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Lecture 2: Optimization

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You Have Learned (Unconstrained) Optimization in Your High School

Let
$$f(x) = ax^2 + bx + c$$
, $a \neq 0$, $x^* = -\frac{b}{2a}$
Case I: $f''(x^*) = a > 0 \Rightarrow x^* \in \arg\min_{x \in R} f(x)$

Case II:
$$f''(x^*) = a < 0 \Rightarrow x^* \in \arg \max_{x \in R} f(x)$$

For minimization problem (Case I),

 $f'(x^*) = 0$ is called the first order optimality condition

 $f''(x^*) = a > 0$ is the second order optimality condition

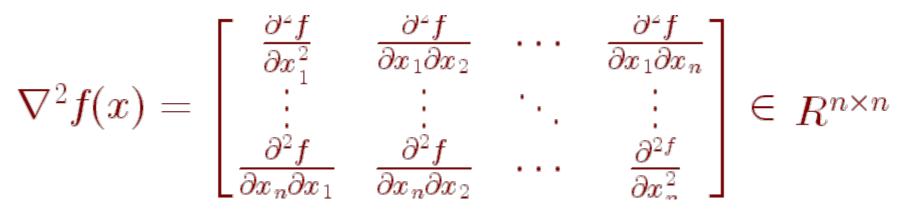
Optimization Examples in this Book

On p.62, Maximum likelihood estimation On p.68, Maximum a Posteriori estimation On p.74, Least squares estimates On p.207, Gradient descent method On p.246, Backpropagation

Gradient and Hessian

• Let $f: \mathbb{R}^n \to \mathbb{R}$ be a differentiable function. The gradient of function f at a point $x \in \mathbb{R}^n$ is defined as $\nabla f(x) = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \dots, \frac{\partial f(x)}{\partial x_n}\right] \in \mathbb{R}^n$

• If $f: \mathbb{R}^n \to \mathbb{R}$ is a twice differentiable function. The Hessian matrix of f at a point $x \in \mathbb{R}^n$ is defined as



Example of Gradient and Hessian

$$\begin{split} f(x) &= x_1^2 + x_2^2 - 2x_1 + 4x_2 \\ &= \frac{1}{2} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} -2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ \nabla f(x) &= \begin{bmatrix} 2x_1 - 2, 2x_2 + 4 \end{bmatrix} \quad \nabla^2 f(x) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \\ \text{By letting } \nabla f(x) &= 0 \text{, we have} \end{split}$$

$$x^* = \begin{bmatrix} 1 \\ -2 \end{bmatrix} \in \operatorname*{arg\,min}_{x \in R^2} f(x)$$

Quadratic Functions (Standard Form) $f(x) = \frac{1}{2}x^THx + p^Tx$

Let $f: R^n \to R$ and $f(x) = \frac{1}{2}x^T H x + p^T x$ where $H \in R^{n \times n}$ is a symmetric matrix and $p \in R^n$ then $\nabla f(x) = Hx + p$ $\nabla^2 f(x) = H$ (Hessian)

Note : If *H* is positive definite, then $x^* = -H^{-1}p$ is the unique solution of $\min f(x)$

Least-squares Problem

$$\min_{x \in \mathbb{R}^{n}} \|Ax - b\|_{2}^{2}, A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^{m}$$

$$f(x) = (Ax - b)^{T}(Ax - b)$$

$$= x^{T}A^{T}Ax - 2b^{T}Ax + b^{T}b$$

$$\nabla f(x) = 2A^{T}Ax - 2A^{T}b$$

$$\nabla^{2}f(x) = 2A^{T}A$$

$$x^{*} = (A^{T}A)^{-1}A^{T}b \in \arg\min_{x \in \mathbb{R}^{n}} \|Ax - b\|_{2}^{2}$$
if $A^{T}A$ is nonsingular matrix \Rightarrow P.D.
Note : x^{*} is an analytical solution

How to Solve an Unconstrained MP

- Get an initial point and iteratively decrease the obj. function value
- Stop once the stopping criteria satisfied
- Steep decent might not be a good choice
- Newton's method is highly recommended
 Local and quadratic convergent algorithm
 - Need to choose a good step size to guarantee global convergence

The First Order Taylor Expansion

Let $f: \mathbb{R}^n \to \mathbb{R}$ be a differentiable function

$$f(x+d) = f(x) + \nabla f(x) \cdot d + \alpha(x,d) \left\| d \right\|$$

where
$$\lim_{d\to 0} \alpha(x,d) = 0$$

If $\nabla f(x)d < 0$ and d is small enough then f(x+d) < f(x).

We call d is a descent direction.

Steep Descent with Exact Line Search

Start with any $x^0 \in \mathbb{R}^n$. Having x^i , stop if $\nabla f(x^i) = 0$ Else compute x^{i+1} as follows:

- (i) Steep descent direction: $d^i = -\nabla f(x^i)$
- (ii) Exact line search: Choose a stepsize $\lambda \in R$ such that

$$rac{df(x^i+\lambda d^i)}{d\lambda} = f'(x^i+\lambda d^i) = 0$$

(iii) Updating: $x^{i+1} = x^i + \lambda d^i$

MATLAB Code for Steep Descent with Exact Line Search (Quadratic Function Only)

function [x, f_value, iter] = grdlines(Q,p, x0, esp)

%

```
% min 0.5*x'Q*x+p'x
```

% Solving unconstrained minimization via % steep descent with exact line search %

```
flag =1;
iter = 0;
while flag > esp
      grad = Q^*xO+p;
      temp1 = grad'*grad;
      if temp1 < 10^{-12}
         flag = esp
       else
         stepsize = temp1/(grad'*Q*grad);
         x1 = x0 - stepsize^{*}grad;
         flag = norm(x1-x0);
         x0 = x1;
      end;
      iter = iter + 1;
end;
x = x0;
f_value = 0.5 * x' * Q * x + p' * x;
```

The Key Idea of Newton's Method

Let $f: \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function $f(x+d) = f(x) + \nabla f(x) \cdot d + \frac{1}{2}x^T \nabla^2 f(x)x + \beta(x,d) ||d||$ where $\lim_{d\to 0} \beta(x,d) = 0$

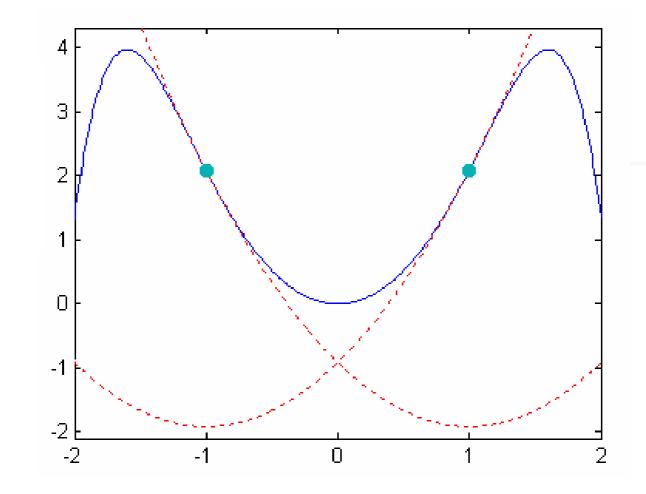
At i^{th} iteration, use a quadratic function to approximate $f(x) \approx f(x^i) + \nabla f(x^i)(x - x^i) + \frac{1}{2}(x - x^i)^T \nabla^2 f(x^i)(x - x^i)$ $x^{i+1} = \arg \min \widetilde{f}(x)$

Newton's Method

Start with $x^0 \in R^n$. Having x^i , stop if $\nabla f(x^i) = 0$ Else compute x^{i+1} as follows:

- (i) Newton direction: $\nabla^2 f(x^i) d^i = -\nabla f(x^i)$. Have to solve a system of linear equations here!
- (ii) Updating: $x^{i+1} = x^i + d^i$

 \succ Converge only when x^0 is close to x^* enough.



 $f(x) = -\frac{1}{6}x^{6} + \frac{1}{4}x^{4} + 2x^{2}$ $g(x) = f(x^{i}) + f'(x^{i})(x - x^{i}) + \frac{1}{2}f''(x^{i})(x - x^{i})$

It can not converge to the optimal solution.

Constrained Optimization Problem

Problem setting: Given functions f, g_i , i = 1, ..., kand h_j , j = 1, ..., m, defined on a domain $\Omega \subseteq R^n$, $\min_{x \in \Omega} f(x)$ subject to $g_i(x) \leqslant 0, \quad \forall i$ $h_j(x) = 0, \quad \forall j$

where f(x) is called the objective function and $g(x) \leq 0$, h(x) = 0 are called constraints.

Example

$$\min f(x) = 2x_1^2 + x_2^2 + 3x_3^2$$

s.t. $2x_1 - 3x_2 + 4x_3 = 49$

<sol>

$$\mathcal{L}(x,\alpha) = f(x) + \beta(2x_1 - 3x_2 + 4x_3 - 49) , \beta \in \mathbb{R}$$

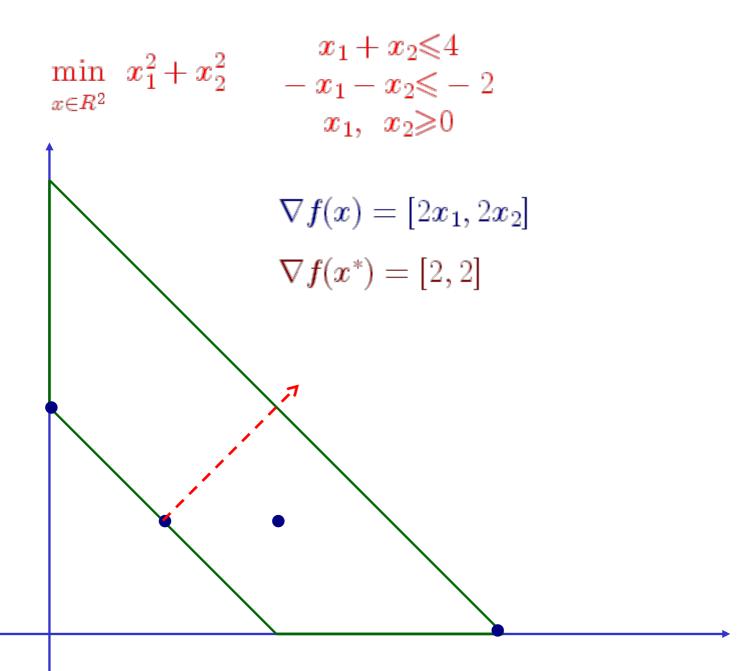
$$\frac{\partial}{\partial x_1} \mathcal{L}(x,\beta) = 0 \implies 4x_1 + 2\beta = 0$$

$$\frac{\partial}{\partial x_2} \mathcal{L}(x,\beta) = 0 \implies 2x_2 - 3\beta = 0$$

$$\frac{\partial}{\partial x_3} \mathcal{L}(x,\beta) = 0 \implies 6x_3 + 4\beta = 0$$

$$2x_1 - 3x_2 + 4x_3 - 49 = 0$$

$$\implies x_1 = 3, \quad x_2 = -9, \quad x_3 = -4$$



Definitions and Notation

• Feasible region:

$$\mathcal{F} = \{ x \in \Omega | \mathbf{g}(x) \leq \mathbf{0}, \mathbf{h}(x) = \mathbf{0} \}$$

where
$$\mathbf{g}(x) = \begin{bmatrix} g_1(x) \\ \vdots \\ g_k(x) \end{bmatrix}$$
 and $\mathbf{h}(x) = \begin{bmatrix} h_1(x) \\ \vdots \\ h_m(x) \end{bmatrix}$

• A solution of the optimization problem is a point $x^* \in \mathcal{F}$ such that $\nexists x \in \mathcal{F}$ for which $f(x) < f(x^*)$ and x^* is called a global minimum.

Definitions and Notation

A point x̄ ∈ ℱ is called a local minimum of the optimization problem if ∃ε > 0 such that f(x)≥f(x̄), ∀x ∈ ℱ and ||x - x̄|| < ε
At the solution x*, an inequality constraint g_i(x) is said to be active if g_i(x*) = 0, otherwise it is called an inactive constraint.

• $g_i(x) \leq 0 \iff g_i(x) + \xi_i = 0, \ \xi_i \geq 0$ where ξ_i is called the slack variable

Definitions and Notation

- Remove an inactive constraint in an optimization problem will NOT affect the optimal solution
 - Very useful feature in SVM
- If $\mathcal{F} = \mathbb{R}^n$ then the problem is called unconstrained minimization problem
 - Least square problem is in this category
 - SSVM formulation is in this category
 - Difficult to find the global minimum without convexity assumption

The Most Important Concepts in Optimization (minimization)

- ♦ A point is said to be an *optimal solution* of a unconstrained minimization if there exists no decent direction → $\nabla f(x^*) = 0$
- ◆ A point is said to be an optimal solution of a constrained minimization if there exists no feasible decent direction → KKT conditions
 - There might exist decent direction but move along this direction will leave out the feasible region

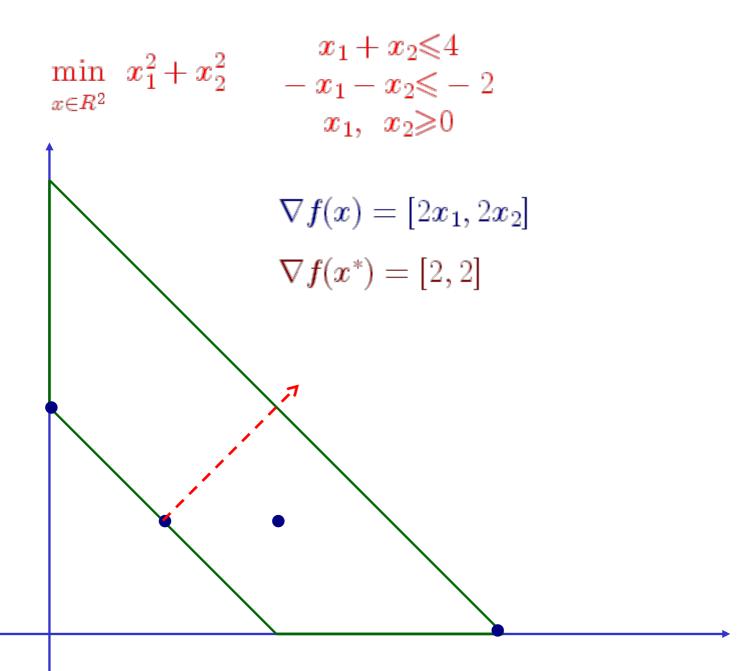
Minimum Principle

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a convex and differentiable function $\mathfrak{F} \subset \mathbb{R}^n$ be the feasible region.

$$x^* \in \arg\min_{x \in \mathcal{F}} f(x) \iff \nabla f(x^*)(x - x^*) \ge 0 \quad \forall x \in \mathcal{F}$$

Example:

min
$$(x-1)^2$$
 s.t. $a \le x \le b$



Linear Programming Problem

- An optimization problem in which the objective function and all constraints are linear functions is called a linear programming problem
 - (LP) min $p^T x$ s.t. $Ax \leq b$ Cx = d $L \leq x \leq U$

Linear Programming Solver in MATLAB

X=LINPROG(f,A,b) attempts to solve the linear programming problem:

min f'*x subject to: A*x <= b

X=LINPROG(f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints $Aeq^*x = beq$.

X=LINPROG(f,A,b,Aeq,beq,LB,UB) defines a set of lower and upper bounds on the design variables, X, so that the solution is in the range LB <= X <= UB.
Use empty matrices for LB and UB if no bounds exist. Set LB(i) = -Inf if X(i) is unbounded below; set UB(i) = Inf if X(i) is unbounded above.

Linear Programming Solver in MATLAB

X=LINPROG(f,A,b,Aeq,beq,LB,UB,X0) sets the starting point to X0. This option is only available with the active-set algorithm. The default interior point algorithm will ignore any non-empty starting point.

You can type "help linprog" in MATLAB to get more information!

 L_1 -Approximation: min $||Ax - b||_1$ $x \in \mathbb{R}^n$ $\left\|z\right\|_1 = \sum_{i=1}^m \left\|z_i\right\|$ $1^T s$ $\min_{x,s} \quad \sum_{i=1}^{n} s_i$ min Or x,sx,ss.t. $-s_i \leqslant A_i x - b_i \leqslant s_i \quad \forall i$ s.t. $-s \leqslant Ax - b \leqslant s$

$$\min_{\substack{x,s \\ \text{s.t.}}} \begin{bmatrix} 0 & \cdots & 0 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x \\ s \end{bmatrix}$$

$$s.t. \quad \begin{bmatrix} A & -I \\ -A & -I \end{bmatrix}_{2m \times (n+m)} \begin{bmatrix} x \\ s \end{bmatrix} \leqslant \begin{bmatrix} b \\ -b \end{bmatrix}$$

Chebyshev Approximation: $\min_{x \in R^n} \left\| Ax - b \right\|_\infty$

$$\left\|z\right\|_{\infty} = \max_{1 \leqslant i \leqslant m} \left\|z_i\right\|$$

$$\min_{\substack{x,\gamma\\ \text{s.t.}}} \quad \gamma \\ -1\gamma \leqslant Ax - b \leqslant 1\gamma$$

$$\min_{\substack{x,\gamma \\ \text{s.t.}}} \begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ \gamma \end{bmatrix}$$

$$\left[\begin{array}{c} A & -1 \\ -A & -1 \end{array} \right]_{2m \times (n+1)} \begin{bmatrix} x \\ \gamma \end{bmatrix} \leqslant \begin{bmatrix} b \\ -b \end{bmatrix}$$

Quadratic Programming Problem

If the objective function is convex quadratic while the constraints are all linear then the problem is called convex quadratic programming problem

(QP) min $\frac{1}{2}x^TQx + p^Tx$ s.t. $Ax \leq b$ Cx = d $L \leq x \leq U$

Quadratic Programming Solver in MATLAB

X=QUADPROG(H,f,A,b) attempts to solve the quadratic programming problem:

```
min 0.5*x'*H*x + f'*x subject to: A*x \le b
```

X=QUADPROG(H,f,A,b,Aeq,beq) solves the problem above while additionally satisfying the equality constraints $Aeq^*x = beq$.

X=QUADPROG(H,f,A,b,Aeq,beq,LB,UB) defines a set of lower and upper bounds on the design variables, X, so that the solution is in the range LB <= X <= UB.
Use empty matrices for LB and UB if no bounds exist. Set LB(i) = -Inf if X(i) is unbounded below; set UB(i) = Inf if X(i) is unbounded above.

Quadratic Programming Solver in MATLAB

X=QUADPROG(H,f,A,b,Aeq,beq,LB,UB,X0) sets the starting point to X0.

You can type "help quadprog" in MATLAB to get more information!

Standard Support Vector Machine

$$\begin{split} \min_{w,b,\xi_A,\xi_B} C(1^T \xi_A + 1^T \xi_B) + \frac{1}{2} \|w\|_2^2 \\ (Aw + 1b) + \xi_A \geqslant 1 \\ (Bw + 1b) - \xi_B \leqslant -1 \\ \xi_A \geqslant 0, \xi_B \geqslant 0 \end{split}$$

Farkas' Lemma

For any matrix $A \in \mathbb{R}^{m \times n}$ and any vector $b \in \mathbb{R}^n$, *either*

 $Ax \ge 0$, b'x < 0 has a solution

Or

 $A'\alpha = b, \quad \alpha \geqslant \mathbf{0} \text{ has a solution}$

but never both.

Minimization Problem
vs.Kuhn-Tucker Stationary-point ProblemMP: $\min_{x \in \Omega} f(x)$ such that
 $\mathbf{g}(x) \leqslant \mathbf{0}$

KTSP: Find $\overline{x} \in \Omega$, $\overline{\alpha} \in R^m$ such that $\nabla f(\overline{x}) + \overline{\alpha}' \nabla \mathbf{g}(\overline{x}) = 0$ $\overline{\alpha}' \mathbf{g}(\overline{x}) = 0$ $\mathbf{g}(\overline{x}) \leq \mathbf{0}, \ \overline{\alpha} \geq \mathbf{0}$ Lagrangian Function $\mathcal{L}(x, \alpha) = f(x) + \alpha' \mathbf{g}(x)$

Let $\mathcal{L}(x,\alpha) = f(x) + \alpha' \mathbf{g}(x)$ and $\alpha \ge \mathbf{0}$

• If f(x), g(x) are convex then $\mathcal{L}(x, \alpha)$ is convex.

- For a fixed $\alpha \ge \mathbf{0}$, if $\overline{x} \in \arg\min\{\mathcal{L}(x,\alpha) | x \in \mathbb{R}^n\}$ then $\frac{\partial \mathcal{L}(x,\alpha)}{\partial x} \Big|_{x=\overline{x}} = \nabla f(\overline{x}) + \alpha' \nabla \mathbf{g}(\overline{x}) = 0$
 - Above result is a sufficient condition if $\mathcal{L}(x, \alpha)$ is convex.

KTSP with Equality Constraints? (Assume h(x) = 0 are linear functions) $\mathbf{h}(x) = \mathbf{0} \Leftrightarrow \mathbf{h}(x) \leq \mathbf{0} \text{ and } - \mathbf{h}(x) \leq \mathbf{0}$ **KTSP**: Find $\overline{x} \in \Omega$, $\overline{\alpha} \in R^k$, $\overline{\beta}_+, \overline{\beta}_- \in R^m$ such that $\nabla f(\overline{x}) + \overline{\alpha}' \nabla \mathbf{g}(\overline{x}) + (\overline{\beta}_{+} - \overline{\beta}_{-})' \nabla \mathbf{h}(\overline{x}) = 0$ $\overline{\alpha}'\mathbf{g}(\overline{x}) = 0, \ (\overline{\beta}_+)'\mathbf{h}(\overline{x}) = 0, \ (\overline{\beta}_-)'(-\mathbf{h}(\overline{x})) = 0$ $\mathbf{g}(\overline{x}) \leqslant \mathbf{0}, \, \mathbf{h}(\overline{x}) = 0$ $\overline{\alpha} \geq , \overline{\beta}_{+}, \overline{\beta}_{-} \geq \mathbf{0}$

KTSP with Equality Constraints

KTSP: Find $\overline{x} \in \Omega$, $\overline{\alpha} \in R^k$, $\overline{\beta} \in R^m$ such that $\nabla f(\overline{x}) + \overline{\alpha}' \nabla \mathbf{g}(\overline{x}) + \overline{\beta} \nabla \mathbf{h}(\overline{x}) = 0$ $\overline{\alpha}' \mathbf{g}(\overline{x}) = 0$, $\mathbf{g}(\overline{x}) \leq \mathbf{0}$, $\mathbf{h}(\overline{x}) = 0$ $\overline{\alpha} \geq \mathbf{0}$

• Let $\overline{\beta} = \overline{\beta}_{+} - \overline{\beta}_{-}$ and $\overline{\beta}_{+}, \overline{\beta}_{-} \ge 0$ then $\overline{\beta}$ is free variable

Generalized Lagrangian Function $\mathcal{L}(x, \alpha, \beta) = f(x) + \alpha' \mathbf{g}(x) + \beta' \mathbf{h}(x)$

Let $\mathcal{L}(x, \alpha, \beta) = f(x) + \alpha' \mathbf{g}(x) + \beta' \mathbf{h}(x)$ and $\alpha \ge \mathbf{0}$

- If f(x), g(x) are convex and h(x) is linear then $\mathcal{L}(x, \alpha, \beta)$ is convex.
- For fixed $\alpha \ge 0, \beta$, if $\overline{x} \in \arg \min\{\mathcal{L}(x, \alpha, \beta) | x \in \mathbb{R}^n\}$ then

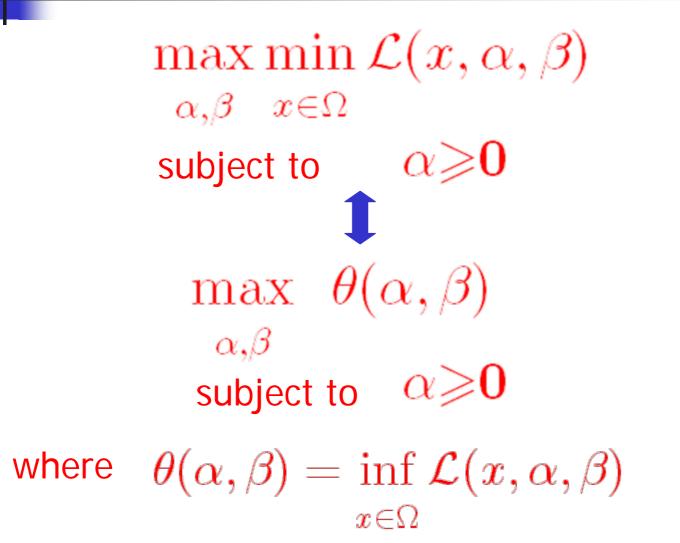
$$\frac{\partial \mathcal{L}(x,\alpha,\beta)}{\partial x}\Big|_{x=\overline{x}} = \nabla f(\overline{x}) + \alpha' \nabla \mathbf{g}(\overline{x}) + \beta' \nabla \mathbf{h}(\overline{x}) = 0$$

• Above result is a sufficient condition if $\mathcal{L}(x, \alpha, \beta)$ is convex.

Lagrangian Dual Problem

$\max \min_{\alpha,\beta} \mathcal{L}(x,\alpha,\beta)$ subject to $\alpha \ge \mathbf{0}$

Lagrangian Dual Problem



Weak Duality Theorem

Let $\overline{x} \in \Omega$ be a feasible solution of the *primal* problem and (α, β) a feasible solution of the *dual* problem. Then $f(\overline{x}) \ge \theta(\alpha, \beta)$

$$heta(lpha,eta) = \inf_{x\in\Omega} \mathcal{L}(x,lpha,eta) \leq \mathcal{L}(ilde{x},lpha,eta)$$

Corollary: $\sup\{\theta(\alpha, \beta) \mid \alpha \ge \mathbf{0}\}$ $\leqslant \inf\{f(x) \mid \mathbf{g}(x) \le \mathbf{0}, \ \mathbf{h}(x) = \mathbf{0}\}$

Weak Duality Theorem

Corollary: If $f(x^*) = \theta(\alpha^*, \beta^*)$ where $\alpha^* \ge 0$ and $\mathbf{g}(x^*) \le 0$, $\mathbf{h}(x^*) = \mathbf{0}$, then x^* and (α^*, β^*) solve the *primal* and *dual* problem respectively. In this case,

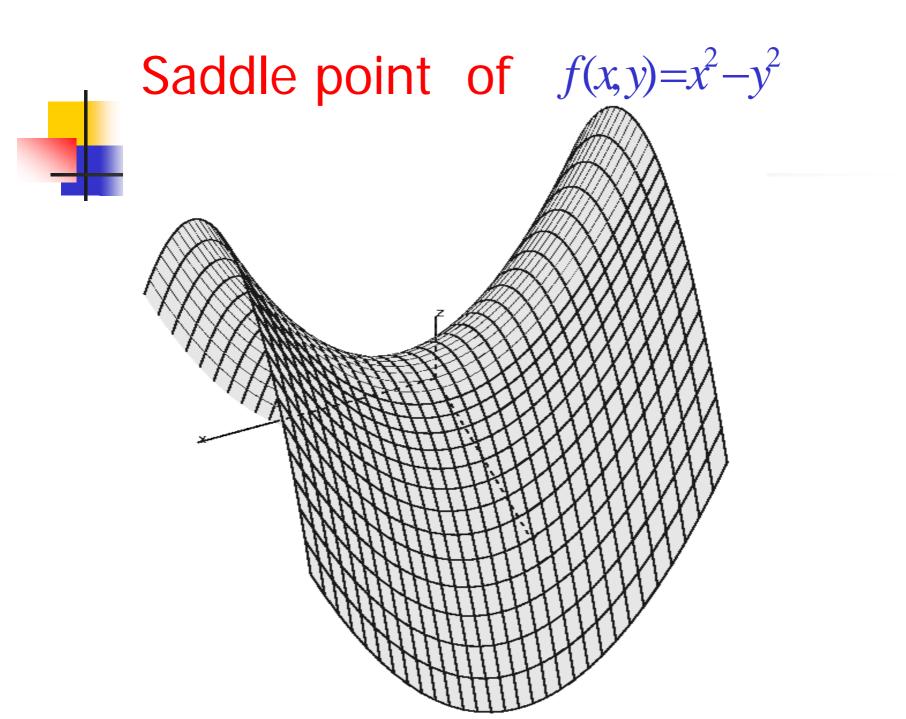
$$\mathbf{0} \leqslant \alpha \perp \mathbf{g}(x) \leqslant \mathbf{0}$$

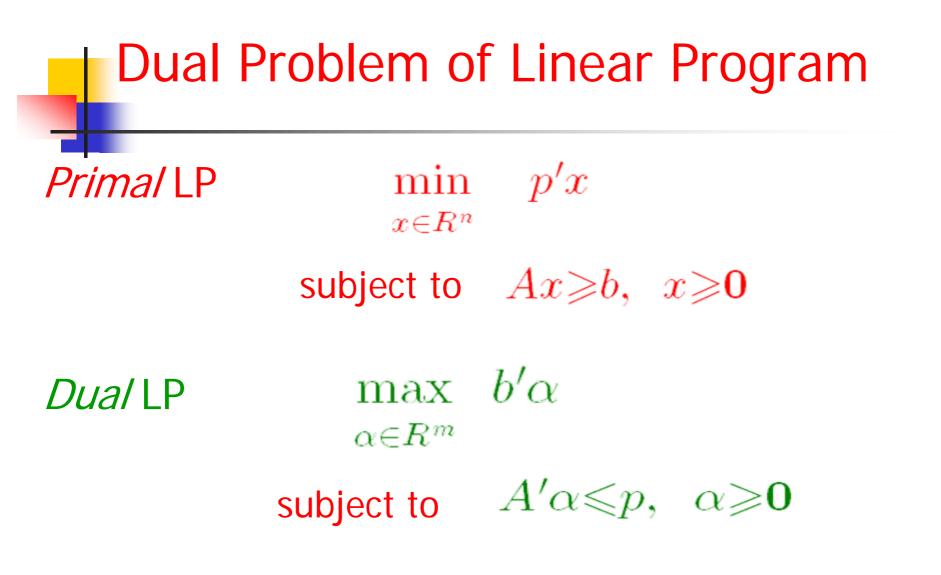
Saddle Point of Lagrangian

Let $x^* \in \Omega, \alpha^* \ge 0, \beta^* \in \mathbb{R}^m$ satisfying

 $\mathcal{L}(x^*, \alpha, \beta) \leq \mathcal{L}(x^*, \alpha^*, \beta^*) \leq \mathcal{L}(x, \alpha^*, \beta^*),$ $\forall x \in \Omega, \ \alpha \geq \mathbf{0}.$ Then (x^*, α^*, β^*) is called

The saddle point of the Lagrangian function





X All duality theorems hold and work perfectly!

Lagrangian Function of Primal LP $\mathcal{L}(x, \alpha) = p'x + \alpha'_1(b - Ax) + \alpha'_2(-x)$

 $\max_{\alpha_1,\alpha_2 \geqslant 0} \min_{x \in \mathbb{R}^n} \mathcal{L}(x,\alpha_1,\alpha_2) \iff$

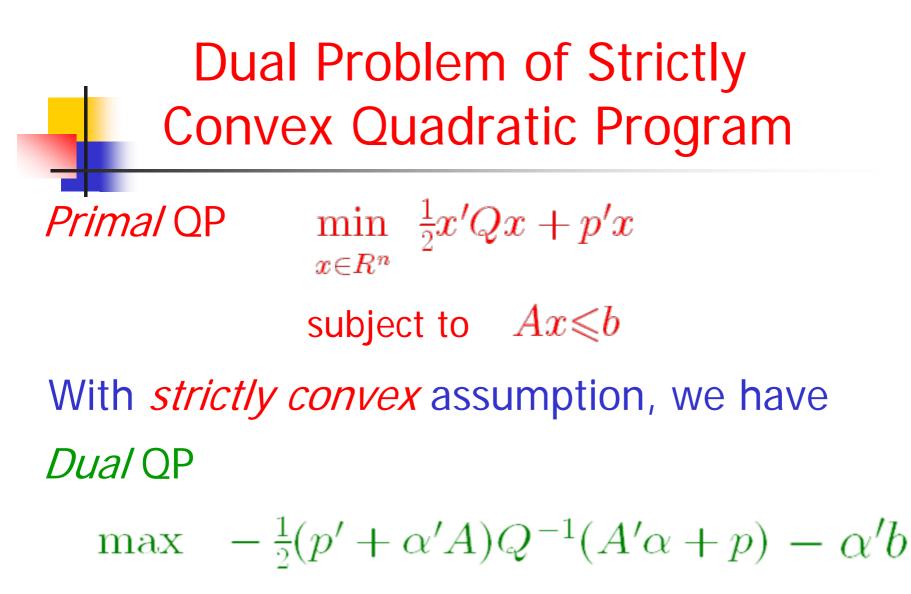
 $\max_{\alpha_1,\alpha_2 \ge 0} p'x + \alpha'_1(b - Ax) + \alpha'_2(-x)$

$$p - A'\alpha_1 - \alpha_2 = 0$$
$$(\nabla_x \mathcal{L}(x, \alpha_1, \alpha_2) = 0)$$

Application of LP DualityLSQ-Normal Equation Always Has a SolutionFor any matrix $A \in R^{m \times n}$ and any vector $b \in R^m$,consider $\min_{x \in R^n} ||Ax - b||_2^2$

 $x^* \in \arg\min\{||Ax - b||_2^2\} \quad \Leftrightarrow A'Ax^* = A'b$

Claim: A'Ax = A'b always has a solution.



subject to $\alpha \ge 0$