SWCON253: Machine Learning

Lecture 12 Constrained Optimization

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References

- Chapter 7, Mathematics for Machine Learning by Deisenroth, Faisal, and Ong (https://mml-book.com)
- Intro to Deep Learning & Generative Models by Sebastian Raschka (http://pages.stat.wisc.edu/~sraschka/teaching/stat453-ss2020/)
- 패턴 인식 by 오일석, 기계 확습 by 오일석



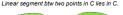


(Cf.) Convex Set & Convex Function

Convex Set

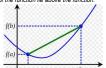
Definition 7.2. A set C is a convex set if for any $x, y \in C$ and for any scalar θ with $0 \le \theta \le 1$, we have

$$\theta x + (1 - \theta)y \in \mathcal{C}. \tag{7.29}$$





A straight line between any two points of the function lie above the function



Convex Function

Definition 7.3. Let function $f: \mathbb{R}^D \to \mathbb{R}$ be a function whose domain is a convex set. The function f is a convex function if for all x, y in the domain of f, and for any scalar θ with $0 \le \theta \le 1$, we have

$$f(\theta x + (1 - \theta)y) \le \theta f(x) + (1 - \theta)f(y)$$
. (7.30)

Remark. A concave function is the negative of a convex function.

NOTE:

All the derivations in this lecture assume **convexity** of the variables & functions.



1. Constrained Optimization Problems

With No Constraints

minimize f(x)

- Unconstrained Optimization
- Solution: $\nabla_{\mathbf{x}} f(\mathbf{x}) = \mathbf{0}$

등니게하는 건건 With Equality Constraints

 $\label{eq:force_force} \begin{aligned} & \text{minimize } f(\underline{x}) \\ & \text{subject to } g(\underline{x}) = 0 \end{aligned}$

모든 변립 발생나 g를 반속하다 무를 과도와 하는 X

$$f(x_1, x_2) = x_1^2 + x_2^2 - 1$$

$$g(x_1, x_2) = x_1 + x_2 - 1$$

◆ With *Inequality* Constraints

 $\begin{aligned} & \text{minimize } f(\underline{x}) \\ & \text{subject to } g(\underline{x}) \leq 0 \end{aligned}$

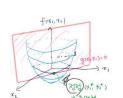
 $minimize(-x \cdot y)$ subject to <math>2x + 2y - 1 < 0

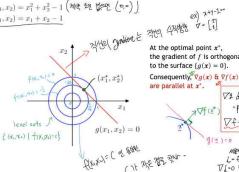
2. Lagrange Multiplier for Equality Constraints

An Illustrative Example

minimize
$$f(\underline{x})$$

subject to $g(\underline{x}) = 0$





the gradient of f is orthogonal to the surface $\{g(x) = 0\}$.

Consequently, $\nabla g(x)$ & $\nabla f(x)$ are parallel at x'.



L-f+ 12 = 301.



2. Lagrange Multiplier for Equality Constraints (cont'd)

Equality Constrained Optimization

$$\begin{array}{l} \text{minimize } f(\underline{x}) \\ \text{subject to } g(\underline{x}) = 0 \end{array}$$

- At the optimal point x^* , $\nabla_x g(x)$ and $\nabla_x f(x)$ are parallel.
 - \star Hence, there exists some $\lambda \in R$ such that $\nabla_x f(x) + \lambda \nabla_x g(x) = 0$.
- We define the Lagrangian function $L(x, \lambda) = f(x) + \lambda g(x)$, where $\lambda \in R$ is called Lagrangian multiplier.
- Now observe that:

$$\star \quad \nabla_{x} f(x) + \lambda \nabla_{x} g(x) = 0 \quad \Leftrightarrow \quad \nabla_{x} L(x, \lambda) = 0$$

$$\star \quad g(x) = 0 \quad \Leftrightarrow \quad \nabla_{x} L(x, \lambda) = 0$$

Example

$$f(x_1, x_2) = x_1^2 + x_2^2 - 1$$

 $g(x_1, x_2) = x_1 + x_2 - 1$

$$L(x, \lambda) = x_1^2 + x_2^2 - 1 + \lambda(x_1 + x_2 - 1)$$

$$\nabla_{x_1} L(x, \lambda) = 2x_1 + \lambda = 0$$

$$\nabla_{x_2} L(x, \lambda) = 2x_2 + \lambda = 0$$

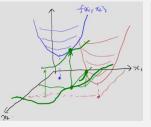
$$\nabla_{x_1} L(x, \lambda) = x_1 + x_2 - 1 = 0$$

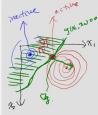
$$\dot{x}(x_1^*, x_2^*) = (0.5, 0.5)$$

3. Lagrange Multiplier for *Inequality* Constraints (cont'd)



- 고대(제의 방향: 제양조건이 g(x)≤ 0.이므로 g의 과목 경계(g(x)=0)에서 최대 → 경계 안쪽(g(x)) ()으로 갈수록 g값이 경계보다 줄어듦 → g의 증가방향은 경계 바깥 방향
- 세약조건이 active: 제약조건을 만족하는 f의 최소라(최절해)이 경계(g(x)= 0)에 존재하다는 뜻
 → f의 원래 최소라이 경계 바깥쪽(g(x)≥ 0)에 존재 → f의 증가방향은 경계 안쪽 방향
 - 제암조건이 inactive: 제약조건을 만족하는 (의 최소라(최절해)이 경계 안쪽(g(x)<0)에 존재한다는 뜻
 → f의 원래 최소라이 경계 안쪽 (참고: f의 증가 방향은 경계 바깥 방향)





At the optimal point ,

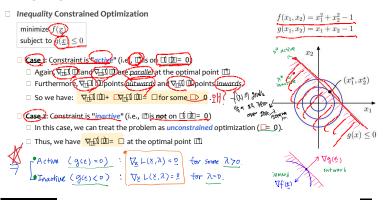
1) If active:

- ∇. D points outward
- √ inwards

2) If inactive:

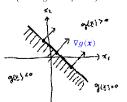
(unconstrained optimization)

3. Lagrange Multiplier for *Inequality* Constraints



3. Lagrange Multiplier for *Inequality* Constraints (cont'd)

- ◆ [Note 1] Gradient of g
 - Inequality constraint: $g(x) \le 0$
 - $\nabla q(x)$ is outward the boundary
 - ★ since at the boundary g(x) increases on the outward direction (from negative to positive).

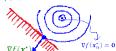


- ♦ [Note 2] Gradient of f
 - Inactive case (i.e., solution is inside the boundary)
 - ★ The unconstrained solution must reside *inside* the boundary \rightarrow $\nabla f(x^*) = 0$ $(x^* = x^*_{anc})$



- Active case (i.e., solution is on the boundary)
- \bigstar The unconstrained solution must reside either on or outside the boundary $\Rightarrow \nabla f(x^*)$ is either zero or inward the boundary.



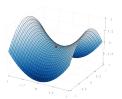


3. Lagrange Multiplier for Inequality Constraints (cont'd)

- Inequality Constrained Optimization (cont'd)
 - We can summarize both cases using the Lagrangian again.



A saddle point on the graph of z=x2-y2 (hyperbolic paraboloid)

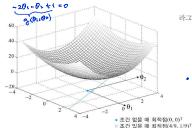


wikinedia ora/wiki/Saddle point#/media/File:Saddle_point.svg

- The conditions in the vellow box is called the Karush-Kuhn-Tucker (KKT) condition
- ★ It is sometimes also called as first-order necessary condition.

<> Examples - Equality Constraint

- 등식 조건부 최적화 문제: $J(\theta) = \theta_1^2 + 2\theta_2^2$
 - 조건이 없을 때 최소 점은 (o,o)^T
 - '2θ,+θ, = 1' 이라는 조건 하에 최소점을 구하면?



3(8,8)

라그랑제 함수: $L(\theta, \lambda_1) = (\theta_1^2 + 2\theta_2^2)$ ($\lambda_1(2\theta_1 + \theta_2 - 1)$)

$$oldsymbol{\theta}$$
로 미분한 식을 $oldsymbol{0}$ 으로 등:
$$\begin{cases} \dfrac{\partial L}{\partial \theta_1} = 2\theta_1 - 2\lambda_1 = 0 \\ \dfrac{\partial L}{\partial \theta_2} = 4\theta_2 - \lambda_1 = 0 \end{cases}$$

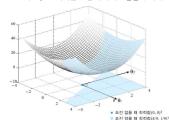
• λ 로 미분한 식을 0으로 뚬: $\frac{\partial L}{\partial \lambda} = -(2\theta_1 + \theta_2 - 1) = 0$

이 식을 풀면,
$$\hat{\theta} = (\frac{4}{9}, \frac{1}{9})^T$$
, $\lambda = \frac{4}{9}$ 70

그림 11 11 등신 조건부 최정화 문제의 예

<> Examples – Inequality Constraint

- 부등식 조건부 최적화 문제: $J(\mathbf{\theta}) = \theta_1^2 + 2\theta_2^2$
 - '20,+0,≥1'이라는 조건 하에 최소점을 구하라.



(a) $f_1(\theta) = 2\theta_1 + \theta_2 - 1 \ge 0$

라그랑제 함수: $L(\theta, \lambda_1) = (\theta_1^2 + 2\theta_2^2) - \lambda_1(2\theta_1 + \theta_2 - 1)$

$$\begin{array}{c} \text{KKT } \text{ \&Z-} \\ \begin{cases} \left[\begin{array}{c} \frac{\partial L}{\partial \theta_1} = 2\theta_1 - 2\lambda_1 = 0 \\ \\ \frac{\partial L}{\partial \theta_2} = 4\theta_2 - \lambda_1 = 0 \\ \\ \lambda_1 \geq 0 \\ \lambda_1 (2\theta_1 + \theta_2 - 1) = 0 \end{array} \right] \end{cases}$$

이제 KKT 조건을 풀어 이름 만족하는 해 θ름 구하면 된다. 이 예는 라그락제 슷수 를 하나만 가지므로 쉽게 풀 수 있다. 마지막 식에서 $\lambda_1 = 0$ 이거나 $2\theta_1 + \theta_2 - 1 = 0$ 이어 야 한다. 먼저 $\lambda_1=0$ 이라고 가정해 보자. 그럼 $\theta_1=\theta_2=0$ 이 되어 주어진 조건 $f_1(\theta)=$ $2\theta_1 + \theta_2 - 1 \ge 0$ 을 만족하지 못한다. 두 번째 경우를 가지고 풀어 보면 $\hat{\theta} = (\frac{4}{0}, \frac{1}{0})^T$ 을





0= 9 + g(0)=170(X)

4. Lagrange Multiplier for Multiple Constraints

Multiple Constraints (including both equality & inequality constraints)

minimize
$$f_0(\underline{x})$$
 subject to $f_i(\underline{x}) \leq 0 \ (i=1,...,m)$ $h_j(\underline{x}) = 0 \ (j=1,...,k)$

$$L(\underline{x},\underline{\lambda},\underline{y}) = f_0(\underline{x}) + \sum_{i=1}^m \lambda_i f_i(\underline{x}) + \sum_{i=1}^k \nu_i h_j(\underline{x}) \quad \text{a. } \quad f_\bullet(\underline{x}) \quad \text{a. } \underline{\lambda}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \text{a. } \underline{\chi}^\mathsf{T} \ \underline{f} \in \mathcal{T} \ \ \underline{f} \in \mathcal{T}$$

- ★ λ_i : Lagrange multiplier associated with $f_i(x_i) \leq 0$.
- $\star v_i$: Lagrange multiplier associated with $h_i(x_i) = 0$.
- Note: Let x₀ be a feasible point of the primal problem (that is a point that satisfies all the constraints), then we have:

$$\sum_{i=1}^{m} \underbrace{\lambda_{i}}_{\geq 0} \underbrace{f_{i}(x_{0})}_{\leq 0} + \sum_{i=1}^{k} \underbrace{\nu_{j} h_{j}(x_{0})}_{\leq 0} \leq 0 \qquad \Rightarrow \qquad L(x_{0}, \lambda, \nu) = f_{0}(x_{0}) + \sum_{i=1}^{m} \lambda_{i} f_{i}(x_{0}) + \sum_{j=1}^{k} \nu_{j} h_{j}(x_{0}) \leq \quad f_{0}(x_{0})$$



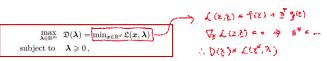


5. Lagrangian Duality

- Duality in Optimization
 - The idea of converting an optimization problem in one set of variables x (called the primal variables) into another set of variables λ (called the dual variables).
- Primal Problem

$$\min_{m{x}} \quad f(m{x})$$
 subject to $g_i(m{x}) \leqslant 0$ for all $i=1,\ldots,m$

Lagrangian Dual Problem



5. Lagrangian Duality - Linear Programming

Consider the special case when all the preceding functions are linear, i.e.,

Consider the special case when all the preceding functions are linear, i.e.,
$$\min_{x \in \mathbb{R}^d} \quad c^{\top}x \tag{7.39}$$
 subject to $Ax \leqslant b$.

where $A \in \mathbb{R}^{m \times d}$ and $b \in \mathbb{R}^{m}$.

The Lagrangian is given by

$$\mathfrak{L}(x, \lambda) = c^{\top}x + \lambda^{\top}(Ax - b) = (c + A^{\top}\lambda)^{\top}x - \lambda^{\top}b$$
.

Taking the derivative of $\mathfrak{L}(x,\lambda)$ with respect to x and setting it to zero $(x,\lambda)=0$

dual optimization problem

$$egin{array}{ll} \max_{oldsymbol{\lambda} \in \mathbb{R}^m} & - oldsymbol{b}^{ op} oldsymbol{\lambda} \ & ext{subject to} & oldsymbol{c} + oldsymbol{A}^{ op} oldsymbol{\lambda} = oldsymbol{0} \end{array}$$

 $\lambda \geqslant 0$.

We have the choice of solving the primal or the dual program depending on whether m or d is larger.

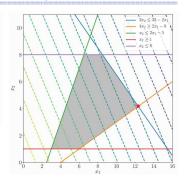
5. Lagrangian Duality – Linear Programming (cont'd)

Example 7.5 (Linear Program) Consider the linear program

$$\min_{x \in \mathbb{R}^2} - \begin{bmatrix} 5 \\ 3 \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$
subject to
$$\begin{bmatrix} 2 & 2 \\ 2 & -4 \\ -2 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leqslant \begin{bmatrix} 33 \\ 8 \\ 5 \\ -1 \\ 2 \end{bmatrix}$$
 (7.44)

with two variables. This program is also shown in Figure 7.9. The objective function is linear, resulting in linear contour lines. The constraint set in standard form is translated into the legend. The optimal value must lie in the shaded (feasible) region, and is indicated by the star.





5. Lagrangian Duality - Quadratic Programming

Consider the case of a convex quadratic objctive function, where the constraints are affine, i.e.,

$$\min_{\boldsymbol{x} \in \mathbb{R}^d} \frac{1}{2} \boldsymbol{x}^{\mathsf{T}} \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^{\mathsf{T}} \boldsymbol{x}$$
 (7.45) subject to $\boldsymbol{A} \boldsymbol{x} \leq \boldsymbol{b}$.

where $\mathbf{A} \in \mathbb{R}^{m \times d}$, $\mathbf{b} \in \mathbb{R}^m$, and $\mathbf{c} \in \mathbb{R}^d$.

The square symmetric matrix $Q \in \mathbb{R}^{d \times d}$ is positive definite, and therefore the objective function is convex.

The Lagrangian is given by
$$\mathfrak{L}(x, \pmb{\lambda}) = \frac{1}{2} \pmb{x}^\top \pmb{Q} \pmb{x} + \pmb{c}^\top \pmb{x} + \pmb{\lambda}^\top (\pmb{A} \pmb{x} - \pmb{b}) = \frac{1}{2} \pmb{x}^\top \pmb{Q} \pmb{x} + (\pmb{c} + \pmb{A}^\top \pmb{\lambda})^\top \pmb{x} - \pmb{\lambda}^\top \pmb{b} \,,$$

Taking the derivative of $\mathfrak{L}(x,\lambda)$ with respect to x and setting it to zero gives $Qx + (c + A^{\top}\lambda) = 0$.

Assuming that
$$Q$$
 is invertible, we get $x = -Q^{-1}(c + A^{T}\lambda)$.

Therefore, the dual optimization problem is given by
$$\max_{\boldsymbol{\lambda} \in \mathbb{R}^m} \quad -\frac{1}{2} (\boldsymbol{c} + \boldsymbol{A}^{\mathsf{T}} \boldsymbol{\lambda})^{\mathsf{T}} \boldsymbol{Q}^{-1} (\boldsymbol{c} + \boldsymbol{A}^{\mathsf{T}} \boldsymbol{\lambda}) - \boldsymbol{\lambda}^{\mathsf{T}} \boldsymbol{b}$$
 subject to $\quad \boldsymbol{\lambda} \geq \boldsymbol{0}$.

We have the choice of solving the primal or the dual program depending on whether *m* or *d* is larger.

5. Lagrangian Duality - Quadratic Programming (cont'd)

- Example: Converting into the standard QP form and then solving the dual problem
 - Primal Problem

$$\min_{\mathbf{x}} J(\mathbf{x}) = x_1^2 + 2x_2^2$$

$$\text{s.t.} \quad g(\mathbf{x}) = -2x_1 - x_2 + 1 \le 0$$

$$\lim_{\mathbf{x} \in \mathbb{R}^d} \frac{1}{2} \mathbf{v}^T Q \mathbf{x} + \mathbf{v}^T \mathbf{x}$$

$$\text{subject to} \quad \mathbf{A} \mathbf{x} \le \mathbf{b},$$

$$\mathbf{A} \mathbf{x} \cdot \mathbf{b} \le \mathbf{c} = \mathbf{c}$$

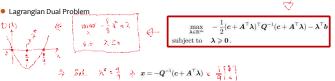
$$\mathbf{A} \mathbf{x} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{c}$$

$$\mathbf{A} \mathbf{x} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c}$$

$$\mathbf{A} \mathbf{x} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c}$$

$$\mathbf{A} \mathbf{x} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c} \cdot \mathbf{c}$$

$$\mathbf{A} \mathbf{x} \cdot \mathbf{c} \cdot$$

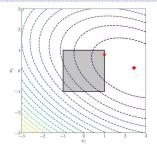




5. Lagrangian Duality - Quadratic Programming (cont'd)

Example 7.6 (Quadratic Program) Consider the quadratic program

of two variables. The program is also illustrated in Figure 7.4. The objective function is quadratic with a positive semidefinite matrix Q, resulting in elliptical contour lines. The optimal value must lie in the shaded (feasible) region, and is indicated by the star.



The unconstrained problem (indicated by the contour lines) has a minimum on the right side (indicated by the circle).

The box constraints $(-1 \le x_1 \le 1 \text{ and } -1 \le x_2 \le 1)$ require that the optimal solution is within the box, resulting in an optimal value indicated by the star.