Bayesian shrinkage prediction for the regression problem

Kei Kobayashi∗ and Fumiyasu Komaki†

Abstract

We consider Bayesian shrinkage predictions for the Normal regression problem under the frequentist Kullback-Leibler risk function.

Firstly, we consider the multivariate Normal model with an unknown mean and a known covariance. While the unknown mean is fixed, the covariance of future samples can be different from training samples. We show that the Bayesian predictive distribution based on the uniform prior is dominated by that based on a class of priors if the prior distributions for the covariance and future covariance matrices are rotation invariant.

Then, we consider a class of priors for the mean parameters depending on the future covariance matrix. With such a prior, we can construct a Bayesian predictive distribution dominating that based on the uniform prior.

Lastly, applying this result to the prediction of response variables in the Normal linear regression model, we show that there exists a Bayesian predictive distribution dominating that based on the uniform prior. Minimaxity of these Bayesian predictions follows from these results.

Key words: Bayesian prediction, shrinkage estimation, Normal regression, superharmonic function, minimaxity, Kullback-Leibler divergence.

1 Introduction

Suppose that we have observations \( y \sim N_d(y; \mu, \Sigma) \). Here \( N_d \) is the density function of the \( d \)-dimensional multivariate Normal distribution with mean vector \( \mu \) and covariance matrix \( \Sigma \). We consider the prediction of \( \tilde{y} \sim N_d(\tilde{y}; \mu, \tilde{\Sigma}) \) using a predictive density \( \hat{p}(\tilde{y}|y) \). We assume that the mean of the distribution of unobserved (future) samples is the same as the one of the observed samples. However, the covariance matrices, \( \Sigma \) and \( \tilde{\Sigma} \), are not necessarily the same or proportional to each other. We call a problem with such settings the “problem with changeable covariances.” As we will show below, the

∗kei@ism.ac.jp
†komaki@mist.i.u-tokyo.ac.jp
changeable covariance is a natural assumption when we consider the linear regression problems.

In the present work, we assume that the mean vector $\mu$ is unknown and the covariance matrix $\Sigma$ is known. We consider both cases where the future covariance $\tilde{\Sigma}$ is known and unknown.

We evaluate predictive densities $\hat{p}(\tilde{y}|y)$ by the KL loss function

$$D(\hat{p}(\tilde{y}|\theta)||\hat{p}(\tilde{y}|y)) := \int \hat{p}(\tilde{y}|\theta) \log \frac{\hat{p}(\tilde{y}|\theta)}{\hat{p}(\tilde{y}|y)} d\tilde{y}$$ \hspace{1cm} (1)

and the (frequentist) risk function

$$R_{KL}(\hat{p}, \theta) := \int p(y|\theta) D(\hat{p}(\tilde{y}|\theta)||\hat{p}(\tilde{y}|y))d\tilde{y}.$$ \hspace{1cm} (2)

We consider the Bayesian predictive density

$$p_\pi(\tilde{y}|y) := \frac{\int \hat{p}(\tilde{y}|\theta)p(y|\theta)\pi(\theta)d\theta}{\int p(y|\theta)\pi(\theta)d\theta}$$

with prior $\pi(\theta)$. For the Normal model, the Bayesian predictive density with the uniform prior $\pi_I(\mu) = 1$ becomes

$$p_\pi(\tilde{y}|y; \Sigma, \tilde{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\Sigma + \tilde{\Sigma}|^{1/2}} \exp \left( - \frac{\|\tilde{y} - y\|^2}{2} \right),$$

as we will see in Section 2. Let $p_\pi(\tilde{y}|y; \Sigma, \tilde{\Sigma})$ denote $p_\pi(\tilde{y}|y)$ for short.

When $\tilde{\Sigma}$ is proportional to $\Sigma$, i.e. $\tilde{\Sigma} = a\Sigma$ for $a > 0$, the problem is reduced to the one with $\Sigma = vI_d$ and $\tilde{\Sigma} = \tilde{v}I_d$ for positive scalar values $v$ and $\tilde{v}$. This case with ‘unchangeable covariances’ has been well studied. The Bayesian predictive density

$$p_1(\tilde{y}|y; \Sigma, \tilde{\Sigma}) = \frac{1}{\{2\pi(v + \tilde{v})\}^{d/2}} \exp \left( - \frac{\|\tilde{y} - y\|^2}{2(v + \tilde{v})} \right)$$

based on the uniform prior $\pi_I(\mu) = 1$ dominates the plug-in density

$$p(\tilde{y}|\hat{\mu}) = \frac{1}{\{2\pi\tilde{v}\}^{d/2}} \exp \left( - \frac{\|\tilde{y} - y\|^2}{2\tilde{v}} \right)$$

with MLE, where $\hat{\mu} = y$. Moreover, by Murray (1977) and Ng (1980), the Bayesian predictive density $p_1(\tilde{y}|y)$ is the best predictive density that is invariant under the translation group. In Liang & Barron (2004) and George et al. (2006), the minimaxity of $p_1$ was proved.

In Komaki (2001), it was proved that the Bayesian predictive density $p_S(\tilde{y}|y)$ with Stein prior

$$\pi_S(\mu) := \|\mu\|^{-(d-2)}$$ \hspace{1cm} (3)
dominates the Bayesian predictive density \( p_1(\hat{y}|y) \) with the uniform prior \( \pi_1(\mu) \).

George et al. (2006) generalized the result of Komaki (2001). Define the marginal distribution \( m_\pi \) by

\[
m_\pi(z; \Sigma) := \int N(z; \mu, \Sigma) \pi(\mu) \, d\mu.
\]

(4)

As we will see in Theorem 2.4 below, George et al. (2006) proved a sufficient condition on the prior \( \pi(\mu) \) or the marginal distribution \( m_\pi \) for \( p_\pi(\hat{y}|y) \) to dominate \( p_1(\hat{y}|y) \) when \( \Sigma \) is proportional to \( \hat{\Sigma} \). In the present work, we generalize the results of Komaki (2001) and George et al. (2006) to the corresponding problem with the changeable covariances, considering only finite sample cases. Asymptotic properties of Bayesian prediction are studied in Komaki (1996), Corcuera & Giunnolo (2000), and Komaki (2006).

2 Prior distributions independent of the future covariance

In this section, we develop and prove our main results concerning properties of \( p_\pi(\hat{y}|y) \) in the problem with changeable covariances.

First we give three lemmas generalizing results proved in George et al. (2006) for the problem with “unchangeable” variances.

Define the marginal distribution \( m_\pi \) by (4).

**Lemma 2.1** If \( m_\pi(z; \Sigma) < \infty \) for all \( z \), then \( p_\pi(\hat{y}|y) \) is a proper probability density. Moreover, the mean of \( p_\pi(\hat{y}|y) \) is equal to the posterior mean \( E_\pi[\mu|y] \) if it exists.

Let

\[
w := (\Sigma^{-1} + \hat{\Sigma}^{-1})^{-1}(\Sigma^{-1}y + \hat{\Sigma}^{-1}\hat{y})
\]

and

\[
\Sigma_w := (\Sigma^{-1} + \hat{\Sigma}^{-1})^{-1}.
\]

(5)

As a function of the predictive density based on the uniform prior, the Bayesian predictive density based on a prior \( \pi(\mu) \) becomes as follows:

**Lemma 2.2**

\[
p_\pi(\hat{y}|y) = p_1(\hat{y}|y) \frac{m_\pi(w; \Sigma_w)}{m_\pi(y; \Sigma)}.
\]

The following lemma is used for proving minimaxity of \( p_\pi(\hat{y}|y) \).

**Lemma 2.3** The Bayesian predictive density \( p_1(\hat{y}|y) \) is minimax under KL risk function \( R_{KL}(\hat{p}, \mu) \).
Since the proofs of Lemma 2.1 and Lemma 2.3 are almost same as those of Lemma 1 and Lemma 3 in George et al. (2006), we omit them. We prove only Lemma 2.2.

**Proof of Lemma 2.2**

\[
p(y | \mu, \Sigma)p(\tilde{y} | \mu, \tilde{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp \left( - \frac{(y - \mu)^\top \Sigma^{-1}(y - \mu)}{2} \right) \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp \left( - \frac{(\tilde{y} - \mu)^\top \tilde{\Sigma}^{-1}(\tilde{y} - \mu)}{2} \right)
\]

\[
= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp \left( - \frac{(w - \mu)^\top \Sigma^{-1}_w (w - \mu)}{2} \right) \exp \left( - \frac{y^\top \Sigma^{-1} y}{2} - \frac{\tilde{y}^\top \tilde{\Sigma}^{-1} \tilde{y}}{2} \right)
\]

\[
= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp \left( - \frac{(w - \mu)^\top \Sigma^{-1}_w (w - \mu)}{2} \right) \exp \left( - \frac{(y - \tilde{y})^\top (\Sigma + \tilde{\Sigma})^{-1}(y - \tilde{y})}{2} \right)
\]

In the last equation, we use

\[
\Sigma^{-1}(\Sigma^{-1} + \tilde{\Sigma}^{-1})^{-1} = \Sigma^{-1}(\Sigma^{-1} + \tilde{\Sigma}^{-1})^{-1} - \Sigma^{-1}(\Sigma^{-1} + \tilde{\Sigma}^{-1})^{-1}(\Sigma^{-1} + \tilde{\Sigma}^{-1})
\]

\[
= -\Sigma^{-1} + \tilde{\Sigma}^{-1} - \Sigma^{-1}
\]

From (6), the predictive density with the uniform prior \(I(\mu) = 1\) is given by

\[
p_1(\tilde{y} | y) = \frac{\int p(y | \mu, \Sigma)p(\tilde{y} | \mu, \tilde{\Sigma}) \, d\mu}{\int p(y | \mu, \Sigma) \, d\mu}
\]

\[
= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} |\Sigma^{-1} + \tilde{\Sigma}^{-1}|^{-1/2} (2\pi)^{d/2} \exp \left( - \frac{(y - \tilde{y})^\top (\Sigma + \tilde{\Sigma})^{-1}(y - \tilde{y})}{2} \right)
\]

\[
= (2\pi)^{-d/2}|\Sigma + \tilde{\Sigma}|^{-1/2} \exp \left( - \frac{(y - \tilde{y})^\top (\Sigma + \tilde{\Sigma})^{-1}(y - \tilde{y})}{2} \right).
\]

Therefore

\[
p_\pi(\tilde{y} | y) = \frac{\int p(y | \mu, \Sigma)p(\tilde{y} | \mu, \tilde{\Sigma}) \pi(\mu) \, d\mu}{\int p(y | \mu, \Sigma) \pi(\mu) \, d\mu}
\]

\[
= \frac{p_1(\tilde{y} | y)}{\int N(y | \mu, \Sigma) \pi(\mu) \, d\mu}
\]

\[
= \frac{p_1(\tilde{y} | y) m_\pi(w | \Sigma_w)}{m_\pi(y | \Sigma)}.
\]
Next, the difference of the risk functions of the two priors is evaluated. Let

\[ R_{KL}(\pi, \mu) := \int p(y|\mu, \Sigma) D(p(\tilde{y}|\mu, \tilde{\Sigma}) \parallel p_\pi(\tilde{y}|y)) \, dy \]

\[ \phi_\pi(\mu, \Sigma) := \int N(z; \mu, \Sigma) \log m_\pi(z; \Sigma) \, dz. \]

Then from Lemma 2.2

\[ R_{KL}(\pi, \mu) - R_{KL}(\pi_I, \mu) = \int p(y|\mu, \Sigma)p(\tilde{y}|\mu, \tilde{\Sigma}) \log \frac{p_\pi(\tilde{y}|y)}{p_\pi(\tilde{y}|y)} \, dy \, d\tilde{y} \]

\[ = \int p(y|\mu, \Sigma)p(\tilde{y}|\mu, \tilde{\Sigma}) \log \frac{m_\pi(y; \Sigma)}{m_\pi(w; \Sigma_w)} \, dy \, d\tilde{y} \]

\[ = \phi_\pi(\mu, \Sigma) - \phi_\pi(\mu, \Sigma_w). \]  

(7)

Now \( \Sigma_w = (\Sigma^{-1} + \tilde{\Sigma}^{-1})^{-1} \prec \Sigma \). In order to prove \( R_{KL}(\pi, \mu) < R_{KL}(\pi_I, \mu) \), it suffices to prove \( \phi_\pi(\mu, \Sigma) < \phi_\pi(\mu, \Sigma_w) \).

Before stating the main results for the problem with changeable covariances, we review some results with a special setting, i.e., unchangeable covariances.

An extended real-valued function \( \pi(\mu) \) on an open set \( R \subset \mathbb{R}^p \) is said to be superharmonic when it satisfies the following properties:

1. \(-\infty < \pi(\mu) \leq \infty \) and \( \pi(\mu) \neq \infty \) on any component of \( R \).

2. \( \pi(\mu) \) is lower semi-continuous on \( R \).

3. If \( G \) is an open subset of \( R \) with compact closure \( \bar{G} \subset R \), \( w(\mu) \) is a continuous function on \( \bar{G} \), \( w(\mu) \) is harmonic on \( G \), and \( \pi(\mu) \geq w(\mu) \) on \( \partial G \), then \( \pi(\mu) \geq w(\mu) \) on \( G \).

If \( \pi(\mu) \) is a \( C^2 \) function, then \( \pi(\mu) \) is superharmonic on \( R \) if and only if \( \Delta \pi \leq 0 \) on \( R \).

**Theorem 2.4 (Komaki (2001) and George et al. (2006))**

Assume \( d \geq 3 \).

(i) If \( \pi(\mu) \) is the Stein prior \( \pi_S(\mu) \),

\[ v_1 > v_2 > 0 \Rightarrow \phi_{\pi_S}(\mu, v_1I_d) < \phi_{\pi_S}(\mu, v_2I_d) \text{ for all } \mu. \]

(ii) If \( \pi(\mu) \) is a superharmonic function and \( m_\pi(z; vI_d) < \infty \) for any \( z \) and \( v \),

\[ v_1 > v_2 > 0 \Rightarrow \phi_{\pi}(\mu, v_1I_d) \leq \phi_{\pi}(\mu, v_2I_d) \text{ for all } \mu. \]

Furthermore, if \( m_\pi(z; vI_d) \) is also not constant for all \( v_2 \leq v \leq v_1 \), the inequality holds strictly.
(iii) If $\sqrt{m_\pi(z; vI_d)}$ is a superharmonic function for any $v$ and $m_\pi(z; vI_d) < \infty$ for any $z$ and $v$,

$$v_1 > v_2 > 0 \Rightarrow \phi_\pi(\mu, v_1 I_d) \leq \phi_\pi(\mu, v_2 I_d) \text{ for all } \mu.$$ Furthermore, if $m_\pi(z; vI_d)$ is also not constant for any $v_2 \leq v \leq v_1$, the inequality holds strictly.

We note that (iii) implies (ii) and (ii) implies (i). (i) was proved in Komaki (2001). (ii) and (iii) were proved in George et al. (2006).

Theorem 2.5 is a generalization of (ii) of Theorem 2.4 to the problem with changeable covariances. For each prior $\pi_\Sigma(\mu)$, define a rescaled prior with respect to a positive definite $d \times d$ matrix $\Sigma^*$ by

$$\pi_{\Sigma^*}(\mu) := \pi(\Sigma^* - 1/2 \mu).$$

In particular, call $\pi_{S; \Sigma^*}(\mu) := \pi(S; \Sigma^* - 1/2 \mu)$ as a rescaled Stein prior with respect to $\Sigma^*$.

We consider Bayesian risk with priors $p(\Sigma)$ and $\tilde{p}(\tilde{\Sigma})$:

$$R_{KL}(\pi, \mu) = \int p(\Sigma)\tilde{p}(\tilde{\Sigma})R_{KL}(\pi, \mu)d\Sigma d\tilde{\Sigma},$$

where $d\Sigma$ means a Lebesgue measure for a vector space of all components of a matrix $\Sigma$. Define

$$\varphi_\pi(\mu) := \int p(\Sigma)\tilde{p}(\tilde{\Sigma})\phi_\pi(\mu, \Sigma)d\Sigma d\tilde{\Sigma}$$

$$= \int p(\Sigma)\tilde{p}(\tilde{\Sigma})N(z; \mu, \Sigma) \log m_\pi(z; \Sigma) dz d\Sigma d\tilde{\Sigma} \quad (8)$$

$$\varphi_\pi^w(\mu) := \int p(\Sigma)\tilde{p}(\tilde{\Sigma})\phi_\pi(\mu, \Sigma^w)d\Sigma d\tilde{\Sigma}$$

$$= \int p(\Sigma)\tilde{p}(\tilde{\Sigma})N(z; \mu, \Sigma^w) \log m_\pi(z; \Sigma^w) dz d\Sigma d\tilde{\Sigma}. \quad (9)$$

Then from (7),

$$R_{KL}(\pi, \mu) - R_{KL}(\pi_1, \mu) = \varphi_\pi(\mu) - \varphi_\pi^w(\mu). \quad (10)$$

We consider the case where $p(\Sigma)$, $\tilde{p}(\tilde{\Sigma})$, and $\pi(\mu)$ are rotation invariant. Here, a function $f(\Sigma)$ of a matrix $\Sigma \in \mathbb{R}^{d \times d}$ and a function $f(\mu)$ of a vector $\mu \in \mathbb{R}^{d \times d}$ are said to be rotation invariant if $f(\Sigma) = f(PS \Sigma^P^T)$ and $g(\mu) = g(P \mu)$, respectively, for every orthogonal matrix $P \in \mathbb{R}^{d \times d}$.

Theorem 2.5

Let $d \geq 3$. If $p(\Sigma)$ and $\tilde{p}(\tilde{\Sigma})$ are rotation invariant functions and $\pi$ is a rotation invariant superharmonic prior, then

$$R_{KL}(\pi_{\Sigma}, \mu) \leq R_{KL}(\pi_1, \mu)$$

for any $\mu$. In particular, the Bayesian predictive distribution $p_{\Sigma}(y|\tilde{y})$ with $\pi_\Sigma$ dominates that based on $\pi_1$ if $\pi$ is also not constant.
Proof. We note that \( m_{\pi}(z; \Sigma) < \infty \) for every \( z \in \mathbb{R}^d \) and positive definite matrix \( \Sigma \in \mathbb{R}^{d \times d} \) from Lemma A.1 in the appendix.

First, we prove invariance of \( \varphi_{\pi\Sigma}(\mu) \) and \( \varphi_{w\Sigma}(\mu) \) under rotations of \( \mu \).

Let \( P \) be a \( d \times d \) orthogonal matrix, then

\[
\varphi_{\pi\Sigma}(P\mu) = \int p(\Sigma)\bar{p}(\bar{\Sigma})N(z; P\mu, \Sigma) \log \int N(z; \mu', \Sigma)\pi_{\Sigma}(\mu')d\mu'dz\Sigma d\bar{\Sigma} \\
= \int p(\Sigma)\bar{p}(\bar{\Sigma})N(\bar{z}; \mu, P^\top \Sigma P) \log \int N(\bar{z}; \bar{\mu}', P^\top \Sigma P)\pi(\Sigma^{-1/2}P\bar{\mu}')d\bar{\mu}'d\bar{z}\Sigma d\bar{\Sigma} \\
= \int p(P\Sigma P^\top)\bar{p}(\bar{\Sigma})N(\bar{z}; \mu, \Sigma) \log \int N(\bar{z}; \bar{\mu}', \Sigma)\pi(\Sigma^{-1/2}\bar{\mu}')d\bar{\mu}'d\bar{z}\Sigma d\bar{\Sigma} \\
= \varphi_{\pi\Sigma}(\mu).
\]

Proof of the rotation invariance of \( \varphi_{\pi\Sigma}(\mu) \) is nearly the same.

We define

\[
\mu^* := \arg \max_{\|\mu'\| = \|\mu\|} \frac{\|\Sigma^{-1/2}\mu'\|}{\|\Sigma_w^{-1/2}\mu'\|}
\]

and

\[
\tau := \frac{\|\Sigma^{-1/2}\mu^*\|}{\|\Sigma_w^{-1/2}\mu^*\|}.
\]

Note that \( 0 < \tau < 1 \), because \( \tilde{\Sigma} \) is positive definite. Moreover,

\[
\|\tau \Sigma_w^{-1/2}\bar{\mu}'\| = \tau \|\Sigma_w^{-1/2}\bar{\mu}'\| \geq \frac{\|\Sigma^{-1/2}\bar{\mu}'\|}{\|\Sigma_w^{-1/2}\bar{\mu}'\|} \|\Sigma_w^{-1/2}\bar{\mu}'\| = \|\Sigma^{-1/2}\bar{\mu}'\|
\]

for every \( \bar{\mu}' \).

From the rotation invariance of \( \phi_{\pi\Sigma} \),

\[
\varphi_{\pi\Sigma}(\mu) = \varphi_{\pi\Sigma}(\mu^*) \\
= E_{\Sigma,\tilde{\Sigma}}[\int N(z; \mu^*, \Sigma) \log \int N(z; \tilde{\mu}, \Sigma)\pi(\Sigma^{-1/2}\tilde{\mu})d\tilde{\mu}dz] \\
= E_{\Sigma,\tilde{\Sigma}}[\int N(\tilde{z}; \Sigma^{-1/2}\mu^*, I_d) \log \int N(\tilde{z}; \tilde{\mu}', I_d)\pi(\tilde{\mu}')d\tilde{\mu}'d\tilde{z}] \\
= E_{\Sigma,\tilde{\Sigma}}[\int N(\tilde{z}; \tau \Sigma_w^{-1/2}\mu^*, I_d) \log \int N(\tilde{z}; \tilde{\mu}', I_d)\pi(\tilde{\mu}')d\tilde{\mu}'d\tilde{z}] \\
= E_{\Sigma,\tilde{\Sigma}}[\int N(\tilde{z}; \Sigma_w^{-1/2}\mu^*, \tau^{-2}I_d) \log \int N(\tilde{z}; \tilde{\mu}', \tau^{-2}I_d)\pi(\tau\tilde{\mu}')d\tilde{\mu}'d\tilde{z}] \\
\leq E_{\Sigma,\tilde{\Sigma}}[\int N(\tilde{z}; \Sigma_w^{-1/2}\mu^*, I_d) \log \int N(\tilde{z}; \tilde{\mu}', I_d)\pi(\tau\tilde{\mu}')d\tilde{\mu}'d\tilde{z}] \\
= E_{\Sigma,\tilde{\Sigma}}[\int N(\bar{z}; \mu^*, \Sigma_w) \log \int N(\bar{z}; \bar{\mu}', \Sigma_w)\pi(\tau \Sigma_w^{-1/2}\bar{\mu}')d\bar{\mu}'d\bar{z}] \\
\]

Here, inequality (12) is given by Theorem 2.4 (ii).
Since every rotation invariant superharmonic function is radially nonincreasing,
\[ \pi(\tau^{w-1/2}\tilde{\mu}') \leq \pi(\Sigma^{-1/2}\tilde{\mu}') . \]
From this inequality,
\[
E_{\Sigma, \tilde{\Sigma}} \left[ \int N(\tilde{z}; \mu^*, \Sigma_w) \log \int N(\tilde{z}; \tilde{\mu}', \Sigma_w) \pi(\tau^{w-1/2}\tilde{\mu}') d\tilde{\mu}' d\tilde{z} \right] \\
\leq E_{\Sigma, \tilde{\Sigma}} \left[ \int N(\tilde{z}; \mu^*, \Sigma_w) \log \int N(\tilde{z}; \tilde{\mu}', \Sigma_w) \pi(\Sigma^{-1/2}\tilde{\mu}') d\tilde{\mu}' d\tilde{z} \right] \\
= \varphi^w_{\pi_{\Sigma}}(\mu^*) \\
= \varphi^w_{\pi_{\tilde{\Sigma}}}(\mu) \\
(13)
\]
In particular, if \( \pi \) is not constant, inequality (12) holds strictly. Therefore, \( p_{\Sigma} \) dominates \( p_{\tilde{\Sigma}} \).

From Lemma 2.3, \( p_{\Sigma} \) is proved to be minimax.

**Corollary 2.6**
Assume \( d \geq 3 \). Let \( p(\Sigma) \) and \( \tilde{p}(\tilde{\Sigma}) \) be rotation invariant continuous functions. If \( \pi \) is a rotation invariant superharmonic prior, Bayesian predictive density \( p_{\Sigma}(\tilde{y}|y) \) is minimax under \( R_{KL} \).

Theorem 2.5 and Corollary 2.6 can be generalized to the case with a semi-positive definite future covariance matrix \( \tilde{\Sigma} \). Let \( \tilde{\Sigma} \) be a \( d \)-dimensional semi-positive matrix whose rank is \( k > 0 \). Then there is a \( d \times k \) matrix \( L \) satisfying \( \tilde{\Sigma} = LL^\top \). Let \( \{a_i\}_{i=1}^{d-k} \) be a set of orthogonal normalized vectors that are orthogonal to each column vector of \( L \), i.e. \( L^\top a_i = 0 \) and \( a_i^\top a_j = \delta_{ij} \) for \( i, j = 1, \ldots, d-k \). Define the Normal distribution with semi-positive definite covariance matrix by
\[
N_d(y; \mu, \tilde{\Sigma}) = \frac{1}{(2\pi)^{k/2}|L^\top L|^{1/2}} \exp \left( -\frac{(y - \mu)^\top \tilde{\Sigma}^\dagger (y - \mu)}{2} \right) \prod_{i=1}^{d-k} \delta(a_i^\top (y - \mu))
\]
where \( \tilde{\Sigma}^\dagger \) is Moore-Penrose pseudo-inverse of \( \tilde{\Sigma} \).

From the results of functional analysis, \( N_d(y; \mu, \Sigma) \) for any semi-positive definite \( \tilde{\Sigma} \) is equivalent to \( \lim_{\epsilon \to 0} N_d(y; \mu, \Sigma + \epsilon I_d) \) as a functional on Schwartz functions of \( y \).

Using this equivalence and the bounded convergence theorem, equation (11) is valid for a semi-definite future covariance matrix if we define \( \Sigma_w := (\Sigma^{-1} + \tilde{\Sigma}^\dagger)^{-1} \). Because \( \tilde{\Sigma}^\dagger \neq 0 \), \( \tau \) defined by (11) takes value in \( (0, 1) \). Therefore, Theorem 2.5 and Corollary 2.6 hold for each semi-definite future covariance matrix \( \tilde{\Sigma} \).

### 3 Prior distributions depending on the future covariance

In this section, we consider prior distributions depending on the future covariance matrix. Theorem 3.2 below says that every Bayesian prediction with an adequately metrized
prior dominates that based on the uniform prior. Although the assumption that priors can depend on the future covariance may seem strange, this assumption is natural when we consider the linear regression problem, as we will see in Section 4.

First, we generalize Theorem 3.2 to the case with non-identity covariances. Let $\mu$ and $z$ be vectors in $\mathbb{R}^d$ and let $\Sigma \in \mathbb{R}^{d\times d}$ be a positive definite matrix.

Let $\Sigma_1$ and $\Sigma_2$ be positive definite matrices such that $\Sigma_1 \preceq \Sigma_2$. An orthogonal matrix $U$ and a diagonal matrix $\Lambda$ are given by a diagonalization of $\Sigma_1^{1/2} \Sigma_2^{-1} \Sigma_1^{1/2}$, i.e. $\Sigma_1^{1/2} \Sigma_2^{-1} \Sigma_1^{1/2} = U^T \Lambda U$. Let $A^* := \Sigma_1^{1/2} U^T (\Lambda^{-1} - I_d)^{1/2}$.

**Proposition 3.1** If $\pi$ is a prior s.t. $\pi(A^* \mu)$ is a superharmonic function of $\mu$, then

$$
\phi_\pi(\mu, \Sigma_1) \geq \phi_\pi(\mu, \Sigma_2)
$$

for any $\mu \in \mathbb{R}^d$. Inequality (14) becomes strict if $\pi$ is not a constant function.

The following theorem is a direct result of Proposition 3.1.

**Theorem 3.2** If $\pi(A^* \mu)$ is a superharmonic function of $\mu$, then $R_{KL}(\pi, \mu) \leq R_{KL}(\pi_1, \mu)$. Furthermore, if $\pi$ is not a constant function, a Bayesian predictive distribution $p_\pi$ dominates the one with the uniform prior $\pi_1$.

Note that $\pi(A^* \mu)$ can be superharmonic only if $\text{rank}(\Sigma_2 - \Sigma_1) \geq 3$.

**Proof of Proposition 3.1 and Theorem 3.2** Assume $0 \prec \Sigma_1 \preceq \Sigma_2$ and let $\Sigma_1^{1/2} \Sigma_2^{-1} \Sigma_1^{1/2} = U^T \Lambda U$ be a diagonalization. Then,

$$
\phi_\pi(\mu, \Sigma) = \int \log \left\{ \int \pi(\nu) \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp \left( -\frac{(x - \nu)^T \Sigma^{-1} (x - \nu)}{2} \right) d\nu \right\} \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp \left( -\frac{(x - \mu)^T \Sigma^{-1} (x - \mu)}{2} \right) dx.
$$

Let $\tilde{x} := U^{1/2} x$, $\tilde{\mu} = U^{1/2} \mu$, and $\tilde{\nu} = U^{1/2} \nu$. By $|\Sigma_2|^{-1/2} |\Sigma_1|^{1/2} = |\Lambda|^{1/2}$,

$$
\phi_\pi(\mu, \Sigma_2) = \int \log \left\{ \int \pi(\Sigma_1^{1/2} U^T \nu) \frac{1}{(2\pi)^{d/2} |\Lambda|^{1/2}} \exp \left( -\frac{(\tilde{x} - \tilde{\nu})^T \Lambda^{-1} (\tilde{x} - \tilde{\nu})}{2} \right) d\tilde{\nu} \right\} \frac{1}{(2\pi)^{d/2} |\Lambda|^{1/2}} \exp \left( -\frac{(\tilde{x} - \tilde{\mu})^T \Lambda^{-1} (\tilde{x} - \tilde{\mu})}{2} \right) d\tilde{x}
$$

$$
= \phi_{\pi(\Sigma_1^{1/2} U^T \cdot)}(\tilde{\mu}, \Lambda^{-1}),
$$

(15)

where $\pi(\Sigma_1^{1/2} U^T \cdot)$ is a prior distribution whose density function is represented by $\pi(\Sigma_1^{1/2} U^T \mu)$ with a prior density $p_\pi$.

Putting $\Sigma_2 = \Sigma_1$, we get

$$
\phi_\pi(\mu, \Sigma_1) = \phi_{\pi(\Sigma_1^{1/2} U^T \cdot)}(\tilde{\mu}, I_d),
$$

(16)
where \( I_d \) is the \( d \)-dimensional identity matrix.

We denote each diagonal component of \( \Lambda \) by \( \lambda_i \). Now \( 0 < \lambda_i \leq 1 \) for each \( i \) since \( \Sigma_1 \preceq \Sigma_2 \). Let \( a_i(t) := 1 + t(\lambda_i^{-1} - 1) \) and \( A := \text{diag}(a_i) \). Then

\[
\phi_\pi(\mu, \Sigma_2) - \phi_\pi(\mu, \Sigma_1) = \phi_\pi((\Sigma_1^{-1/2}U^\top)(\hat{\mu}, \Lambda^{-1}) - \phi_\pi((\Sigma_1^{-1/2}U^\top)(\hat{\mu}, I_d))
= \int_{t=0}^1 \sum_{i=1}^d \frac{\partial a_i(t)}{\partial t} \frac{\partial}{\partial a_i} \phi_\pi((\Sigma_1^{-1/2}U^\top)(\hat{\mu}, A)} \bigg|_{a_i(t)} \, dt
= \int_{t=0}^1 \sum_{i=1}^d \frac{\partial \hat{a}_i(t)}{\partial t} \frac{\partial}{\partial \hat{a}_i} \phi_\pi(\Lambda^{\ast})(\hat{\mu}, \tilde{A}) \bigg|_{\tilde{a}_i(t)} \, dt
= \int_{t=0}^1 \sum_{i=1}^d \frac{\partial}{\partial \hat{a}_i} \phi_\pi(\Lambda^{\ast})(\hat{\mu}, \tilde{A}) \bigg|_{\tilde{a}_i(t)} \, dt
\]

where \( \tilde{a}_i := (\lambda_i^{-1} - 1)^{-1}a_i \) and \( \hat{\mu} := (\Lambda^{-1} - I_d)^{-1/2}\hat{\mu} \).

By assumption, \( \pi(\Lambda^{\ast}) \) for \( \Lambda^{\ast} = \Sigma_1^{-1/2}U^\top(\Lambda^{-1} - I_d)^{1/2} \) is superharmonic. Now it is sufficient to prove Lemma 3.3 iii) below. \( \square \)

**Lemma 3.3**

i) \( \Sigma_i \frac{\partial}{\partial \Sigma_i} N(x; \mu, A) = \frac{1}{2} \Delta N(x; \mu, A) \).

ii) \( \int f(x-t) \, d\mu(t) \) is a superharmonic function of \( x \) if \( f \) is a superharmonic function and \( \mu \) is a positive measure on \( \mathbb{R}^d \).

iii) \( \Sigma_i \frac{\partial}{\partial a_i} \phi_\pi(\mu, A) \leq 0 \) for any \( \mu \in \mathbb{R}^d \), \( a_i > 0 \), and \( A = \text{diag}(a_i) \) for each superharmonic prior \( \pi \).

**Proof of Lemma 3.3**

Lemma i) follows from direct calculation. For a proof of ii), see Problem 1.7.16 of Lehmann & Casella (1998).

\[
\sum_{i=1}^d \frac{\partial}{\partial a_i} \phi_\pi(\mu, A) = \sum_{i=1}^d \frac{\partial}{\partial a_i} \int \log \left\{ \int \pi(\nu) N(x; \nu, A) \, d\nu \right\} N(x; \mu, A) \, dx
= \int \sum_{i=1}^d \frac{\partial}{\partial a_i} \int \pi(\nu) N(x; \nu, A) \, d\nu \int \pi(\nu) N(x; \nu, A) \, d\nu N(x; \mu, A) \, dx
+ \int \log \left\{ \int \pi(\nu) N(x; \nu, A) \, d\nu \right\} \sum_{i=1}^d \frac{\partial}{\partial a_i} N(x; \mu, A) \, dx.
\]

Now,

\[
\sum_{i=1}^d \frac{\partial}{\partial a_i} \int \pi(\nu) N(x; \nu, A) \, d\nu = \frac{1}{2} \Delta \int \pi(\nu) N(x; \nu, A) \, d\nu \leq 0
\]

10
from Lemma 3.3 i) and ii). Thus, the first term of the right-hand side of (17) is non-positive. The second term of the right-hand side of (17) becomes

\[
\frac{1}{2} \int \log \left\{ \int \pi(\nu) N(x; \nu, A) d\nu \right\} \Delta N(x; \mu, A) dx \\
= \frac{1}{2} \int \Delta \log \left\{ \int \pi(\nu) N(x; \nu, A) d\nu \right\} N(x; \mu, A) dx
\]

(18)

by i) and the self-adjoint property of the Laplacian. Since the logarithm of a superharmonic function is superharmonic (see Problem 1.7.16 of Lehmann & Casella (1998)), (18) is non-positive from ii). Thus Lemma 3.3 iii) is proved. □

Example 3.4 A rescaled Stein prior

\[
\pi_{S, \Sigma_2 - \Sigma_1}(\mu) = \| (\Sigma_2 - \Sigma_1)^{-1/2} \mu \|^{-(d-2)}
\]
satisfies the condition of Proposition 3.1 and Theorem 3.2. This is because

\[
\| (\Sigma_2 - \Sigma_1)^{-1/2} \mu \|^{-(d-2)} = (\mu^\top \Sigma_1^{-1/2} (\Sigma_1^{-1/2} \Sigma_2 \Sigma_1^{-1/2} - I_d)^{-1} \Sigma_1^{-1/2} \mu)^{-(d-2)/2} \\
= (\mu^\top \Sigma_1^{-1/2} U^\top (\Lambda^{-1} - I_d)^{-1} U \Sigma_1^{-1/2} \mu)^{-(d-2)/2}.
\]

Thus, \( \pi_{S, \Sigma_2 - \Sigma_1}(A^* \mu) = \pi_S(\mu). \)

4 Application to the Normal linear regression problem

In this section, we apply the results in the previous section to the Normal linear regression problem.

Consider a Normal linear model

\[
y = X^\top \beta + \epsilon, \hspace{1cm} (19)
\]

\[
\epsilon \sim N_p(0, \sigma^2 I_p),
\]

where the target variable \( y \) is a \( p \) dimensional vector, \( X \) is a \( d \times p \) matrix composed of the explanatory variables, \( \sigma^2 > 0 \) is an unknown variance, and \( \beta \) is an unknown \( d \)-dimensional vector. When the rightmost column of \( X \) is the constant vector \((1, \ldots, 1)^\top\), the model (19) is a model with a intercept, \( y = X^\top \beta + \beta_0 + \epsilon. \)

We suppose that a future sample \( \tilde{y} \) is generated by

\[
\tilde{y} = \tilde{X}^\top \beta + \tilde{\epsilon}, \hspace{1cm} (20)
\]

\[
\tilde{\epsilon} \sim N_p(0, \tilde{\sigma}^2 I_p),
\]
where $\tilde{y}$ is a $\tilde{p}$ dimensional vector, $\tilde{X}$ is a $d \times \tilde{p}$ matrix, and $\sigma^2 > 0$ is an unknown variance.

In the present work, we assume that $p \geq d$ and $XX^\top$ is regular, however neither $\tilde{p} \geq d$ nor regularity of $\tilde{X} \tilde{X}^\top$ is necessary.

We consider the prediction problem for the linear regression models (19) and (20) with KL risk function

$$\tilde{R}_{KL}(\beta, \tilde{p}_\pi, X, \tilde{X}) := \int p(y|X; \beta, \sigma^2) D(p(\tilde{y}|\tilde{X}; \beta, \tilde{\sigma}^2)\|p_\pi(\tilde{y}|\tilde{X}, y, X; \sigma^2, \tilde{\sigma}^2)) dy.$$ 

and partial Bayesian risk function with prior $p(X)$ and $\tilde{p}(\tilde{X})$:

$$\tilde{R}_{KL}(\beta, \tilde{p}_\pi) := \int p(X)\tilde{p}(\tilde{X}) \tilde{R}_{KL}(\beta, \tilde{p}_\pi, X, \tilde{X}) dX d\tilde{X}.$$ 

Note that we do not assume any prior for $\beta$.

Next, the regression model is reduced to a Normal model discussed in Section 2. Let $y_1 := (XX^\top)^{-1}Xy$ and $y_2 := y - X^\top(XX^\top)^{-1}Xy$. Then

$$\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp \left( -\frac{(X^\top \beta - y)^\top XX^\top (X^\top \beta - y)}{2\sigma^2} \right) dy_1 dy_2,$$

where

$$\Sigma := \sigma^2(XX^\top)^{-1}$$

and $g(y_2; \sigma^2)$ is a density function of $y_2$ that is independent of $y_1$ and $\beta$.

When $y$ is given, $y_1$ is a sufficient statistic of $\beta$, the maximum likelihood estimator, and the least-square estimator of $\beta$. Thus, the regression model (19) is reduced to a Normal model

$$p(y_1; \beta, \Sigma) = N_d(y_1; \beta, \Sigma).$$

Similarly, the regression model (20) for the future samples is reduced to a Normal model

$$\tilde{p}(\tilde{y}_1; \beta, \tilde{\Sigma}) = N_d(\tilde{y}_1; \beta, \tilde{\Sigma})$$

with semi-positive definite covariance matrix. Here $\tilde{y}_1 := (\tilde{X} \tilde{X}^\top)^\dagger \tilde{X} \tilde{y}$ and

$$\tilde{\Sigma} := \tilde{\sigma}^2(\tilde{X} \tilde{X}^\top)^\dagger.$$ 

The KL risk of the Bayesian predictive density with a prior $\pi(\beta)$ for the regression problem becomes
Bayesian prediction for the Normal regression problem.

To a prediction problem (22) and (23). Using the result in Section 2, we construct a risk

Theorem 4.1

Define Σ, ˜Σ, and Σw

\[ R_{KL}(p_\pi, \beta) = \int p(y \mid X; \beta, \sigma^2)D(p(\tilde{y} \mid \tilde{X}; \beta, \tilde{\sigma}^2)\|p_\pi(\tilde{y} \mid \tilde{X}, y, X)dy \]

\[ = \int p(y \mid X; \beta, \sigma^2) \int \frac{N_d(y_1; \beta, \tilde{\Sigma}) \pi(y_2; \tilde{\sigma}^2)}{\int N_d(y_1; \beta, \tilde{\Sigma}) \pi(y_2; \tilde{\sigma}^2) N_d(y_1; \beta, \Sigma) \pi(y_2; \sigma^2) \pi(\beta) d\beta} dy_1 \int \frac{N_d(\tilde{y}_2; \tilde{\Sigma}) g(\tilde{y}_2; \tilde{\sigma}^2)}{\int N_d(\tilde{y}_2; \tilde{\Sigma}) g(\tilde{y}_2; \tilde{\sigma}^2) N_d(y_1; \beta, \Sigma) g(y_2; \sigma^2) \pi(\beta) d\beta} dy_2 dy_1 \]

\[ = \int \frac{N_d(y_1; \beta, \Sigma) \pi(y_2; \sigma^2) \pi(\beta) d\beta}{\int N_d(y_1; \beta, \Sigma) \pi(y_2; \sigma^2) \pi(\beta) d\beta} \int \frac{N_d(\tilde{y}_2; \tilde{\Sigma}) g(\tilde{y}_2; \tilde{\sigma}^2)}{\int N_d(y_1; \beta, \Sigma) g(y_2; \sigma^2) \pi(\beta) d\beta} dy_2 \]

\[ = R_{KL}(\pi(y_1 \mid y_1)) := \frac{\int N_d(y_1; \beta, \tilde{\Sigma}) N_d(y_1; \beta, \Sigma) \pi(\beta) d\beta}{\int N_d(y_1; \beta, \Sigma) \pi(\beta) d\beta} \]

where

\[ q_\pi(\tilde{y}_1 \mid y_1) := \frac{\int N_d(\tilde{y}_1; \beta, \tilde{\Sigma}) N_d(y_1; \beta, \Sigma) \pi(\beta) d\beta}{\int N_d(y_1; \beta, \Sigma) \pi(\beta) d\beta} \]

Theorem 4.1

Let \( \pi_\Sigma(\beta) = \pi(\Sigma^{-1/2} \beta) \). Let \( p(X) \) and \( \tilde{p}(\tilde{X}) \) be rotation invariant continuous functions.

(i) If \( \pi \) is a non-constant rotation invariant superharmonic function, then the Bayesian predictive density \( p_\Sigma \) with a prior \( \pi_\Sigma \) dominates \( p_1 \) with the uniform prior \( \pi_1 \) under the risk \( \tilde{R}_{KL} \).

(ii) If \( \pi \) is a rotation invariant superharmonic function, then \( p_\Sigma \) is minimax under the KL risk \( \tilde{R}_{KL} \).

Proof. If \( p(X) \) and \( \tilde{p}(\tilde{X}) \) are rotation invariant, then the distributions of \( \Sigma = \sigma^2(XX^\top)^{-1} \) and \( \Sigma_w = (\sigma^{-2}(XX^\top) + \tilde{\sigma}^{-2}(\tilde{X}\tilde{X}^\top))^{-1} \) are also rotation invariant.

From Theorem 2.5 and Corollary 2.6, the theorem is derived directly. □

The assumption of rotation invariance of \( p(x) \) and \( p(\tilde{x}) \) is sometimes not realistic. If we consider priors depending on the future explanatory variables, we can construct a Bayesian prediction dominating the one with the uniform prior and, therefore, being a minimax prediction.

Define an orthogonal matrix \( U \) and a diagonal matrix \( \Lambda \) by a diagonalization of \( \Sigma_u^{-1/2} \Sigma_u^{-1} \Sigma_u^{-1/2} \), i.e., \( \Sigma_u^{-1/2} \Sigma_u^{-1} \Sigma_u^{-1/2} = U^\top \Lambda U \). Let \( A^* := \Sigma_u^{-1/2} U^\top (\Lambda^{-1} - I_d)^{1/2} \). Then the following theorem is a direct consequence of Theorem 3.2.
Theorem 4.2 (i) If $\pi(A^*\beta)$ is superharmonic w.r.t. $\beta$ and $\pi$ is non-constant, then the Bayesian prediction based on the prior $\pi$ dominates that based on the uniform prior. (ii) If $\pi(A^*\beta)$ is superharmonic, then the Bayesian prediction based on the prior $\pi$ is minimax.

Note that $\pi(A^*\beta)$ can be superharmonic only if the number of the future samples is more than two.

5 Experimental results

We show several experimental results on the Bayesian prediction with shrinkage priors for regression problems.

Figures 1 and 2 are examples of the regression problem. We consider the five dimensional Normal regression models, without an intercept term (Figure 1) and with an intercept term (Figure 2). We set the true parameter $\beta = (1, 0, \ldots, 0) \in \mathbb{R}^5$. An explanatory variable $X$ is sampled from the uniform distribution $U([-1, 1]^{5\times10})$ and corresponding target variable $y$ is sampled from $N_{10}(X^T\beta, I_{10})$. The target variable $\tilde{y}$ for each explanatory variable $\tilde{x} = (\tilde{x}_1, 0, \ldots, 0)$ where $\tilde{x}_1 \in [0, 2]$ is predicted by the Bayesian predictive density based on the uniform prior $\pi_1$ and that based on a rescaled Stein prior $\pi_{S;\Sigma}$ where $\Sigma = XX^T$.

Two lines in Figures 1 and 2 are $y = \tilde{\beta}_\pi^T\tilde{x}$ for $\pi_1$ and $\pi_{S;\Sigma}$, respectively, where $\tilde{\beta}_\pi$ is the posterior mean with prior $\pi$. In both figures, the slope of the line with rescaled Stein prior is smaller than the one with the uniform prior because the slope parameter $\beta$ is shrunk to $\beta = 0$. Moreover in Figure 2, the intercept parameter is also shrunk.

Figure 3 shows the distribution functions of the predictive density $p_1(\tilde{y}|\tilde{x}, y, X)$ with $\pi_1$ and $p_{S;\Sigma}(\tilde{y}|\tilde{x}, y, X)$ with $\pi_{S;\Sigma}$, respectively, for $\beta = \tilde{x} = e_1 := (1, 0, \ldots, 0) \in \mathbb{R}^d$. 

Figure 1: An example of the Bayesian prediction based on the uniform prior and a rescaled Stein prior for the Normal regression model without an intercept term.
Figure 2: An example of the Bayesian prediction based on the uniform prior and a rescaled Stein prior for the Normal regression model with an intercept term $\beta_0 = 1$.

Next, we show an example of Bayesian prediction whose prior depends on the explanatory variables of future samples. We set $x_1 = (\sqrt{3}/2, 1/2, 0)^\top$, $x_2 = (\sqrt{3}/2, -1/2, 0)^\top$, $x_3 = (0, 0, 1)^\top$, $y_1 = \sqrt{3}/2 + 1/2$, $y_2 = \sqrt{3}/2 - 1/2$ and $y_3 = 0$. Figure 5 is a graph of $E_{\pi_{S,A^*}}[\tilde{y}|\tilde{x}, y, x]$ for each value of $\tilde{x} = (\tilde{x}(1), \tilde{x}(2), 0) \in \mathbb{R} \times \mathbb{R} \times \{0\}$ with the rescaled Stein prior $\pi_{S,A^*}$. Here, the Bayesian estimation based on the uniform prior corresponds to the MLE $\hat{\beta} = (1, 1, 0)$, i.e. $y = x^{(1)} + x^{(2)}$.

We can see that the amount of shrinkage by the Bayesian prediction increases as the direction of $\tilde{x}$ becomes closer to $x^{(1)}$ than $x^{(2)}$, i.e. $\tilde{x}^\top e_1$ becomes larger than $\tilde{x}^\top e_2$. This fact is intuitively explained as follows: when explanatory variables of training samples are closer to $x^{(1)}$, $\tilde{x}$ whose direction is close to $x^{(1)}$ has more information than ones whose direction is close to $x^{(2)}$. Thus $\tilde{x}$ close to $x^{(1)}$ need not be shrunk.

Figure 4 shows the risk functions of $p_I$ and $p_\Sigma$ for $d = 3, 5, 7, 9$ and $\|\beta\| \in [0, 2]$. The model has no intercept term. Here we assume that the columns of $X$ and $\tilde{X}$ are independently sampled from $N_{10}(0, I_{10})$.

Figure 6 compares five predictive densities: the Bayesian predictive density based on $p_I$ and $p_\Sigma$, the ridge regression prior with regularization parameters $\lambda \in \{\sqrt{10}, 10\}$, and the plug-in density of MLE.

The ridge regression prior is

$$
\pi_{RR}(\beta; \lambda) = \frac{\lambda^{d/2}}{(2\pi)^{d/2}} \exp\left(-\lambda \|\beta\|^2/2\right)
$$

with a regularization parameter $\lambda > 0$. We note that the posterior mean with the ridge regression prior is equivalent to the ridge regression estimator

$$
\hat{\beta}_{RR} = (XX^\top + \lambda I)^{-1}Xy.
$$

When $\|\beta\|$ is close to 0, the center of shrinkage, the risk based on the ridge regression prior $\pi_{RR}$ becomes smaller than that based on $\pi_\Sigma$. However, when $\|\beta\|$ increases, the
Figure 3: Distribution functions of \( p_I(\tilde{y} | \tilde{x}, y, X) \) and \( p_{S;\Sigma}(\tilde{y} | \tilde{x}, y, X) \) where \( \beta = \tilde{x} = e_1 := (1, 0, \ldots, 0) \in \mathbb{R}^d \), \( X \) is a sample from \( U([-1, 1]^{d_\times p}) \), \( y \) is a sample from \( N_p(y; X^T \beta, 10I_p) \), and \( \tilde{p}(\tilde{y} | \tilde{x}) = N(\tilde{y}; \tilde{x}^T \beta, 10) \). We generate \( 10^4 \) samples of \( \tilde{y} \) from each predictive distribution. Sample means of \( P_I \) and \( P_{S;\Sigma} \) are 1.3134 and 0.6898, respectively.

prediction with \( \pi_{RR} \) becomes worse than the one with \( \pi_I \) and even worse than the plug-in distribution of the MLE.

6 Conclusions and discussions

In this paper, we considered the multivariate Normal model with an unknown mean and a known covariance. The covariance matrix can be changed after the first sampling. We assumed rotation invariant priors of the covariance matrix and the future covariance matrix. We showed that the shrinkage predictive density with the rescaled rotation invariant superharmonic priors is minimax under the Kullback-Leibler risk. Moreover, if the prior is not constant, Bayesian predictive density based on the prior dominates the one with the uniform prior.

In this case, the rescaled priors are independent of the covariance matrix of future samples. Therefore, we can calculate the posterior distribution and the mean of the predictive distribution (i.e. the posterior mean and the Bayesian estimate for quadratic loss) based on some of the rescaled Stein priors without knowledge of future covariance. Since the predictive density with the uniform prior is minimax, the one with each rescaled Stein prior is also minimax.

Next we considered Bayesian predictions whose prior can depend on the future covariance. In this case, we proved that the Bayesian prediction based on a rescaled superharmonic prior dominates the one with the uniform prior without assuming the rotation invariance.

Applying these results to the prediction of response variables in the Normal regres-
Figure 4: The risk difference of $p_I$ and $p_{S, \Sigma}$ for $d = 3, 5, 7, 9$ and $\|\beta\| \in [0, 2]$. We generate $10^4$ independent samples of $X$ and $\tilde{X}$ from $N_{10}(0, I_{10})$. Each line in the figure represents the sample mean of risk difference $R_{KL}(\beta, p_I) - R_{KL}(\beta, p_{S, \Sigma})$. Each error bar represents the standard deviation.

sion model, we show that there exists the prior distribution such that the corresponding Bayesian predictive density dominates that based on the uniform prior. Since the prior distribution is independent of future explanatory variables, both the posterior distribution and the mean of the predictive distribution are independent of the future explanatory variables.

The robustness of some shrinkage methods as Stein estimators has been studied (see, for example, the bibliography in Robert (2001)). The Stein effect has robustness in the sense that it depends on the loss function rather than the true distribution of the observations. Our result shows that the Stein effect has robustness with respect to the covariance of the true distribution of the future observations.

As the dimension of the model becomes large, the risk improvement by the shrinkage with the rescaled Stein prior $\pi_\Sigma$ increases as in Figure 4. An important example of the high dimensional model is the kernel methods (see Hastie et al. (2001)). As noted in Cristianini & Shawe-Taylor (2000), the feature space of kernel methods is a kernel reproducing Hilbert space whose dimension is as large as the sample size. Therefore Bayesian prediction based on shrinkage priors could be efficient for kernel methods. This is a future problem.

7 Acknowledgment

The authors appreciate Mr. Vu, Vincent Q. for precious comments on an earlier version of this paper.
A Finiteness of the marginal distribution

Here, we prove finiteness of the marginal distribution $m_\pi(\mu, \Sigma)$.

Lemma A.1 If $\pi$ is a superharmonic prior density function, the marginal distribution $m_\pi(x, \Sigma)$ is finite for every vector $x \in \mathbb{R}^d$ and positive definite matrix $\Sigma \in \mathbb{R}^{d \times d}$.

Proof. Fix a vector $x \in \mathbb{R}^d$ From the definition of superharmonic functions, $\pi \not\equiv \infty$. Thus, $\exists x_0 \in \mathbb{R}^d$ s.t. $\pi(x_0) < \infty$. If we set $\tilde{\pi}(\mu) := \pi(\mu + x_0)$, then $\tilde{\pi}$ is superharmonic and $\tilde{\pi}(0) < \infty$.

Let $\lambda_{\text{max}}$ be the maximal eigenvalue of $\Sigma$ and $r_0 := \|x + x_0\|$, then

$$m_\pi(x, \Sigma) \leq \int \exp \left( -\frac{\|x + x_0 - \mu\|^2}{2\lambda_{\text{max}}} \right) \tilde{\pi}(\mu) d\mu$$

$$\leq \int_{\|\mu\| \leq 2r_0} \exp \left( -\frac{\|x + x_0 - \mu\|^2}{2\lambda_{\text{max}}} \right) \tilde{\pi}(\mu) d\mu + \int_{\|\mu\| > 2r_0} \exp \left( -\frac{\|\mu\|^2}{8\lambda_{\text{max}}} \right) \tilde{\pi}(\mu) d\mu$$

(26)

The first term of the right-hand side of (26) is finite because the integral of a superharmonic function over a compact subspace of $\mathbb{R}^d$ is finite (see Theorem 4.10 of Helms (1969)).

The second term is also finite because

$$\sum_{n=2}^{\infty} \int_{nr_0 < \|\mu\| \leq (n+1)r_0} \exp \left( -\frac{\|\mu\|^2}{8\lambda_{\text{max}}} \right) \tilde{\pi}(\mu) d\mu \leq C \sum_{n=2}^{\infty} \exp \left( -\frac{(nr_0)^2}{8\lambda_{\text{max}}} \right) \tilde{\pi}(0) \{n + 1\}^d$$

for a positive constant $C$. Here we used a fact $\int_{\|\mu\| < r} \tilde{\pi}(\mu) d\mu < C\tilde{\pi}(0)r^d$ by Theorem 4.9 of Helms (1969). Therefore, $m_\pi(x, \Sigma) < \infty$. □
Figure 6: Comparison of the risk values by five predictive densities: the Bayesian predictive density based on $p_I$ and $p_{\Sigma}$, the ridge regression prior with regularization parameters $\lambda = 10$ and $\lambda = \sqrt{10} = 3.16$, and the plug-in density of the MLE. The model is five dimensional and has no intercept term. We generate $10^4$ independent samples of $X$ and $\tilde{X}$ from $N_{10}(0, I_{10})$. Each line in the figure represents the sample mean of the risk $R_{KL}(\beta, \hat{p})$ for the predictive density $\hat{p}$.

From this lemma, we see the assumption $m_{\pi}(z, v_{Id}) < \infty$ in Theorem 2.4 (ii) is redundant.

References

Corcuera, J. M. & Giummolé, F. (2000). First-order optimal prediction densities. In Applications of differential geometry to econometrics, P. Marriott & M. Salmon, eds. Cambridge: Cambridge University Press, pp. 214–229.

Cristianini, N. & Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines. Cambridge University Press.

George, E. I., Liang, F. & Xu, X. (2006). Improved minimax prediction under Kullback-Leibler loss. Annals of Statistics 34, 78–91.

Hastie, T., Tibshirani, R. & Friedman, J. (2001). The elements of statistical learning – Data mining, inference, and prediction. Springer series in statistics. New York: Springer.

Helms, L. L. (1969). Introduction to Potential Theory. New York: Wiley-Interscience.

Komaki, F. (1996). On asymptotic properties of predictive distributions. Biometrika 83, 299–313.
Komaki, F. (2001). A shrinkage predictive distribution for multivariate Normal observ-
ables. *Biometrika* **88**, 859–864.

Komaki, F. (2006). Shrinkage priors for bayesian prediction. *Annals of Statistics* **34**, 808–819.

Lehmann, E. L. & Casella, G. (1998). *Theory of point estimation*. New York: Springer, 2nd ed.

Liang, F. & Barron, A. (2004). Exact minimax strategies for predictive density es-
   timation, data compression, and model selection. *Ieee Transactions on Information Theory* **50**, 2708–2726.

Murray, G. D. (1977). A note on the estimation of probability density functions. 
   *Biometrika* **64**, 150–152.

Ng, V. M. (1980). On the estimation of parametric density functions. *Biometrika* **67**, 505–506.

Robert, C. P. (2001). *The Bayesian Choice*. New York: Springer-Verlag, 2nd ed.