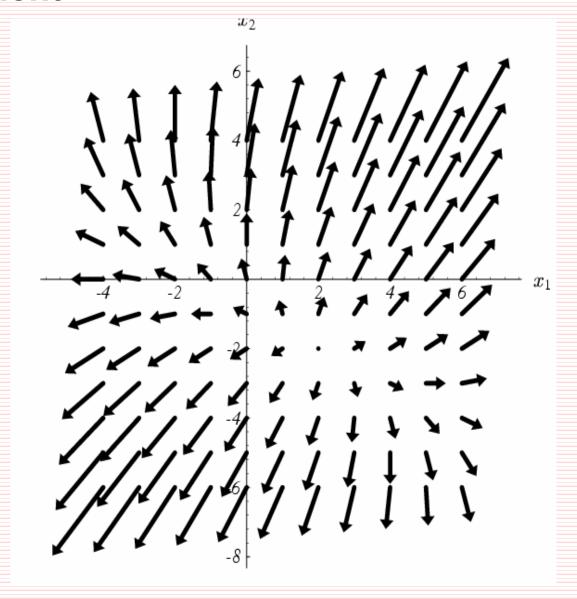
$$\mathbf{Q}\mathbf{x} = \mathbf{b}$$
 solving it is minimizing  $\mathbf{E}(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Q}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$ 



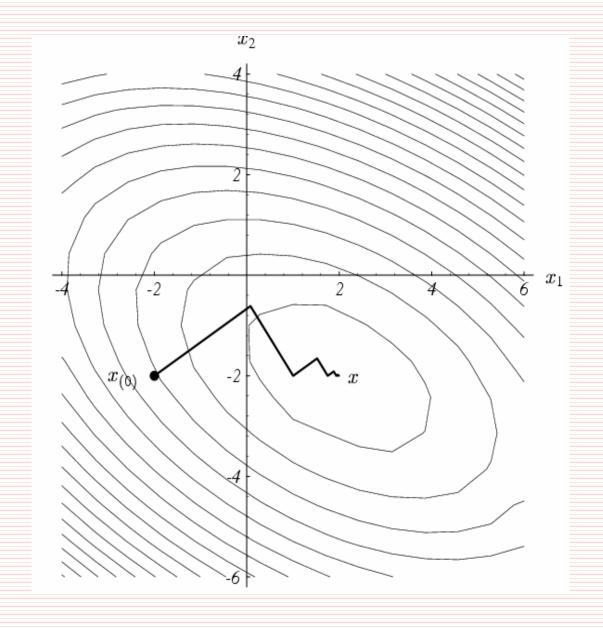
#### The Contours



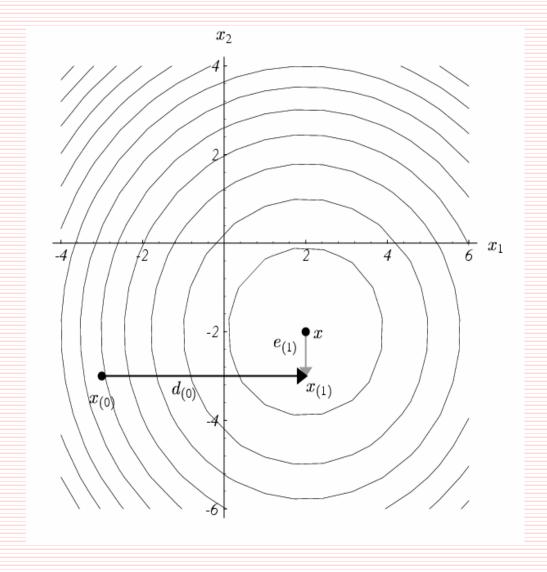
#### **The Gradient**



#### **Directions of Steepest Descent**



## **Conjugate Directions**



#### To find conjugate directions

$$J(\mathbf{x}) = \frac{1}{2} \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x} - \mathbf{b}^{\mathrm{T}} \mathbf{x}$$

$$\mathbf{x}_{\mathrm{F}} = \min_{\mathbf{x}} J(\mathbf{x})$$

$$\mathbf{e}_{i} = \mathbf{x}_{i} - \mathbf{x}_{\mathrm{F}}$$

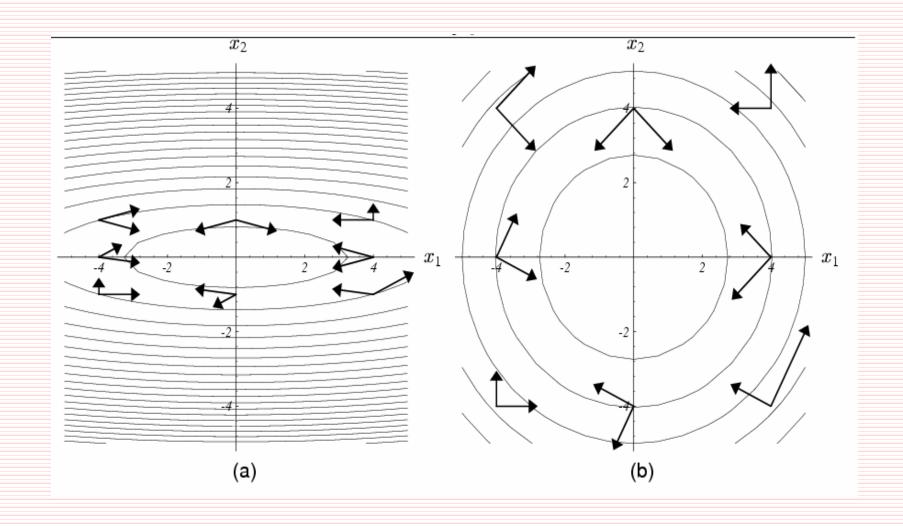
$$\mathbf{x}_{i+1} = \mathbf{x}_{i} + \alpha_{i} \mathbf{d}_{i}$$

$$\mathbf{d}_{i}^{T}\mathbf{e}_{i+1} = 0$$
 for conjugate direction

$$\mathbf{e}_{i+1} = \mathbf{x}_{i+1} - \mathbf{x}_{F} = \mathbf{x}_{i} + \alpha_{i} \mathbf{d}_{i} - \mathbf{x}_{F} = \mathbf{e}_{i} + \alpha_{i} \mathbf{d}_{i}$$

$$\alpha_i = -\frac{\mathbf{d}_i^T \mathbf{e}_i}{\mathbf{d}_i^T \mathbf{d}_i}$$
 but  $\mathbf{e}_i$  is not known

Therefore instead of making the directions e othorgonal make it A orthogonal



$$\mathbf{x}_{i+1} = \mathbf{x}_{i} + \alpha_{i} \mathbf{d}_{i}$$

$$\frac{dJ(\mathbf{x}_{i+1})}{d\alpha} = 0$$

$$J'(\mathbf{x}_{i+1}) \frac{d\mathbf{x}_{i+1}}{d\alpha} = 0$$

$$-\mathbf{r}_{i+1}^{T} \mathbf{d}_{i} = 0 \quad \left[ \because \mathbf{r}_{i+1} = \mathbf{b} - \mathbf{A} \mathbf{x}_{i+1} \right]$$

$$-\mathbf{r}_{i+1}^{T}\mathbf{d}_{i} = 0$$

$$\mathbf{d}_{i}^{T}\mathbf{A}\mathbf{e}_{i+1} = 0$$

$$\left[ :: \mathbf{b} - \mathbf{A}\mathbf{x}_{F} = 0 \rightarrow \mathbf{b} = \mathbf{A}\mathbf{x}_{F} \rightarrow \mathbf{r}_{i+1} = \mathbf{b} - \mathbf{A}\mathbf{x}_{i+1} \rightarrow \mathbf{A}\left(\mathbf{x}_{F} - \mathbf{x}_{i+1}\right)\right]$$

$$\mathbf{d}_{i}^{T}\mathbf{A}\left(\mathbf{x}_{i+1} - \mathbf{x}_{F}\right) = 0$$

$$\mathbf{d}_{i}^{T}\mathbf{A}\left(\mathbf{x}_{i} + \alpha\mathbf{d}_{i} - \mathbf{x}_{F}\right) = 0$$

$$\alpha = \frac{\mathbf{d}_{i}^{T}\mathbf{r}_{i}}{\mathbf{d}_{i}^{T}\mathbf{A}\mathbf{d}_{i}}$$

#### **Gram-Schmidt Conjugation**

All that is needed now is a set of A-orthogonal search directions

 $\mathbf{u_0}, \mathbf{u_1}, \dots, \mathbf{u_n}$  n independent vectors

$$d_{(i)} = u_i + \sum_{k=0}^{i-1} \beta_{ik} d_{(k)},$$

where

 $\beta_{ik}$  is defined for i > k

## Algorithm Fletcher-Reeves Conjugate Gradient Method

Step 1. start with any  $\mathbf{x}_0 \in \mathbb{R}^{n \times 1}$ 

Step 2. Compute 
$$\mathbf{g}_0 = \nabla_{\mathbf{x}} \mathcal{E}(\mathbf{x}_k) \Big|_{k=0}$$

Step 3. 
$$\mathbf{d}_0 = -\mathbf{g}_0$$

Step 4. 
$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$$
 such that  $\min_{\alpha \ge 0} \mathcal{E}(\mathbf{x}_k + \alpha \mathbf{d}_k)$ 

Step 5. 
$$\mathbf{g}_k = \nabla_x \boldsymbol{\mathcal{E}}(\mathbf{x}_{k+1})$$

Step 6. 
$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$$
 and  $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{d}_k}$ 

steps 4 through 6 are carried out for  $k = 0, 1, \dots, n-1$ 

Step 7. Replace  $\mathbf{x}_0$  by  $\mathbf{x}_n$  and go to step 1

Step 8. Continue untill convergence is achieved. Termination criterion is

$$\|\mathbf{d}_k\| < \varepsilon$$

## Conjugate Gradient Algorithm

 $\mathbf{Q}\mathbf{x} = \mathbf{b}$  solving it is minimizing  $\mathbf{E}(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Q}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$ 

## Algorithm Conjugate Gradient Method

Step 1. start with any  $\mathbf{x}_0 \in \mathbb{R}^{n \times 1}$ . define the initial vector as

$$|\mathbf{d}_{0} = -\mathbf{g}_{0} = -\nabla_{x} \mathcal{E}(\mathbf{x}_{k})|_{k=0} = \mathbf{b} - \mathbf{Q}\mathbf{x}_{0}$$

Step 2. 
$$\alpha_k = -\frac{\mathbf{g}_k^T \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{Q} \mathbf{d}_k}$$
 where  $\mathbf{g}_k = \mathbf{Q} \mathbf{x}_k - \mathbf{b}$ 

Step 3. 
$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$$

Step 4. 
$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$$
 and  $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{Q} \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{Q} \mathbf{d}_k}$ 

an alternate form is

$$\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{g}_{k+1}}{\mathbf{g}_k^T \mathbf{g}_k}$$

Step 5. Go to step 2

## **Constrained Optimization**

minimize  $f_0(\mathbf{x})$ 

subject to 
$$f_i(\mathbf{x}) \le 0$$
  $i = 1, 2, \dots, m$ 

$$h_i\left(\mathbf{x}\right) = 0 \qquad i = 1, 2, \dots, p$$

$$\mathbf{x} \in \mathbf{R}^n$$
  $D = \bigcap_{i=1}^m \mathbf{dom} \, f_i \, \cap \, \bigcap_{i=1}^p \mathbf{dom} \, h_i \text{ is nonempty}$ 

let the optimal value is  $p^*$ 

Define Lagrangian associated with the above problem as

$$L: \mathbf{R}^n \times \mathbf{R}^m \times \mathbf{R}^p \to \mathbf{R}$$

$$L(\mathbf{x}, \lambda, \mathbf{v}) = f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{h} \nu_i h_i(\mathbf{x})$$

 $\lambda_i$  and  $\nu_i$  are dual variables and the **dual function** is

$$g(\lambda, \mathbf{v}) = \inf_{\mathbf{x} \in \mathbf{D}} L(\mathbf{x}, \lambda, \mathbf{v}) = \inf_{\mathbf{x} \in \mathbf{D}} \left[ f_0(\mathbf{x}) + \sum_{i=1}^m \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^h \nu_i h_i(\mathbf{x}) \right]$$

For dual variables  $\lambda_i$  and  $\nu_i$  positive

the dual problems always gives values less than  $p^*$ 

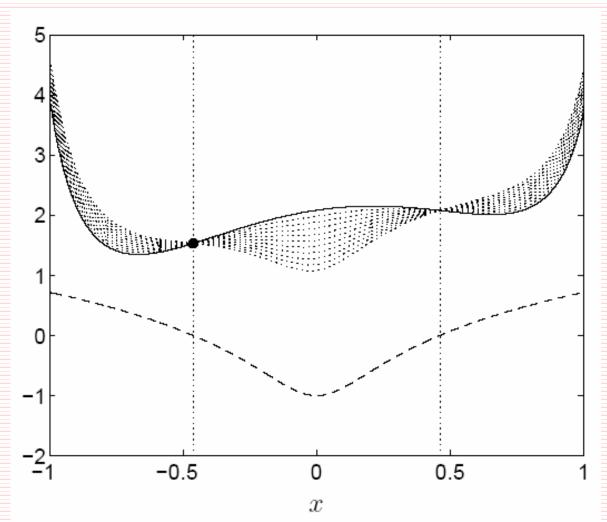
$$g(\lambda, \nu) \le p^*$$

Suppose  $\tilde{\mathbf{x}}$  is a feasible point then

$$\sum_{i=1}^{m} \lambda_{i} f_{i}\left(\tilde{\mathbf{x}}\right) + \sum_{i=1}^{h} \nu_{i} h_{i}\left(\tilde{\mathbf{x}}\right) \leq 0$$

$$L(\tilde{\mathbf{x}}, \lambda, \mathbf{v}) = f_0(\tilde{\mathbf{x}}) + \sum_{i=1}^{m} \lambda_i f_i(\tilde{\mathbf{x}}) + \sum_{i=1}^{h} \nu_i h_i(\tilde{\mathbf{x}}) \le f_0(\tilde{\mathbf{x}})$$

$$g(\lambda, \mathbf{v}) = \inf_{\mathbf{x} \in \mathbf{D}} L(\mathbf{x}, \lambda, \mathbf{v}) \le L(\tilde{\mathbf{x}}, \lambda, \mathbf{v}) \le f_0(\tilde{\mathbf{x}})$$



Lower bound from a dual feasible point. The solid curve shows the objective function  $f_0$ , and the dashed curve shows the constraint function  $f_1$ . The feasible set is the interval [-0.46, 0.46] indicated by two dotted vertical lines. The optimal value is at -0.46,  $p^*=1.54$ 

#### Lagrange's Dual Problem

To find out  $p^*$  is to find the upper bound of  $g(\lambda, \nu)$ 

$$\max \operatorname{maximize} g(\lambda, \nu)$$
$$\lambda > 0$$

say the maximum value  $g(\lambda, \nu)$  is  $d^*$ 

Then always  $d^* \le p^*$  [for convex problems equality holds "Strong Duality"]

 $(p^* - d^*)$  is knowns as the duality gap

#### **Example: Least Square Solution**

minimize 
$$\mathbf{x}^T \mathbf{x}$$

subject to 
$$\mathbf{A}\mathbf{x} = b$$

Augmented function

minimize 
$$L(\mathbf{x}, \mathbf{v}) = \mathbf{x}^T \mathbf{x} + \mathbf{v} (A\mathbf{x} - b)$$

$$\nabla L(\mathbf{x}, \nu) = 2\mathbf{x} + \mathbf{A}^T \nu = 0$$

$$\mathbf{x} = -\frac{1}{2}\mathbf{A}^{\mathsf{T}}\mathbf{v}$$

**Dual Function** 

$$g(v) = L\left(-\left(\frac{1}{2}\right)A^{T}v,v\right) = -\left(\frac{1}{4}\right)v^{T}AA^{T}v - b^{T}v$$

#### KKT [Karush-Kuhn-Tucker Conditions]

Assume the functions  $f_0, f_1, \dots, f_m, h_1, \dots, h_p$  are differentiable at the optimal point

Thus we have

$$\begin{split} &h_i\!\left(\mathbf{x}^*\right)\!=\!0, \qquad i\!=\!1,\!\cdots, p\\ &f_i\!\left(\mathbf{x}^*\right)\!\leq\!0, \qquad i\!=\!1,\!\cdots, m\\ &\lambda_i^*\geq\!0, \qquad i\!=\!1,\!\cdots, m\\ &\lambda_i^*\cdot f_i\!\left(\mathbf{x}^*\right)\!=\!0, \, i\!=\!1,\!\cdots, m\\ &\nabla f_0\!\left(\mathbf{x}^*\right)\!+\!\sum_{\mathrm{i}=1}^{m}\lambda_\mathrm{i}^*\nabla f_i\!\left(\mathbf{x}^*\right)\!+\!\sum_{\mathrm{i}=1}^{p}\nu_\mathrm{i}^*\nabla h_i\!\left(\mathbf{x}^*\right)\!=\!0 \end{split}$$

These are known as **KKT** conditions