HW5 Handwritten Assignment

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As the final exam approaches, we will select some problems from old assignments and exams to help students review the course materials. Problems 1, 2, 3, and 5 must be completed, while only one among Problem 4 or Problem 6 has to be answered (which will be graded).

Problem 1 (Trace Optimization)(1%)

1. Let $\Sigma \in \mathbb{R}^{m \times m}$ be a symmetric positive semi-definite matrix, $\mu \in \mathbb{R}^m$. Please construct a set of points $x_1, ..., x_n \in \mathbb{R}^m$ such that

$$\frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)(x_i - \mu)^T = \Sigma, \quad \frac{1}{n} \sum_{i=1}^{n} x_i = \mu$$

Hint: n is not given by the problem. WLOG, you may assume $\mu = 0 \in \mathbb{R}^d$.

Solution: WLOG (Without Loss of Generality), let $\mu = 0$. Since Σ is a symmetric positive semi-definite matrix, we can perform eigen decomposition as follows:

$$\Sigma = UDU^T = \sum_{i=1}^{m} (d_i u_i u_i^T).$$

where U and U^T are orthogonal matrix. Let n=2m and construct a set of points $x_1,...,x_m,...,x_{2m}$ where $x_i = \sqrt{d_i}u_i$ and $x_{m+i} = -\sqrt{d_i}u_i \ \forall \ 1 \le i \le m$. Then,

$$\frac{1}{n} \sum_{i=1}^{n} x_i = \mu = 0$$

$$\frac{1}{n} \sum_{i=1}^{n} x_i x_i^T = \sum_{i=1}^{m} (d_i u_i u_i^T) = UDU^T = \Sigma$$

Note that lots of students just use the covariance of eigen decomposition to construct $\{x_i\}_{i=1}^n$. However, It should satisfy the condition that $\frac{1}{n}\sum_{i=1}^n x_i = \mu$

2. Let $1 \le k \le m$, solve the following optimization problem and justify with proof:

minimize $Trace(\Phi^T \Sigma \Phi)$ subject to $\Phi^T \Phi = I_k$ variables $\Phi \in R^{m \times k}$

In other words, you need to find Φ and verify that your Φ minimize the trace.

Solution: Method 1: Let ϕ_1, \dots, ϕ_k be the columns of Φ . Then

$$Trace(\Phi^{T} \Sigma \Phi) = \sum_{i=1}^{k} \phi_{i}^{T} \Sigma \phi_{i} = \sum_{i=1}^{k} \phi_{i}^{T} (\sum_{j=1}^{m} (d_{j} u_{j} u_{j}^{T})) \phi_{i} = \sum_{j=1}^{m} d_{j} \sum_{i=1}^{k} \langle u_{j}, \phi_{i} \rangle^{2} = \sum_{j=1}^{m} c_{j} d_{j}$$

where $\langle \cdot, \cdot \rangle$ is standard inner product in Euclidean space, $c_j := \sum_{i=1}^k \langle u_j, \phi_i \rangle^2$ for each $j=1,\cdots,m$ and $d_1 \geq d_2 \geq \cdots \geq d_m \geq 0$ Claim: $0 \leq c_j \leq 1$ and $\sum_{j=1}^m c_j = k$ Clearly, $c_j \geq 0$. Extending ϕ_1, \cdots, ϕ_k to $\phi_1, \cdots, \phi_k, \phi_{k+1}, \cdots, \phi_m$ for \mathbb{R}^m . Then, for each $j=1,\cdots,m$

$$c_j = \sum_{i=1}^k \langle u_j, \phi_i \rangle^2 \le \sum_{i=1}^m \langle u_j, \phi_i \rangle^2 = 1$$

Finally, since u_1, \dots, u_m is an orthonormal basis for \mathbb{R}^m ,

$$\sum_{j=1}^{m} c_j = \sum_{j=1}^{m} \sum_{i=1}^{k} \langle u_j, \phi_i \rangle^2 = \sum_{i=1}^{k} \sum_{j=1}^{m} \langle u_j, \phi_i \rangle^2 = \sum_{i=1}^{k} \|\phi_i\|_2^2 = k$$

Hence, the minimum value of $\sum_{j=1}^m c_j d_j$ over all choice of $c_1, c_2, \cdots, c_m \in [0,1]$ with $\sum_{j=1}^k c_j = k$ is d_{m-k+1}, \cdots, d_m . This is achieved when $c_1, \cdots, c_{m-k} = 0$ and $c_{m-k+1} = \cdots = c_m = 1$. Notice: Many students proceed the proof as the following. By the symmetry of Σ , we have

$$\Sigma = U\Lambda U^T$$
, U orthonormal.

Let $V = U^T \Phi$ and hence $\Phi = UV$. Then

$$Tr(\Phi^{\top}\Sigma\Phi) = Tr(\Phi^{\top}U\Lambda U^{\top}\Phi) = Tr(V^{\top}\Lambda V).$$

Note that $\Lambda \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{m \times k}$, and $V^{\top} \Lambda V \in \mathbb{R}^{k \times k}$. Then

$$Tr(V^{\top}\Lambda V) = \sum_{i=1}^{k} \lambda_i v_i^{\top} v_i = \sum_{i=1}^{k} \lambda_i$$

"because V is orthonormal", which is not true because $U^{\top}\Phi$ is not necessarily orthonormal.

Problem 2 (Gradient Boosting)(1%)

Consider the binary classification problem, where we are given training data set $\{(x_i, y_i)\}_{i=1}^N$ with $x_i \in \mathbb{R}^d$ and $y_i \in \{1, -1\}$. Let $F = \{f \mid f : \mathbb{R}^d \to \{1, -1\}\}$ be the collection of classifiers. Given number of epochs $T \in \mathbb{N}$. Suppose that we want to find the function

$$g(x) = \sum_{t=1}^{N} \alpha_t f_t(x)$$

where $f_t \in F$ and $\alpha_t \in \mathbb{R}$ for all $t = 1, \dots, T$, by which the aggregated classifier is given by

$$h(x) = \begin{cases} 1, & \text{if } g(x) > 0 \\ -1, & \text{if } g(x) \le 0. \end{cases}$$

Please apply gradient boosting to show how the functions f_t and the coefficients α_t are computed with an aim to minimize the following loss function

$$L(g) = \sum_{i=1}^{N} \log \left(1 + e^{-y_i g(x_i)} \right).$$

Problem 3 (EM algorithm for mixture of exponential model)(1%)

Given N samples $x_1, \ldots, x_N \in [0, \infty)$, we would like to cluster them into K clusters. Assume the samples are generated according to Exponential mixture models

$$X \sim \sum_{j=1}^{K} \pi_j Exp(\tau_j)$$

where $\pi_1 + \ldots + \pi_K = 1$, and $Exp(\tau)$ denotes the exponential distribution with probability density function

$$f_{\tau}(x) = \begin{cases} (1/\tau)e^{-x/\tau} &, x \ge 0\\ 0 &, x < 0. \end{cases}$$

We would like to apply Expectation Maximization algorithm to find the maximum likelihood estimation of parameters $\theta = \{(\pi_k, \tau_k)\}_{k=1}^K$.

(a) Please write down the E-step and M-step and show that the parameters are updated from $\theta^{(t)} = \left\{ (\pi_k^{(t)}, \tau_k^{(t)}) \right\}_{k=1}^K$ to $\theta^{(t+1)} = \left\{ (\pi_k^{(t+1)}, \tau_k^{(t+1)}) \right\}_{k=1}^K$ in the following form:

$$\tau_k^{(t+1)} = \frac{\sum_{i=1}^N \delta_{ik}^{(t)} x_i}{\sum_{i=1}^N \delta_{ik}^{(t)}}, \quad \pi_k^{(t+1)} = \frac{1}{N} \sum_{i=1}^N \delta_{ik}^{(t)}$$

(b) What is the closed form expression of $\delta_{ik}^{(t)}$?

Solution: Denote $\mathcal{X} = (\mathbf{x}_i)_{i=1}^N$ and latent variables $\mathcal{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \{1, \dots, K\}^N$, and consider the joint probability distribution as

$$p(\mathcal{X}, \mathcal{Z}; \boldsymbol{\theta}) = \prod_{i=1}^{N} p(\mathbf{x}_i, z_i; \boldsymbol{\theta}), \text{ where } p(\mathbf{x}, z = k; \boldsymbol{\theta}) = \pi_k \prod_{j=1}^{D} \mu_{kj}^{x^{(j)}} (1 - \mu_{kj})^{1 - x^{(j)}}.$$

Start with initial guess $\boldsymbol{\theta}^{(0)}$, the EM algorithm estimates $\boldsymbol{\theta}^{(t+1)} = (\pi_k^{(t+1)}, \mu_k^{(t+1)})_{k=1}^K$ from $\boldsymbol{\theta}^{(t)} = (\pi_k^{(t)}, \mu_k^{(t)})_{k=1}^K$ as follows:

Expectation Step: Compute

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \mathbb{E}_{\mathcal{Z}|\mathcal{X};\boldsymbol{\theta}^{(t)}}[\log p(\mathcal{X},\mathcal{Z};\boldsymbol{\theta})] = \sum_{i=1}^{N} \mathbb{E}_{z_{i}|\mathbf{x}_{i};\boldsymbol{\theta}^{(t)}}[\log p(\mathbf{x}_{i},z_{i};\boldsymbol{\theta})].$$

The posterior probability of latent variables based on current parameters $\boldsymbol{\theta}^{(t)}$:

$$P[z_i = k | \mathbf{x}_i; \boldsymbol{\theta}^{(t)}] = \frac{p(\mathbf{x}_i, z_i = k; \boldsymbol{\theta}^{(t)})}{\sum_{k'=1}^{K} p(\mathbf{x}_i, z_i = k'; \boldsymbol{\theta}^{(t)})} = \frac{\pi_k^{(t)} \prod_{j=1}^{D} \mu_{kj}^{x_i^{(j)}} (1 - \mu_{kj})^{1 - x_i^{(j)}}}{\sum_{k'=1}^{K} \pi_{k'}^{(t)} \prod_{j=1}^{D} \mu_{k'j}^{x_i^{(j)}} (1 - \mu_{k'j})^{1 - x_i^{(j)}}}.$$

The log-likelihood of parameter θ for jointly generating \mathbf{x}_i and z_i :

$$\log p(\mathbf{x}_i, z_i = k; \boldsymbol{\theta}) = \log \pi_k + \sum_{j=1}^{D} \left(x_i^{(j)} \log \mu_{kj} + (1 - x_i^{(j)}) \log(1 - \mu_{kj}) \right)$$

Hence,

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \sum_{i=1}^{N} \sum_{k=1}^{K} \delta_{ik}^{(t)} \left(\log \pi_k + \sum_{j=1}^{D} \left(x_i^{(j)} \log \mu_{kj} + (1 - x_i^{(j)}) \log(1 - \mu_{kj}) \right) \right),$$

where $\delta_{ik}^{(t)} = P[z_i = k | \mathbf{x}_i; \boldsymbol{\theta}^{(t)}].$

Maximization Step: Choose $\theta^{(t+1)} = \arg \max_{\theta} Q(\theta | \theta^{(t)})$. Note that

$$\frac{\partial}{\partial \mu_{kj}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \sum_{i=1}^{N} \delta_{ik}^{(t)} \left(\frac{x_i^{(j)}}{\mu_{kj}} - \frac{1 - x_i^{(j)}}{1 - \mu_{kj}} \right).$$

By setting the partial derivative to zero, the maximal solution for μ_{kj} is

$$\mu_{kj}^{(t+1)} = \frac{\sum_{i=1}^{N} \delta_{ik}^{(t)} x_i^{(j)}}{\sum_{i=1}^{N} \delta_{ik}^{(t)}}.$$

As for π_k , due to the constraint $\sum_{k=1}^K \pi_k = 1$, we introduce Lagrange multipliers and note

$$\frac{\partial}{\partial \pi_k} \left(Q(\boldsymbol{\theta} | \boldsymbol{\theta}^{(t)}) - \lambda \sum_{k=1}^K \pi_k \right) = \frac{1}{\pi_k} \sum_{i=1}^N \delta_{ik}^{(t)} - \lambda.$$

By setting the above quantities identically zero for all k, we solve $\lambda = N$ and the maximal solution for π_k is

$$\pi_k^{(t+1)} = \frac{1}{N} \sum_{i=1}^N \delta_{ik}^{(t)}.$$

Problem 4 (Sparse SVM)(2%)

Given training data of N input-output pairs $\mathscr{D} = ((x_i, y_i))_{i=1}^N$, where $x_i \in \mathcal{X}$ and $y_i \in \{\pm 1\}$. One can give two types of arguments in favor of the SVM algorithm: one based on the sparsity of the support vectors, another based on the notion of margin. Suppose instead of maximizing the margin, we choose instead to maximize sparsity by minimizing the p-norm of the vector $\alpha = (\alpha_1, ..., \alpha_N)$ that defines the weight vector \mathbf{w} , for some $p \geq 1$. In this question we consider the case p = 2, which leads to the following optimization problem:

which can be rewritten in the following primal problem:

minimize
$$f(\alpha, b, \boldsymbol{\xi}) = \frac{1}{2} \sum_{i=1}^{N} \alpha_i^2 + \sum_{i=1}^{N} C_i \xi_i$$

$$g_{1,i}(\alpha, b, \boldsymbol{\xi}) = 1 - \xi_i - y_i \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_i \cdot \mathbf{x}_j + b \right) \leq 0$$
subject to
$$g_{2,i}(\alpha, b, \boldsymbol{\xi}) = -\alpha_i \leq 0$$

$$g_{3,i}(\alpha, b, \boldsymbol{\xi}) = -\xi_i \leq 0$$
variables
$$\alpha = (\alpha_1, ..., \alpha_N) \in \mathbb{R}^N, b \in \mathbb{R}, \boldsymbol{\xi} = (\xi_1, ..., \xi_N) \in \mathbb{R}^N$$

$$(1)$$

as well as its Lagrangian dual problem:

maximize
$$\theta(\boldsymbol{\omega}, \beta, \boldsymbol{\gamma}) = \inf_{\alpha \in \mathbb{R}^N, b \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^N} L(\alpha, b, \boldsymbol{\xi}, \boldsymbol{\omega}, \beta, \boldsymbol{\gamma})$$

subject to $\omega_i \geq 0, \beta_i \geq 0, \gamma_i \geq 0, i \in [1, N]$
variables $\boldsymbol{\omega} = (\omega_1, ..., \omega_N) \in \mathbb{R}^N, \beta = (\beta_1, ..., \beta_N) \in \mathbb{R}^N, \boldsymbol{\gamma} = (\gamma_1, ..., \gamma_N) \in \mathbb{R}^N$ (2)

- 1. Write down the Lagrangian function $L(\alpha, b, \xi, \omega, \beta, \gamma)$ in explicit form of $\alpha, b, \xi, \omega, \beta, \gamma$.
- 2. Show that the duality gap between (1) and (2) is zero.
- 3. Derive $\theta(\boldsymbol{\omega}, \boldsymbol{\beta}, \boldsymbol{\gamma})$ in explicit form of dual variables $\boldsymbol{\omega}, \boldsymbol{\beta}, \boldsymbol{\gamma}$.
- 4. Show that the dual problem can be simplified as

maximize
$$\sum_{i=1}^{N} \omega_i - \frac{1}{2} \sum_{i=1}^{N} \left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i \right)_+^2$$
subject to
$$\sum_{i=1}^{N} \omega_i y_i = 0$$
variables
$$0 \le \omega_i \le C_i, \ i = 1, \dots, N$$
 (3)

- 5. Suppose $(\bar{\alpha}, \bar{b}, \bar{\xi})$ and $(\bar{\omega}, \bar{\beta}, \bar{\gamma})$ are the optimal solutions to problems (1) and (2) respectively. Denote $\bar{\mathbf{w}} = \sum_{j=1}^{N} \bar{\alpha}_{j} y_{j} \mathbf{x}_{j}$.
 - (a) Prove that

$$\bar{\alpha}_i = \max\left(\sum_{j=1}^N \bar{\omega}_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i, 0\right) \ \forall i = 1, \dots, N$$
 (4)

(b) Prove that

$$\bar{b} = \underset{b \in \mathbb{R}}{\operatorname{arg\,min}} \sum_{i=1}^{N} C_i \max \left(1 - y_i \left(\bar{\mathbf{w}} \cdot \mathbf{x}_i + b \right), 0 \right), \tag{5}$$

- (c) Prove that $\bar{\xi}_i = \max \left(1 y_i \left(\bar{\mathbf{w}} \cdot \mathbf{x}_i + \bar{b}\right), 0\right)$ for all $i = 1, \dots, N$.
- (d) Prove that

$$\begin{array}{ll}
\bar{\omega}_{i} = C_{i}, & \text{if } y_{i} \left(\bar{\mathbf{w}} \cdot \mathbf{x}_{i} + \bar{b} \right) < 1 \\
\bar{\omega}_{i} = 0, & \text{if } y_{i} \left(\bar{\mathbf{w}} \cdot \mathbf{x}_{i} + \bar{b} \right) > 1 \\
0 \leq \bar{\omega}_{i} \leq C_{i}, & \text{if } y_{i} \left(\bar{\mathbf{w}} \cdot \mathbf{x}_{i} + \bar{b} \right) = 1
\end{array} \right\} \quad \forall i = 1, \dots, N$$

Solution: 1. The Lagrangian function can be explicitly written as

$$L(\alpha, \beta, \omega, \gamma) = f(\alpha, b, \xi) + \sum_{i=1}^{N} \omega_i g_1^i(\alpha, b, \xi) + \sum_{i=1}^{N} \gamma_i g_2^i(\alpha, b, \xi),$$

where

$$f(\alpha, b, \xi) = \frac{1}{2} \sum_{i=1}^{N} \alpha_i^2 + \sum_{i=1}^{N} C_i \xi_i + \sum_{i=1}^{N} \left(1 - \xi_i - y_i \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_i + \beta_i \right) \right) + \sum_{i=1}^{N} \beta_i (-\alpha_i) + \sum_{i=1}^{N} \gamma_i (-\xi_i).$$

- 2. We can verify that the problem satisfies the condition of the strong duality theorem. Hence, the duality gap is zero.
- 3. Take partial derivatives of the Lagrangian function L over α, b, ξ yields

$$\frac{\partial}{\partial \alpha_i} L = \alpha_i - \sum_{i=1}^N \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i - \beta_i, \quad \frac{\partial}{\partial b} L = -\sum_{i=1}^N \omega_i y_i, \quad \frac{\partial}{\partial \xi_i} L = C_i - \omega_i - \gamma_i.$$

If the following conditions hold:

$$\sum_{i=1}^{N} \omega_i y_i = 0, \quad \omega_i + \gamma_i = C_i, \ \forall i = 1, \dots, N,$$

then $\theta(\omega, \beta, \gamma) = L(\alpha, b, \xi, \omega, \beta, \gamma)$ if and only if

$$\alpha_i = \sum_{i=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i + \beta_i, \ \forall i \in \{1, N\},$$

at which

$$\theta(\omega, \beta, \gamma) = \sum_{i=1}^{N} \omega_i - \frac{1}{2} \sum_{i=1}^{N} \left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i + \beta_i \right)^2.$$

Otherwise, since $\frac{\partial}{\partial \alpha}L$, $\frac{\partial}{\partial \xi_1}L$, ..., $\frac{\partial}{\partial \xi_N}L$ are constants not identically zero, one has $\theta(\omega, \beta, \gamma) = -\infty$. 4. Because $\beta_i \geq 0$,

$$\left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i + \beta_i\right)^2 = \left(\max\left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i, 0\right)\right)^2 = \left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i\right)^2.$$

By (c), one may rewrite (17) as

maximize
$$\sum_{i=1}^{N} \omega_i - \frac{1}{2} \sum_{i=1}^{N} \left(\sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i \right)^2,$$

subject to

$$\sum_{i=1}^{N} \omega_i y_i = 0, \quad \omega_i + \gamma_i = C_i, \ \forall i = 1, \dots, N,$$

variables $\omega_i \geq 0, \beta_i \geq 0, \gamma_i \geq 0, i = 1, \dots, N$, which can be further simplified as (18).

5. By (b), the duality gap is zero, so the primal and dual optimal solutions satisfy the KKT conditions. Note that in (c) we have shown that the stationary condition $\theta(\omega, \beta, \gamma) = L(\alpha, b, \xi, \omega, \beta, \gamma)$ holds iff (21) and (22) are both satisfied. As such, we may write down the KKT conditions, including Stationary, Primal feasible, Dual feasible, and Complementary conditions, as follows (for all i = 1, ..., N):

(S1)
$$\omega_i + \gamma_i = C_i$$
 (D1) $\omega_i \ge 0$

$$(S2) \quad \sum_{i=1}^{N} \omega_i y_i = 0 \tag{D2} \quad \beta_i \ge 0$$

(S3)
$$\alpha_i = \sum_{j=1}^{N} \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i + \beta_i$$
 (D3) $\gamma_i \ge 0$

(P1)
$$y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \ge 1 - \xi_i$$
 (C1) $\omega_i(1 - \xi_i - y_i(\mathbf{w} \cdot \mathbf{x}_i + b)) = 0$

$$(C2) \quad \xi_i \ge 0 \tag{C2}$$

(P3)
$$\xi_i \ge 0$$
 (C3) $\gamma_i \xi_i = 0$

Given the optimal ω_i , it is clear by (25) and (S3) that $\beta_i = \left(\sum_{j=1}^N \omega_j y_j y_i \mathbf{x}_j \cdot \mathbf{x}_i\right)$ and (19) holds. Given the optimal coefficient vector α , observe that (16) can be rewritten as the following optimization problem:

$$\text{minimize } \frac{1}{2} \sum_{i=1}^{N} \alpha_i^2 + \sum_{i=1}^{N} C_i \max \left(1 - y_i \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \cdot \mathbf{x}_i + b \right), 0 \right),$$

variables $b \in \mathbb{R}$, $\alpha_i \geq 0$, $i \in \{1, N\}$, hence the optimal bias is given by (20).

- If $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) < 1$, then $\xi_i > 0$ by (P1), $\gamma_i = 0$ by (C3), $\omega_i = C_i$ by (S1), $\xi_i = 1 y_i(\mathbf{w} \cdot \mathbf{x}_i + b)$.
- If $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) > 1$, then $\omega_i = 0$ by (P3, C1), so $\gamma_i = C_i$, so $\xi_i = 0$ by (C3).
- If $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) = 1$, then $\xi_i = 0$ by (S1, C1, C2), and $\omega_i = C_i$ by (D1, D3, S1).

Problem 6 (Stationary and Deterministic Policy)(2%)

In this problem, we aim to help students review and understand the proof of existence of stationary and deterministic policy that maximizes the $V^{\pi}(s)$ for all $s \in \mathcal{S}$.

Theorem. Let Π be the set of nonstationary and randomized policies. Define

$$V^*(s) = \sup_{\pi \in \Pi} V^{\pi}(s)$$

$$Q^*(s, a) = \sup_{\pi \in \Pi} Q^{\pi}(s, a).$$

Then there exists a stationary and deterministic policy π such that for all $s \in \mathcal{S}$ and $a \in \mathcal{A}$,

$$V^{\pi}(s) = V^*(s)$$

$$Q^{\pi}(s, a) = Q^*(s, a).$$

Remark. The notations are consistent with those in the lecture notes.

- 1. Verify that V^* and Q^* is bounded between 0 and $\frac{1}{1-\gamma}$. Hence, V^* and Q^* must be finite.
- 2. Show that given $(s_0, a_0, r_0, s_1) = (s, a, r, s')$, the optimal discounted value γV^* , from t = 1 onwards, does not depend on the initial conditions s, a, and r:

$$\sup_{\pi \in \Pi} \mathbb{E} \left[\sum_{t=1}^{\infty} \gamma^t r(s_t, a_t) \mid \pi, (s_0, a_0, r_0, s_1) = (s, a, r, s') \right] = \gamma V^*(s').$$

3. Let π^* be a policy such that

$$\forall s \in \mathcal{S}, \quad \pi^*(s) \in \underset{a \in \mathcal{A}}{\operatorname{arg\,max}} \ r(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot | s, a)}[V^*(s')].$$

- (a) Explain that π^* is deterministic.
- (b) Now suppose that the transition of states and actions is deterministic. In order to show that π^* is an optimal policy, i.e. $V^*(s) = V^{\pi^*}(s)$, we have to show two inequalities: $V^* \geq V^{\pi^*}$ and $V^* \leq V^{\pi^*}$. The first one is trivial since $\pi^* \in \Pi$. Now, please show the other inequality $V^* \leq V^{\pi^*} < \infty$.
- (c) Similarly, show that $Q^{\pi^*} = Q^*$ under the assumption that the transition is deterministic.

Solution: Please check the lecture notes.