Extended Plugin Densities for Curved Exponential Families

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Abstract

Extended plugin densities are proposed as predictive densities for curved exponential families. Bayesian predictive densities are often intractable in numerical calculations, although Bayesian predictive densities are optimal under the Bayes risk based on the Kullback–Leibler divergence. Curved exponential families are embedded in larger full exponential families and plugin densities in the full exponential families, which we call extended plugin densities, are considered. It is shown that the extended plugin density with the posterior mean of the expectation parameter of the full exponential family is optimal regarding the Bayes risk in the extended model. Several information-geometric results for extended plugin densities are obtained in parallel with those for Bayesian predictive densities. Choice of priors for extended plugin densities with Bayes estimators is investigated and a superharmonic condition for a prior to dominate the Jeffreys prior is obtained.

Keywords: Bayes, predictive density, information geometry

1 Introduction

Constructing predictive densities is a fundamental problem in statistical analysis, which aims to predict the behavior of future samples using past observations. Here, we consider a statistical model of a curved exponential family

\[ \mathcal{P} = \{ p(x; u) = s(x) \exp(\theta^i(u)x_i - \Psi(\theta(u))) \mid u := (u^a) \in U, \ a = 1, \ldots, d, \ i = 1, \ldots, m \}, \]

where \( U \subset \mathbb{R}^d \) and \( 1 \leq d \leq m \). Summation over a repeated index is automatically taken according to Einstein’s summation convention: if an index occurs as an upper and lower index in one term, then the summation is implied. Suppose that we have observations \( x^n = \{ x(1), x(2), \ldots, x(n) \} \) independently.
distributed according to a density $p(x; u) \in \mathcal{P}$. The objective is to provide the predictive density of $y = x(n + 1)$ which is independently distributed according to the same density $p(y; u)$.

We adopt the Kullback–Leibler divergence

$$D\{p(y; u); \hat{p}(y; u)\} = \int p(y; u) \log \frac{p(y; u)}{\hat{p}(y; u)} dy$$

as a loss function of a predictive density $\hat{p}(y; u)$. Then, the risk function and the Bayes risk with respect to a prior $\pi(u)$ are

$$E[D\{p(y; u); \hat{p}(y; u)\}] = \int p(x^n; u) D\{p(y; u); \hat{p}(y; u)\} dx^n,$$

and

$$\int \pi(u) \int p(x^n; u) D\{p(y; u); \hat{p}(y; u)\} dx^n du,$$

respectively.

There are two widely used methods for constructing predictive densities, namely (i) plugin densities with an estimator and (ii) Bayesian predictive densities. Plugin densities are constructed by plugging-in an estimator $\hat{u}(x^n)$ to the model, which is always included in $\mathcal{P}$. A Bayesian predictive density is defined by

$$\hat{p}(y \mid x^n) = \int p(y; u) p_\pi(u \mid x^n) du$$

where $p_\pi(u \mid x^n)$ is the posterior density

$$p_\pi(u \mid x^n) = \frac{p(x^n; u) \pi(u)}{\int p(x^n; u) \pi(u) du}$$

of $u$. In many examples, the Bayesian predictive density is not included in the model $\mathcal{P}$. Aitchison (1975) showed that the Bayesian predictive density is optimal about the Bayes risk in terms of the Kullback–Leibler divergence in the family of all probability densities, which we denote as $\mathcal{F}$. This result shows that the Bayesian predictive density is preferable to plugin densities about the Bayes risk.

However, the explicit form of the Bayesian predictive density is often intractable. In such examples, the numerical calculations of Bayesian predictive densities are burdensome because it involves integrations in the space of probability density functions. For multivariate normal models, Xu and Zhou (2011) proposed a class of empirical Bayes predictive densities to avoid intractable implementation of Bayesian predictive densities.

Here, we propose a distinct class of predictive densities and our focus is on models of curved exponential families including full exponential families such as multivariate normal models. The outline of the construction of our proposed predictive densities is as follows. We consider a full exponential family

$$\mathcal{E} = \{p(x; \theta) = s(x) \exp(\theta^i x_i - \Psi(\theta)) \mid \theta := (\theta^i) \in \Theta, \ i = 1, \ldots, m\} \ (\Theta \subseteq \mathbb{R}^m)$$

including $\mathcal{P}$. We refer to plugin densities in $\mathcal{E}$ as extended plugin densities, and investigate the properties of extended plugin densities. The inclusion relation is $\mathcal{P} \subseteq \mathcal{E} \subseteq \mathcal{F}$ and we consider the middle layer of
the three-layer structure. The coordinate system \( \theta = (\theta^i) \) \((i = 1, \ldots, m)\) is called natural parameters of exponential families. Another coordinate system \( \eta = (\eta_i) \) defined by

\[
\eta_i = E[x_i] = \frac{\partial}{\partial \theta^i} \Psi(\theta) \quad (i = 1, \ldots, m),
\]

is called expectation parameters.

In Section 2, we show that the extended plugin density with the posterior mean of \( \eta \) is optimal. Because the Bayesian predictive density is optimal (Aitchison, 1975) under the Bayes risk with the Kullback–Leibler loss, the Bayes risk of the Bayesian predictive density is not greater than that of the extended plugin density. However, evaluating extended plugin densities is less difficult than evaluating Bayesian predictive densities.

The properties of extended plugin densities are investigated from an information-geometric view in the following sections. There have been several previous studies on Bayesian predictive densities from information-geometric perspectives, such as Komaki (1996, 2006). The extended plugin of the Bayes estimator and the Bayesian predictive density are parallel in that the Bayesian predictive density is optimal in \( \mathcal{F} \) and the extended plugin of the Bayes estimator denoted herein as \( p(y; \hat{\eta}_\pi) \) is optimal in \( \mathcal{E} \) regarding the Bayes risk. We show that several geometric results of Bayesian predictive densities also hold for \( p(y; \tilde{\eta}_\pi) \) parallelly.

The rest of this paper is organized as follows. In Section 2, we explain the motivation for dealing with extended plugin densities, and the Bayes estimator of the extended model is obtained. In Section 3, the main results for extended plugin densities are obtained in information-geometric perspectives. In Section 4, we consider the choice of priors for \( p(y; \hat{\eta}_\pi) \) and superharmonic condition to dominate the plugin of the Bayes estimator based on the Jeffreys prior is obtained. Discussions are given in Section 5.

2 Extended plugin densities

We explain the motivation to deal with extended plugin densities. To construct predictive densities, plug-in densities with estimators of \( u \) (e.g., the maximum likelihood estimator \( \hat{u}_{\text{MLE}} \) or the Bayes estimator \( \hat{u}_\pi \)) are often used. The posterior mean of \( u \) is one of the choices for the estimator. The posterior mean of \( u \) for plug-in densities is

\[
\bar{u}_\pi := \frac{\int u p(x^n; u) \pi(du)}{\int p(x^n; u) \pi(du)},
\]

and when we consider the full exponential family, the posterior mean of \( \eta \) for extended plug-in densities is

\[
\bar{\eta}_\pi := \frac{\int \eta p(x^n; \eta(u)) \pi(du)}{\int p(x^n; \eta(u)) \pi(du)}.
\]

Note that \( \bar{\eta}_\pi(x^n) \neq \eta(\bar{u}_\pi(x^n)) \) in general. We show a simple example where the extended plugin of \( \bar{\eta}_\pi \) can be a natural choice of a predictive density.
Example (spike model): We consider inference of the eigenvector and the eigenvalue of the $l$-dimensional Gaussian density $N(0, \Sigma)$ with zero mean vector and unknown covariance matrix. The covariance matrix $\Sigma$ is supposed to be

$$\Sigma = \lambda \omega \omega^\top + I_l,$$

where the vector $\omega \in \mathbb{R}^l$ satisfies $\omega^\top \omega = 1$ and $\lambda > 0$. The eigenvalues of the matrix $\Sigma$ are $\lambda + 1, 1, \ldots, 1$, and $\omega$ is the first eigenvector. The model $\mathcal{P} = \{N(0, \Sigma) \mid (\omega, \lambda)\}$ is parametrized by $(\omega, \lambda)$, and the plugin density with the posterior mean $\omega_\pi, \lambda_\pi$ is $N(0, \Sigma(\omega_\pi, \lambda_\pi))$. On the other hand, the posterior mean of the matrix $\Sigma$ is another natural estimator of $\Sigma$ other than $\Sigma(\omega_\pi, \lambda_\pi)$. In principal component analysis, estimating the matrix and then decomposing the estimated matrix is a natural way to obtain estimators of eigenvalues and eigenvectors. The components of $\Sigma$ comprise the coordinate system $(\eta_i)$ of the extended statistical model $\mathcal{E} = \{N(0, \Sigma) \mid \Sigma\}$, thus $p(y; \Sigma_\pi)$ is the extended plugin density with the posterior mean of $\eta$.

Consequently, $\bar{\eta}_\pi$ appears to be a natural estimator for curved exponential families. We show that $p(y; \bar{\eta}_\pi)$ is the optimal extended plugin density with respect to the Bayes risk based on a prior $\pi$.

**Proposition 2.1.** The Bayes risk of $p(y; \hat{\eta})$, where $\hat{\eta}$ is an estimator of $\eta$, is minimized when $\hat{\eta} = \bar{\eta}_\pi$.

**Proof.** Let $\hat{\theta}$ be an estimator of $\theta$. Note that $\theta$ and $\eta$ are functions of $u$. The Kullback–Leibler loss of $p(y; \hat{\theta})$ is

$$D\{p(y; \theta(u)); p(y; \hat{\theta})\} = \int p(y; \theta) \log \frac{\exp(\theta^i y_i - \Psi(\theta))}{\exp(\hat{\theta}^i y_i - \Psi(\hat{\theta}))} dy$$

$$= (\theta^i - \hat{\theta}^i) \eta_i - (\Psi(\theta) - \Psi(\hat{\theta})).$$

Hence

$$\int p(u \mid x^n) D\{p(y; \theta(\eta)); p(y; \hat{\theta}(\eta))\} du$$

$$= (\theta^i \eta_i - \hat{\theta}^i \bar{\eta}_i) - (\Psi(\theta) - \Psi(\hat{\theta}))$$

$$= (\theta^i (\bar{\eta}_i) - \hat{\theta}^i \bar{\eta}_i) - (\Psi(\theta(\bar{\eta})) - \Psi(\hat{\theta})) + \left(- \theta^i (\bar{\eta}_i) \bar{\eta}_i + \hat{\theta}^i \bar{\eta}_i + \Psi(\theta(\bar{\eta})) - \Psi(\theta)\right)$$

$$= D\{p(y; \bar{\eta}); p(y; \hat{\theta})\} + \left(- \theta^i (\bar{\eta}_i) \bar{\eta}_i + \hat{\theta}^i \bar{\eta}_i + \Psi(\theta(\bar{\eta})) - \Psi(\theta)\right),$$

where, for a function $f(\eta)$,

$$\bar{f}(\eta) = \int p(u \mid x^n) f(\eta) du.$$

The Bayes risk is minimized when $\hat{\theta} = \theta(\bar{\eta}) = \theta(\bar{\eta}_\pi)$. Thus $p(y \mid \bar{\eta}_\pi)$ is optimal with respect to the Bayes risk in the class of extended plugin densities. 

We use a simple example to show the difference of plugin of $\hat{u}_\pi$, extended plugin of $\hat{\eta}_\pi$, and the Bayesian predictive density.
Example (Fisher circle model) We consider two dimensional Gaussian densities $N(\mu, I_2)$ with unknown mean vector $\mu$ and the identity covariance matrix $I_2$. The probability density function is

$$p(x; \mu) = \frac{1}{2\pi} \exp \left( -\frac{1}{2} \left\{ (x_1 - \mu_1)^2 + (x_2 - \mu_2)^2 \right\} \right)$$

$$= \frac{1}{2\pi} \exp \left( -\frac{1}{2} (\bar{x}_1^2 + \bar{x}_2^2) \right) \exp \left( x_1 \mu_1 + x_2 \mu_2 - \frac{1}{2} (\mu_1^2 + \mu_2^2) \right).$$

When the mean vector $\mu$ is expressed as

$$\mu_1 = \cos \omega, \mu_2 = \sin \omega,$$

the 1-dimensional submodel is called the Fisher circle model. Here,

$$\theta^1 = \eta_1 = \mu_1, \ \theta^2 = \eta_2 = \mu_2$$

hold.

We derive the Bayes estimator of $\omega$, the extended plugin of the Bayes estimator $\hat{\eta}_\pi$, and the Bayesian predictive density. For $x^n = \{x(1), x(2), \ldots, x(n)\}$,

$$p(x^n; \omega) = \prod_{t=1}^n \frac{1}{2\pi} \exp \left( -\frac{\|x(t) - \mu(\omega)\|^2}{2} \right)$$

$$= \frac{1}{(2\pi)^n} \exp \left( -\frac{\sum_{t=1}^n (x_1(t) - \mu_1)^2 + x_2(t) - \mu_2)^2}{2} \right) \exp \left( -\frac{n}{2} \|\bar{x} - \mu(\omega)\|^2 \right)$$

where $\bar{x} = \sum_{t=1}^n x(t)/n$. Let $\bar{x} = (\|\bar{x}\| \cos \phi, \|\bar{x}\| \sin \phi)^T$. Then

$$-\frac{n}{2} \|\bar{x} - \mu(\omega)\|^2 = n\|\bar{x}\| \cos(\omega - \phi) + \text{(terms independent of } \omega)$$

and

$$\int_0^{2\pi} \exp(n\|\bar{x}\| \cos(\omega - \phi)) d\omega = 2\pi I_0(n\|\bar{x}\|)$$

where $I_0(\cdot)$ is the modified Bessel function of the first kind. See Fisher (1973, pp. 138–140) for the detail.

When the uniform prior

$$\pi(\omega) \propto 1$$

is adopted, the posterior density is

$$p_\pi(\omega \mid x^n) = \frac{1}{2\pi I_0(n\|\bar{x}\|)} \exp(n\|\bar{x}\| \cos(\omega - \phi)).$$

It follows that the Bayes estimator $\hat{\omega}_\pi$ is $\phi$ and $\hat{\eta}_\pi(\hat{\omega}_\pi)$ is $\bar{x}/\|\bar{x}\|$. The posterior mean of $\eta$ is

$$\hat{\eta}_\pi = \frac{I_1(n\|\bar{x}\|)}{I_0(n\|\bar{x}\|)} \frac{\bar{x}}{\|\bar{x}\|},$$

which is not included in the circle parametrized by $\omega$ and $\hat{\eta}_\pi \neq \eta(\hat{\omega}_\pi)$. On the other hand, the Bayesian predictive density is given by

$$p_\pi(y \mid x^n) = \frac{1}{2\pi} \frac{I_0(\|y + n\bar{x}\|)}{I_0(n\|\bar{x}\|)} \exp \left\{ -\frac{1}{2} (\|y\|^2 + 1) \right\}.$$
Information geometry of extended plugin densities

3.1 Information-geometric notions and asymptotic expansions

First, we prepare some information-geometric notions. For details of the notions and notation in the differential geometry of curved exponential families, refer to Amari (1985).

Let \( a, b, \ldots \) be indices for \( u \). Let \( T_u \mathcal{P} \) be the tangent space of \( \mathcal{P} \) at a point \( u \). The tangent space \( T_u \mathcal{P} \) is identified with the vector space spanned by \( \partial_a p(x; u) \) \( (a = 1, \ldots, d) \), where \( \partial_a \) denotes \( \partial / \partial u^a \). Define inner products in the tangent space by

\[
\langle r, s \rangle = \int r s \frac{1}{p(x; u)} dx.
\]

For a statistical model \( \mathcal{P} \), each component of the Fisher information matrix is defined by

\[
\gamma^{ab}(u) = \langle \partial_a p(x; u), \partial_b p(x; u) \rangle = \int \frac{\partial_a p(x; u) \partial_b p(x; u)}{p(x; u)} dx
\]

and let \( g_{ab} \) be a component of the inverse matrix of \( (\gamma^{ab}) \). The e-connection coefficients and the m-connection coefficients are defined by

\[
\Gamma^e_{abc}(u) = \int p(x; u) \{ \partial_a \log p(x; u) \} \{ \partial_b \log p(x; u) \} dx
\]

and

\[
\Gamma^m_{abc}(u) = \int \frac{\partial_a \partial_b p(x; u) \partial_c p(x; u)}{p(x; u)} dx,
\]

respectively. We define

\[
\Gamma^e_{ab} := \gamma^{bd} \gamma^{dc}, \quad \Gamma^m_{ab} := \gamma^{bd} \gamma^{dc},
\]

and

\[
T_{abc} = \Gamma^m_{abc} - \Gamma^e_{abc}
\]

\[
= \int p(x; u) \{ \partial_a \log p(x; u) \} \{ \partial_b \log p(x; u) \} \{ \partial_c \log p(x; u) \} dx.
\]

The Jeffreys prior density is given by

\[
\pi_J(u) = \sqrt{|\gamma(u)|},
\]

where \( |\gamma(u)| \) is the determinant of the matrix \( (\gamma_{ab}(u)) \).

The coordinate systems \( (\theta^i) \) and \( (\eta_i) \) of the exponential family \( \mathcal{E} \) are dual to each other in the sense that

\[
\left\langle \frac{\partial}{\partial \theta^i} p(x; \theta), \frac{\partial}{\partial \eta_j} p(x; \theta) \right\rangle = \delta^i_j
\]

(2)
where \( \delta^i_j \) is the Kronecker delta. For a curved exponential family, e-connection coefficients and m-connection coefficients are expressed as

\[
\Gamma_{abc} = (\partial_a \partial_b \theta^i)(\partial_c \eta_i) \quad \text{and} \quad \Gamma_{abc}^m = (\partial_a \partial_b \eta_i)(\partial_c \theta^i),
\]

respectively.

Now we proceed to obtain the asymptotic expansion of \( \hat{\eta}_\pi \) around \( \eta(\hat{u}_{\text{MLE}}) \).

**Theorem 3.1.** The posterior mean of \( \eta \), which is the Bayes estimator of \( \eta \), based on a prior \( \pi(u) \) is expanded as

\[
\hat{\eta}_\pi = \eta(\hat{u}_{\text{MLE}}) + \frac{g^{ab}(\hat{u}_{\text{MLE}})}{2n} \left( \partial_a \partial_b \eta(\hat{u}_{\text{MLE}}) - \Gamma_{abc}(\hat{u}_{\text{MLE}}) \partial_c \eta(\hat{u}_{\text{MLE}}) \right) + \frac{g^{ab}(\hat{u}_{\text{MLE}})}{n} \left( \partial_b \log \frac{\pi}{\pi_J} + \frac{T_b(\hat{u}_{\text{MLE}})}{2} \right) \partial_a \eta(\hat{u}_{\text{MLE}}) + o_p(n^{-1}),
\]

where \( T_a = T_{abc}g^{bc} \).

**Proof.** Let \( L(\eta) = \frac{1}{n} \sum_{t=1}^{n} \log p(x(t); \eta) \). Then, \( \hat{\eta}_\pi(x^n) = \{(\hat{\eta}_\pi)_i(x^n)\} \) is given by

\[
(\hat{\eta}_\pi)_i = \hat{\eta}_i + \frac{\hat{J}^{ab}}{2n} \left( \partial_{ab} \hat{\eta}_i + \frac{2(\partial_a \hat{\eta}_i)(\partial_b \hat{\eta})}{\hat{\pi}} \right) + \frac{\hat{J}^{ab} \hat{J}^{cd} \partial_{bcd} \hat{L}}{2n} \partial_a \hat{\eta}_i + O_p(n^{-2}).
\]

Here symbols such as \( \eta(\hat{u}_{\text{MLE}}), \partial_a \eta(\hat{u}_{\text{MLE}}), \) and \( \partial_a \partial_b \eta(\hat{u}_{\text{MLE}}) \) are abbreviated to \( \hat{\eta}, \partial_a \hat{\eta}, \) and \( \partial_{ab} \hat{\eta} \) respectively, \( \hat{J}_{ab} = -\partial_a \hat{L}, \) and \( (\hat{J}^{ab}) \) is the inverse matrix of \( (\hat{J}_{ab}) \). Proof for this approximation is given in Appendix. This approximation follows Kass and Vos (1997, Theorem 4.6.1).

Since \( \hat{J}_{ab} = \hat{g}_{ab} + o_p(1), \partial_{bcd} \hat{L} = E[\partial_{bcd} \hat{L}] + o_p(1) \) by the law of large numbers, and

\[
E[\partial_{bcd} \hat{L}] = -\partial_b g_{cd} - \hat{g}_{cd} = -\partial_b g_{cd} - \Gamma_{cd}^c + T_{b,cd},
\]

and

\[
g^{cd} \partial_b g_{cd} = \partial_b \log |g| = 2 \partial_b \log \pi_J
\]

hold, we obtain

\[
(\hat{\eta}_\pi)_i = \hat{\eta}_i + \frac{\hat{g}^{ab}}{2n} \left( \partial_{ab} \hat{\eta}_i + 2 \partial_a \hat{\eta}_i \partial_b \log \hat{\pi} \right) + \frac{\hat{g}^{ab}}{2n} \left( -2 \partial_b \log \hat{\pi}_J - \hat{g}^{cd} \Gamma_{cd}^c(\hat{u}_{\text{MLE}}) + T_b(\hat{u}_{\text{MLE}}) \right) \partial_a \hat{\eta}_i + o_p(n^{-1})
\]

\[
= \hat{\eta}_i + \frac{\hat{g}^{ab}}{2n} \left( \partial_{ab} \hat{\eta}_i - \Gamma_{abc}(\hat{u}_{\text{MLE}}) \partial_c \hat{\eta}_i \right) + \frac{\hat{g}^{ab}}{n} \left( \partial_b \log \frac{\pi}{\pi_J} + \frac{T_b(\hat{u}_{\text{MLE}})}{2} \right) \partial_a \hat{\eta}_i + o_p(n^{-1}).
\]

\[\square\]
We can obtain the asymptotic expansion of the extended plugin density of the Bayes estimator \( \hat{\eta}_\pi \).

**Theorem 3.2.** The extended plugin density with \( \hat{\eta}_\pi \) is expanded as

\[
p(y; \hat{\eta}_\pi) = p(y; \eta(\hat{u}_{MLE})) + \frac{g^{ab}(\hat{u}_{MLE})}{2n} \left( \partial_a \partial_b \eta_i(\hat{u}_{MLE}) - \frac{\Gamma^{m}_{ab}(\hat{u}_{MLE}) \partial_{\eta_i}(\hat{u}_{MLE})}{2} \right) \partial^i p(y; \hat{u}_{MLE}) \\
+ \frac{g^{ab}(\hat{u}_{MLE})}{n} \left( \partial_b \log \frac{\pi}{\pi_j}(\hat{u}_{MLE}) + \frac{T_b(\hat{u}_{MLE})}{2} \right) \partial_a p(y; \hat{u}_{MLE}) + o_p(n^{-1}),
\]

where \( \hat{u}_{MLE} \) is the maximum likelihood estimator and \( \partial^i = \frac{\partial}{\partial \eta_i} \).

**Proof.** Using the asymptotic expansion in Theorem 3.1 we have

\[
p(y; \hat{\eta}_\pi) = p(y; \hat{\eta}) + \frac{\hat{g}^{ab}}{2n} \left( \partial_{ab} \hat{\eta}_i - \frac{\Gamma^{m}_{ab}(\hat{u}_{MLE}) \partial_{\eta_i}(\hat{u}_{MLE})}{2} \right) \partial^i p(y; \hat{\eta}) \\
+ 0_p(n^{-1}) = p(y; \hat{\eta}) + \frac{\hat{g}^{ab}}{2n} \left( \partial_{ab} \hat{\eta}_i - \frac{\Gamma^{m}_{ab}(\hat{u}_{MLE}) \partial_{\eta_i}(\hat{u}_{MLE})}{2} \right) \partial^i p(y; \hat{\eta}) \\
+ 0_p(n^{-1}).
\]

Komaki (1996) gave an asymptotic expansion of Bayesian predictive densities around the plugin of \( \hat{u}_{MLE} \), and our results are parallel to the results.

### 3.2 Construction of extended plugin densities

In this section, extended plugin densities are specified by shifts from plugin densities of \( \mathcal{P} \).

The shift to \( p(y; \hat{\eta}_\pi) \) in Theorem 3.2 is composed of two components, one “parallel” and the other “orthogonal” to the model \( \mathcal{P} \). That is, the term

\[
\frac{g^{ab}(\hat{u}_{MLE})}{n} \left( \partial_b \log \frac{\pi}{\pi_j}(\hat{u}_{MLE}) + \frac{T_b(\hat{u}_{MLE})}{2} \right) \partial_a p(y; \hat{u}_{MLE})
\]

is included in the space spanned by \( \partial_a p(y; \eta) \ (a = 1, \ldots, d) \) and the term

\[
\frac{g^{ab}(\hat{u}_{MLE})}{2n} \left( \partial_a \partial_b \eta_i(\hat{u}_{MLE}) - \frac{\Gamma^{m}_{ab}(\hat{u}_{MLE}) \partial_{\eta_i}(\hat{u}_{MLE})}{2} \right) \partial^i p(y; \hat{u}_{MLE})
\]

is orthogonal to \( \partial_a p(x; \eta) \ (a = 1, \ldots, d) \) with respect to the inner product \( \langle \cdot, \cdot \rangle \), because

\[
\langle \left( \partial_a \partial_b \eta_i - \frac{\Gamma^{m}_{ab}(\hat{u}_{MLE}) \partial_{\eta_i}(\hat{u}_{MLE})}{2} \right) \partial^i p(y; \eta), \partial_e p(y; \eta) \rangle \\
= \int \partial_a \partial_b \eta_i \frac{\partial p(y; \eta)}{\partial \theta^j} \partial \theta^j \frac{\partial p(y; \eta)}{\partial \theta^j} \frac{1}{p(y; \eta)} dy - \Gamma^{m}_{ab} \delta_{ce} = \partial_a \partial_b \eta_i \partial_e \theta^j - \frac{\Gamma^{m}_{ab}}{\partial \theta^e} = 0
\]
by using (2) and (3).

We divide the tangent vectors of $E$ at $\eta$ into two parts, namely those parallel to $P$ and those orthogonal to $P$. For each point $\eta \in E$, the tangent space $T_\eta E$ is identified with the vector space spanned by

$$\frac{\partial}{\partial \eta_i} p(x; \eta) \ (i = 1, \ldots, m).$$

The tangent space $T_u P$ is a subspace of $T_\eta E$. Let $A(u)$ be an $(m - d)$-dimensional smooth submanifold of $E$ attached to each point $u \in P$ and assume that $A(u)$ orthogonally transverses $P$ at $\eta(u)$. Such a family of submanifolds $\{A(u) \mid u \in U\}$ is called an ancillary family. We introduce an adequate coordinate system $v = (v^\kappa)$ ($\kappa = d + 1, \ldots, m$) to $A(u)$ so that a pair $(u, v)$ uniquely specifies a point of $E$ in the neighborhood of $\eta(u)$. We adopt a coordinate system $v$ on $A(u)$ such that $\eta(u, v) \in P$ if $v = 0$. Then, we have

$$\text{span} \{ \partial^i p(x; \eta) \} = \text{span} \{ \partial_a p(x; \eta), \partial_\kappa p(x; \eta) \}$$

where $\partial_\kappa p(x; \eta) = \frac{\partial}{\partial \eta_\kappa} p(x; \eta)$. Since $A(u)$ orthogonally transverses $E$, we have

$$\langle \partial_a p(x; \eta), \partial_\kappa p(x; \eta) \rangle = 0 \quad (a = 1, \ldots, d, \ \kappa = d + 1, \ldots, m).$$

In the following discussion, we consider extended plugin densities $p(y; \tilde{\eta})$ with estimators $\tilde{\eta} = \eta(\hat{u}, \hat{v})$ where $\hat{u}, \hat{v}$ can be expressed in the form

$$\hat{u} = \hat{u}_{\text{MLE}} + \frac{1}{n} \alpha(\hat{u}_{\text{MLE}}) + o_p(n^{-1}), \quad \hat{v} = \frac{1}{n} \beta(\hat{u}_{\text{MLE}}) + o_p(n^{-1}),$$

respectively. Here $\alpha^a(u), \beta^\kappa(u)$ are smooth functions of $O_p(1)$. Those densities can be expanded as

$$p_{ab}(y; \hat{u}_{\text{MLE}}) = p(y; \hat{u}_{\text{MLE}}) + \frac{1}{n} \alpha^a(\hat{u}_{\text{MLE}}) \partial_a p(y; \eta(\hat{u}_{\text{MLE}})) + \frac{1}{n} \beta^\kappa(\hat{u}_{\text{MLE}}) \partial_\kappa p(y; \eta(\hat{u}_{\text{MLE}})) + o_p(n^{-1}). \quad (5)$$

The results in the following sections hold for asymptotically efficient estimators of $u$ other than $\hat{u}_{\text{MLE}}$ as in Komaki (1996), although here we consider $\hat{u}_{\text{MLE}}$ for simplicity.

This class of extended plugin densities include $p(x; \hat{u}_{\text{MLE}})$ and $p(x; \hat{\eta}_n)$. For $\hat{u} = \hat{u}_{\text{MLE}}$ and $\hat{v} = 0$, the density is the plugin density with the maximum likelihood estimator $\hat{u}_{\text{MLE}}$. The extended plugin density with the Bayes estimator $\hat{\eta}_n$ in Theorem 3.1 is given by

$$\alpha^a(\hat{u}_{\text{MLE}}) = g^{ab}(\hat{u}_{\text{MLE}}) \left( \partial_b \log \frac{\pi}{\pi_J} + \frac{T_b}{2} \right), \quad \beta^\kappa = \frac{1}{2} \tilde{H}_{ab}^\kappa(\hat{u}_{\text{MLE}}) g^{ab}(\hat{u}_{\text{MLE}})$$

where

$$\tilde{H}_{ab}^\kappa = \langle \partial_a \partial_b p(x; u), \partial_\kappa p(x; \eta) \rangle = \langle \partial_a \partial_b \eta_i(u) \rangle \partial_\kappa p(x; \eta),$$

is the mixture embedding curvature of $P$ in $E$ and $\tilde{H}_{ab}^\kappa = \tilde{H}_{ab\lambda} g^{\kappa\lambda}$. This can be confirmed as follows. Let

$$h_{ab} = (\partial_a \partial_b \eta_i(u)) \partial_\kappa p(x; \eta) - \Gamma_{ab}^\kappa \partial_\kappa p(x; u),$$

where
then the orthogonal component in Theorem 3.2 is
\[ \frac{g^{ab}(\hat{u}_{\text{MLE}})}{2n} h_{ab}(\hat{u}_{\text{MLE}}). \]
Since \( h_{ab} \ (a, b = 1, \ldots, d) \) are included in the space spanned by \( \partial_\kappa p(x; u) \) \( (\kappa = d + 1, \ldots, m) \),
\[ h_{ab} = \langle h_{ab}, \partial_\lambda p(x; \eta) \rangle g^{\kappa \lambda} \partial_\kappa p(x; \eta) \]
\[ = \left\langle \partial_a \partial_b \eta_i(u) \partial^i p(x; \eta) - \frac{m}{2} \partial_c p(x; u), \partial_\lambda p(x; \eta) \right\rangle g^{\kappa \lambda} \partial_\kappa p(x; \eta). \]
Because \( \langle \partial_c p(x; \eta), \partial_\lambda p(x; \eta) \rangle = 0 \),
\[ h_{ab} = \langle \partial_a \partial_b \eta_i(u) \partial^i p(x; \eta), \partial_\lambda p(x; \eta) \rangle g^{\kappa \lambda} \partial_\kappa p(x; \eta) \]
\[ = \partial_a \partial_b \eta_i(u) \partial_\lambda g^{\kappa \lambda} \partial_\kappa p(x; \eta) \]
\[ = H_{ab}^\kappa \partial_\kappa p(x; \eta). \]

### 3.3 Optimal orthogonal shift

In this section, it is shown that orthogonal shifts from \( \mathcal{P} \) to extended plugin densities can asymptotically improve the Kullback–Leibler risk. The optimal orthogonal shift is also obtained. The extended plugin density with a Bayes estimator has the optimal orthogonal shift.

We derive the Kullback–Leibler risk of the extended plugin densities.

**Proposition 3.1.** The Kullback–Leibler risk of an extended plugin density \( p_{\alpha, \beta}(y; \hat{u}_{\text{MLE}}) \) in (5) is asymptotically expanded as
\[ \frac{E[D(p(y; u), p_{\alpha, \beta}(y; \hat{u}_{\text{MLE}}))]}{d} = \frac{1}{2n^2} g_{ab}(u) \alpha^a(u) \beta^b(u) + \frac{1}{2n^2} \nabla_\alpha^a(u) + \frac{1}{2n^2} g_{\kappa \lambda}(u) \beta^\kappa(u) \beta^\lambda(u) - \frac{1}{2n^2} H_{ab}^\kappa(u) g^{ab}(u) \beta^\kappa(u) \]
\[ + (\text{terms independent of } \alpha, \beta) + o(n^{-2}), \]  
(6)

where \( \nabla_\alpha^a = \partial_a \alpha^b + \Gamma^b_{ac} \alpha^c \).

**Proof.** See Appendix.

The risk (6) can be improved by choosing an appropriate orthogonal shift \( \beta \). We obtain the optimal orthogonal shift.

**Theorem 3.3.** The optimal \( \beta^\kappa \) in (5) is given by
\[ \beta^\kappa_{\text{opt}}(u) = \frac{1}{2} H_{ab}^\kappa(u) g^{ab}(u). \]  
(7)
Proof. The risk in Proposition 3.1 is
\[
E[D\{p(y; u), p_{\alpha,\beta}(y; \hat{u}_{MLE})\}] = \frac{1}{2n^2}g_{ab}\alpha^a\alpha^b + \frac{1}{n^2}\nabla_u\alpha^a(u)
+ \frac{1}{2n^2}g_{\kappa\lambda}\left(\beta^\lambda - \frac{1}{2}H_{ab}g^{ab}\right)\left(\beta^\kappa - \frac{1}{2}H_{cd}g^{cd}\right) - \frac{1}{8n^2}H_{ab}H_{cd}g^{ab}g^{cd}g_{\kappa\lambda}
+ (\text{terms independent of } \alpha, \beta) + o(n^{-2}).
\]
Thus \(\beta\) is optimal when
\[
\beta^\kappa(u) = \frac{1}{2}H_{ab}(u)g^{ab}(u).
\]

Therefore, the orthogonal component of the shift in Theorem 3.2 is optimal. The extended plugin density with \(\hat{\eta}_\pi\) has the optimal shift. The risk difference between a plugin density \(p_{\alpha,0}(y; \hat{u}_{MLE})\) and an extended plugin density \(p_{\alpha,\beta_{opt}}(y; \hat{u}_{MLE})\) with the optimal orthogonal shift is given by
\[
E[D\{p(y; u), p_{\alpha,0}(y; \hat{u}_{MLE})\}] - E[D\{p(y; u), p_{\alpha,\beta_{opt}}(y; \hat{u}_{MLE})\}]
= \frac{1}{8n^2}H_{ab}H_{cd}g^{ab}g^{cd}g_{\kappa\lambda} + o(n^{-2}).
\]
Here, \(H_{ab}H_{cd}g^{ab}g^{cd}g_{\kappa\lambda}\) is the mixture mean curvature of \(P\) embedded in \(E\) at \(u\).

In Komaki (1996), the Bayesian predictive densities are constructed by the shift from the model \(P\), and a different class of shifts from ours are considered. In the class, the optimal orthogonal shift coincides with the shift to the Bayesian predictive density. The optimal orthogonal shift obtained by Komaki (1996) is not in the tangent space of exponential families \(E\). Thus, the shifted plugin density is not included in \(E\). Our optimal shift is included in the tangent space of \(E\), and the shifted plugin density is included in \(E\). The optimal orthogonal shift of Komaki (1996) is
\[
g^{ab}(\hat{u}_{MLE}) \left(\partial_a\partial_b p(y; \hat{u}_{MLE}) - \frac{m}{m}\Gamma^c_{ab}(\hat{u}_{MLE})\partial_c p(y; \hat{u}_{MLE})\right).
\]
(8)
Our optimal shift is a projection of (8) onto the tangent space of \(E\) because
\[
\left\langle g^{ab}(\hat{u}_{MLE}) \left(\partial_a\partial_b p(y; \hat{u}_{MLE}) - \frac{m}{m}\Gamma^c_{ab}(\hat{u}_{MLE})\partial_c p(y; \hat{u}_{MLE})\right), \partial_c p(y; \hat{u}_{MLE})\right\rangle g^{\lambda\kappa}\partial_\lambda p(y; \hat{u}_{MLE})
= g^{ab}(\hat{u}_{MLE}) \left(\partial_a\partial_b p(y; \hat{u}_{MLE}), \partial_c p(y; \hat{u}_{MLE})\right) g^{\lambda\kappa}\partial_\lambda p(y; \hat{u}_{MLE})
= g^{ab}(\hat{u}_{MLE}) H_{ab}\partial_\kappa p(y; \hat{u}_{MLE}).
\]
Example (Fisher circle model, continued) We have $g_{\omega\omega} = 1$ and $m_{\omega\omega} = 0$. Thus, the optimal orthogonal shift is

$$h_{\omega\omega}(x; \eta) = \left( \partial_{\omega\omega} \eta - m_{\omega\omega} \partial_{\omega\omega} \eta \right) \partial_{i} p(x; \eta) = p(x; \eta) (-\cos \omega (x_1 - \eta_1) - \sin \omega (x_2 - \eta_2))$$

and the risk improvement by the optimal orthogonal shift is

$$\mathbb{E}[D(p(y; \omega), p_{\alpha,0}(y; \hat{\omega}_{\text{MLE}}))] - \mathbb{E}[D(p(y; \omega), p_{\alpha,\hat{\omega}_{\text{opt}}}(y; \hat{\omega}_{\text{MLE}}))] = 1 \frac{8}{n^2} m_{\omega\omega} g_{\omega\omega} + o(n^{-2})$$

The risk improvement by the optimal shift (8) is $\frac{3}{8n^2} + o(n^{-2})$.

If the variance of $x_1, x_2$ is $\sigma^2$, the risk improvements by the optimal orthogonal shift and by the shift (8) are

$$\frac{\sigma^2}{8n^2}, \frac{\sigma^2 + 2}{8n^2},$$

respectively. Therefore when $\sigma^2$ is large, the risk improvement by $p(y; \hat{\eta}_{\pi})$ becomes relatively large, and the performance of the extended plugin density is close to that of the Bayesian predictive density. From an information-geometric point of view, the orthogonal shift to $p(y; \hat{\eta}_{\pi})$ is the projection of the orthogonal shift to the Bayesian predictive density onto the tangent space of $E$, and the cosine of the angle between the two shift vectors is

$$\sqrt{\frac{\sigma^2}{8n^2}} \sqrt{\frac{\sigma^2 + 2}{8n^2}} = \sqrt{\frac{\sigma^2}{\sigma^2 + 2}}.$$ 

Thus the angle between those shifts approaches to 0 as $\sigma^2$ grows.

Example (2-dimensional spike model): In Section [2] we saw in the $l$-dimensional spike model, the extended plugin density with the Bayes estimator is a natural predictive density. Here we consider the 2-dimensional spike model, namely 2-dimensional Gaussian densities with zero mean vector and unknown covariance matrix that is expressed as

$$\Sigma = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} \lambda + 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix},$$

where $\lambda > 0$. The eigenvalues of $\Sigma$ are $\lambda + 1$ and 1. The model $\mathcal{P} = \{N(0, \Sigma) \mid (\lambda, \phi)\}$ is parametrized by $(\lambda, \phi)$. The components of $\Sigma$ are the coordinate system $(\hat{\eta}_{\pi})$ of the extended statistical model $E = \{N(0, \Sigma) \mid \Sigma\}$, thus $p(y; \hat{\Sigma}_{\pi})$ is the extended plugin density with the posterior mean of $\eta$. 

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In this model,
\[
g_{\phi\phi} = \frac{\lambda^2}{\lambda + 1}, \quad g_{\lambda\lambda} = \frac{1}{2(\lambda + 1)}, \quad g_{\lambda\phi} = 0,
\]
\[
m\Gamma_{\phi\phi\lambda} = -\frac{\lambda}{(\lambda + 1)^2}, \quad m\Gamma_{\phi\lambda\phi} = \frac{\lambda}{\lambda + 1}, \quad m\Gamma_{\phi\phi\phi} = m\Gamma_{\phi\lambda\lambda} = m\Gamma_{\lambda\lambda\lambda} = m\Gamma_{\lambda\lambda\phi} = 0
\]
hold. The optimal orthogonal shift is
\[
g_{ab}^{opt} = \frac{\lambda + 1}{2n}(\partial_{ab}\eta - m\nabla_a\nabla_b\eta) = \lambda + 1
\]
\[
\partial_{p}(p(y; \eta)) = \lambda + 1
\]
\[
E[D(p(y; \omega), p(y; ^{\hat{\eta}}\pi)) - E[D(p(y; \omega), p_{\alpha,\beta,\gamma}(y; ^{\hat{\omega}}\text{MLE}))]
\]
\[
= \frac{1}{8n^2} E \left[ \left( \frac{\lambda + 1}{\lambda} \right) \left( (-y_1 \sin \phi + y_2 \cos \phi)^2 - 1 \right) \right] + o(n^{-2})
\]
\[
= \frac{1}{4n^2} \left( \frac{\lambda + 1}{\lambda} \right)^2 + o(n^{-2}),
\]
which grows as \( \lambda \) approaches to zero. The risk improvement by the optimal shift (8) is
\[
\frac{1}{4n^2} \left( \frac{\lambda + 1}{\lambda} \right)^2 + o(n^{-2}).
\]
In such an example, the extended plugin is a promising option for constructing predictive densities, because much less numerical computation is required to obtain extended plugin densities than to obtain Bayesian predictive densities.

4 Shrinkage priors

We consider the choice of priors for the extended plugin with the Bayes estimator \( ^{\hat{\eta}}\pi \). From Proposition 3.1, the risk of \( p(y; ^{\hat{\eta}}\pi) \) is expanded as
\[
E[D(p(y; \omega), p_{\alpha,\beta,\gamma}(y; ^{\hat{\omega}}\text{MLE}))]
\]
\[
= \frac{1}{2n^2} g_{ab} \alpha^a \alpha^b + \frac{1}{n^2} \nabla_a \alpha^a + (\text{terms independent of } \pi) + o(n^{-2})
\]
where \( \alpha^a = g^{ab}(^{\hat{\omega}}\text{MLE}) \left( \partial_b \log \frac{\pi}{\pi_{\text{MLE}}}^{\hat{\omega}}(^{\hat{\omega}}\text{MLE}) \right) - \frac{1}{2} \nabla_a \alpha^a \).

The Laplacian \( \Delta \) on a manifold with the Riemannian metric \( g_{ab} \) is defined by
\[
\Delta f := |g|^{-1/2} \partial_a (|g|^{1/2} g^{ab} \partial_b f),
\]
where \( f \) is a smooth function on the model manifold. A \( C^2 \) function \( f \) is called superharmonic if \( \Delta f \leq 0 \).

**Theorem 4.1.** Suppose that \( \pi \) is a smooth positive function on the model manifold \( \mathcal{P} \). The extended plugin density \( p(y; ^{\hat{\eta}}\pi) \) based on \( \pi \) asymptotically dominates the extended plugin density \( p(y; ^{\hat{\eta}}\pi_j) \) based on the Jeffreys prior \( \pi_j \) if and only if \( (\pi/\pi_j)^{1/2} \) is a non-constant positive superharmonic function.
Proof. Let
\[\nabla_a \alpha^b = \partial_a \alpha^b + \left(\Gamma_{ac}^b(\hat{\mu}_{MLE}) + \frac{T_e(\hat{\mu}_{MLE})}{2}\right)\alpha^c.\]
The asymptotic risk difference is
\[n^2 \{E[D(p(y; u); p(y; \hat{\eta}_{\pi_j})]) - E[D(p(y; u); p(y; \hat{\eta}_{\pi})])\}
= \frac{1}{8} g^{ab}(T_a T_b + \nabla_a \left( g^{ac} T_c \right) - \frac{1}{2} g^{ab} \left( \partial_a \log \frac{\pi}{\pi_j} + \frac{T_a}{2} \right) \left( \partial_b \log \frac{\pi}{\pi_j} + \frac{T_b}{2} \right) - \nabla_a \left\{ g^{ab} \left( \partial_{ab} \log \frac{\pi}{\pi_j} + \frac{T_{ab}}{2} \right) \right\} + o(1)
= - \frac{\pi_j}{\pi} \nabla_a \left( \frac{\pi}{\pi_j} \right) g^{ab} \frac{\partial_a \left( \frac{\pi}{\pi_j} \right)}{\partial b} \frac{\partial_b \left( \frac{\pi}{\pi_j} \right)}{\partial b} + o(1)
= - \frac{\pi_j}{\pi} \nabla_a \left( \frac{\pi}{\pi_j} \right) + \frac{1}{2} g^{ab} \left( \partial_a \log \frac{\pi}{\pi_j} \right) \left( \partial_b \log \frac{\pi}{\pi_j} \right) + o(1).
\]
Because for an arbitrary function \(f\)
\[f^{-1/2} \Delta f^{1/2} = f^{-1/2} \nabla_a (g^{ab} \partial_b f^{1/2})
= \frac{1}{2} f^{-1/2} \nabla_a (g^{ab} f^{-1/2} \partial_b f)
= \frac{1}{2} f^{-1} \Delta f - \frac{1}{4} g^{ab} \partial_a \log f \partial_b \log f
\]
holds, the risk difference is
\[E[D(p(y; u); p(y; \hat{\eta}_{\pi_j})]) - E[D(p(y; u); p(y; \hat{\eta}_{\pi})])
= - \frac{2}{n^2} \left( \frac{\pi_j}{\pi} \right)^{1/2} \Delta \left( \frac{\pi}{\pi_j} \right)^{1/2} + o(n^{-2}).\]

The superharmonic condition for priors for Bayesian predictive densities is obtained in Komaki (2006), and Theorem 4.1 is its parallel result for extended plugin densities of Bayes estimators.

Shrinkage priors are closely related to the superharmonic condition. For example, the Stein prior \(\pi(\mu) = ||\mu||^{-(d-2)}\) for the estimation of mean vector \(\mu\) of \(d\)-dimensional Gaussian densities satisfies the superharmonic condition when \(d > 2\). For a discussion on the treatment of the origin \(\mu = 0\), see Komaki (2006). Consequently, Theorem 4.1 suggests that shrinkage priors are effective for constructing the extended plugin of the Bayes estimator. For the multivariate normal model with known covariance
matrix, finite sample theories have been developed, see Komaki (2001), George et al. (2006), and George et al. (2012).

Example (4-dimensional curved normal) We consider 4-dimensional Gaussian densities \( N(\mu, I_4) \) with the identity covariance matrix \( I_4 \) and unknown mean vector \( \mu \) which is expressed as \( \mu_1 = u_1, \mu_2 = u_2, \mu_3 = u_3, \mu_4 = u_3^2 \) by parameters \( u = (u_1, u_2, u_3) \). We embed this model in the full exponential family \( \{ N(\mu, I_4) \mid \mu \in \mathbb{R}^4 \} \).

The Fisher information matrix of the curved exponential family is denoted by

\[
\begin{align*}
g_{11} &= g_{22} = 1, & g_{33} &= 1 + 4u_3^2, & g_{12} = g_{13} = g_{23} &= 0.
\end{align*}
\]

Change the variables \( u \) to \( \xi \) by

\[
\begin{align*}
\xi_1 &= u_1, \quad \xi_2 = u_2, \quad \xi_3 = \frac{1}{4} \log \left( u_3 + \sqrt{u_3^2 + \frac{1}{4}} \right) + u_3 \sqrt{u_3^2 + \frac{1}{4}} + \frac{1}{4} \log 2,
\end{align*}
\]

where \( \xi_3 \) satisfies

\[
\frac{\partial}{\partial u_3} \xi_3 = \sqrt{4u_3^2 + 1}.
\]

The Fisher information matrix for \( \xi \) is the identity matrix, and the density of the Jeffreys prior is \( \pi_J(\xi) \propto 1 \).

The Stein prior for \( \xi \) is \( \pi(\xi) = ||\xi||^{-1} \) and \( \pi/\pi_J \) is a harmonic function, and \( \pi \) satisfies \( \Delta(\pi/\pi_J)^{1/2} \leq 0 \).

The asymptotic risk improvement is

\[
\begin{align*}
E[D(p(y; u); p(y; \hat{\eta}_\pi))] - E[D(p(y; u); p(y; \hat{\eta}_I))] &= -\frac{2}{n^2} \left( \frac{\pi_J}{\pi} \right)^{1/2} \Delta \left( \frac{\pi}{\pi_J} \right)^{1/2} + o(n^{-2}) \\
&= \frac{1}{2n^2} ||\xi||^{-1} + o(n^{-2}).
\end{align*}
\]

5 Discussions

We proposed extended plugin densities for constructing predictive densities for curved exponential families. The extended plugin density with the posterior mean of the expectation parameter \( \eta \) of the full exponential family is shown to be optimal regarding the Bayes risk based on the Kullback–Leibler divergence if we choose a predictive density from the full exponential family. Several results are obtained from information-geometric perspectives. The results are parallel to those for Bayesian predictive densities. It is shown that plugin densities in \( \mathcal{P} \) can be improved regarding the Kullback–Leibler risk by shifting them in orthogonal directions. It is also shown that the optimal orthogonal shift coincides with the shift to the extended plugin with the Bayes estimator. We also consider priors for the extended plugin with the Bayes estimator and show the superharmonic condition for a prior to dominate the Jeffreys prior. This result suggests that shrinkage priors are effective for the extended plugin with the Bayes estimator.
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Appendix

Proof of asymptotic expansion of $\hat{\eta}_\pi$

We approximate $\hat{\eta}_\pi$ by the Laplace method (e.g., Kass and Vos (1997, Sec. 3.6 and Sec. 4.6), and Tierney and Kadane (1986)). First we expand $\pi(u) \exp(nL(u))$ around $u = \hat{u}_{MLE}$. In the following, symbols such as $\eta(\hat{u}_{MLE})$, $\partial_u \eta(\hat{u}_{MLE})$, and $\partial_u \partial_{\mu} \eta(\hat{u}_{MLE})$ are abbreviated to $\hat{\eta}$, $\partial_u \hat{\eta}$, and $\partial_u \partial_{\mu} \hat{\eta}$ respectively. Let $u = \hat{u}_{MLE} + \phi/\sqrt{n}$.

$$\pi(u) \exp(nL(u)) = \left( \hat{\pi} + \frac{\partial_u \hat{\pi}}{\sqrt{n}} + \frac{(\partial_u \partial_u \hat{\pi})}{6n} + \frac{(\partial_u \partial_u \partial_u \hat{\pi})}{24n} + O_p(n^{-2}) \right) \exp \left( nL + \frac{(\partial_u \partial_u L)}{2} \right)$$

$$= \hat{\pi} e^{nL} \left( 1 + \frac{(\partial_u \hat{L})}{\sqrt{n}} + \frac{(\partial_u \partial_u \hat{L})}{2n} + \frac{(\partial_u \partial_u \partial_u \hat{L})}{6n} + O_p(n^{-2}) \right)$$

$$\times \left( 1 + \frac{(\partial_u \hat{L})}{6n} + \frac{(\partial_u \partial_u \hat{L})}{24n} + \frac{(\partial_u \partial_u \partial_u \hat{L})}{72n} + O_p(n^{-2}) \right)$$

$$= \hat{\pi} e^{nL} \left( 1 + \frac{(\partial_u \hat{L})}{\sqrt{n}} + \frac{(\partial_u \partial_u \hat{L})}{6n} + \frac{(\partial_u \partial_u \partial_u \hat{L})}{144n} + O_p(n^{-2}) \right)$$

$$+ \frac{(\partial_u \hat{L})(\partial_u \partial_u \hat{L})}{12n} + \frac{(\partial_u \hat{L})(\partial_u \partial_u \partial_u \hat{L})}{24n} + \frac{(\partial_u \partial_u \hat{L})(\partial_u \partial_u \partial_u \hat{L})}{144n} + O_p(n^{-2}) \right) \right) .$$

Here $\hat{J}_{ab} = -\partial_u \partial_u \hat{L}$ and we denote terms which do not depend on $\pi$ as $C_1/\sqrt{n}$, which is $O_p(n^{-1/2})$.
Integrate both sides of the above equation and we obtain (let \((\hat{J}^{ab})\) be the inverse matrix of \((\hat{J}_{ab})\))

\[
\int \pi(u) \exp(nL(u))du = C_2 \hat{\eta} \left( 1 + \frac{(\partial_a \hat{\eta} \hat{J}^{ab})}{2\hat{\eta} \pi n} + \frac{(\partial_a \hat{\eta})(\partial_{bcd} \hat{L})(\hat{J}^{ab} \hat{J}^{cd} + \hat{J}^{ac} \hat{J}^{bd} + \hat{J}^{ad} \hat{J}^{bc})}{6\pi n} + \frac{C_3}{n} + O_p(n^{-2}) \right)
\]

Here \(C_2\) and \(C_3\) do not depend on \(\pi\) and \(C_3/n = O_p(n^{-1})\). Replace \(\pi(u)\) by \(\eta_i(u)\pi(u)\) and we have

\[
\int \eta_i(u) \pi(u) \exp(nL(u))du = C_2 \hat{\eta}_i \left( 1 + \frac{(\partial_a (\hat{\eta}_i \hat{J}^{ab}))}{2\hat{\eta}_i \pi n} + \frac{(\partial_a (\hat{\eta}_i))(\partial_{bcd} \hat{L})(\hat{J}^{ab} \hat{J}^{cd} + \hat{J}^{ac} \hat{J}^{bd} + \hat{J}^{ad} \hat{J}^{bc})}{6\pi n} + \frac{C_3}{n} + O_p(n^{-2}) \right).
\]

Therefore, the posterior mean of \(\hat{\eta}_i\) is expanded as follows:

\[
(\hat{\eta}_i)_i = \frac{\int \eta_i \exp(nL(u))\pi(u)du}{\int \exp(nL(u))\pi(u)du} = C_2 \hat{\eta}_i \left( 1 + \frac{(\partial_a (\hat{\eta}_i \hat{J}^{ab}))}{2\hat{\eta}_i \pi n} + \frac{(\partial_a (\hat{\eta}_i))(\partial_{bcd} \hat{L})(\hat{J}^{ab} \hat{J}^{cd} + \hat{J}^{ac} \hat{J}^{bd} + \hat{J}^{ad} \hat{J}^{bc})}{6\pi n} + \frac{C_3}{n} + O_p(n^{-2}) \right)
\]

\[
= \hat{\eta}_i \left( 1 + \frac{\hat{J}^{ab}}{2n} \left( \frac{(\partial_a (\hat{\eta}_i \hat{J}^{ab}))}{\hat{\eta}_i \pi} - \frac{(\partial_a \hat{\eta}_i)}{\pi} \right) \right) + \frac{\hat{J}^{ab} \hat{J}^{cd} \partial_{bcd} \hat{L}}{2n} \left( \frac{(\partial_a (\hat{\eta}_i \hat{J}^{ab}))}{\hat{\eta}_i \pi} - \frac{(\partial_a \hat{\eta}_i)}{\pi} \right) + O_p(n^{-2})
\]

\[
= \hat{\eta}_i + \frac{\hat{J}^{ab}}{2n} \left( \partial_a \hat{\eta}_i + \frac{2(\partial_a (\hat{\eta}_i))(\hat{J}^{ab})}{\pi} \right) + \frac{\hat{J}^{ab} \hat{J}^{cd} \partial_{bcd} \hat{L}}{2n} \partial_a \hat{\eta}_i + O_p(n^{-2}).
\]

Proof of Proposition 3.11

We abbreviate symbols such as \(g_{ab}(u)\) and \(H_{abc}(u)\) to \(g_{ab}\) and \(H_{abc}\), respectively.

The Kullback-Leibler divergence from \(p(y; u)\) to \(P_{\alpha,\beta}(y; \hat{u}_{\text{MLE}})\) is expanded as

\[
D(p(y; u), P_{\alpha,\beta}(y; \hat{u}_{\text{MLE}})) = \frac{1}{2} g_{ab} \hat{u}^{a} \hat{u}^{b} + \frac{1}{2n^2} g_{\kappa\lambda} \tilde{v}^{\kappa} \tilde{v}^{\lambda} + \left( \frac{1}{2} \Gamma_{abc} - \frac{1}{3} T_{abc} \right) \tilde{u}^{a} \tilde{u}^{b} \tilde{u}^{c}
\]

\[
+ \frac{1}{n} \left\{ \frac{m}{2} (\Gamma_{abc} + \Gamma_{abc} + \Gamma_{abc}) - T_{abc} \right\} \tilde{u}^{a}_{\text{MLE}} \tilde{u}^{b}_{\text{MLE}} \tilde{v}^{c} + K_{abcd} \tilde{u}^{a}_{\text{MLE}} \tilde{u}^{b}_{\text{MLE}} \tilde{v}^{c}_{\text{MLE}} \tilde{u}^{d}_{\text{MLE}} + o_p(n^{-2}),
\]

where \(\tilde{u} = \hat{u} - u\), \(\hat{u}_{\text{MLE}} = \hat{u}_{\text{MLE}} - u\) and

\[
K_{abcd} = \frac{1}{24} \int \left\{ 6 \left( \frac{\partial_a p}{p} \frac{\partial_b p}{p} \frac{\partial_c p}{p} \frac{\partial_d p}{p} \right) - 12 \left( \frac{\partial_a p}{p} \frac{\partial_b p}{p} \partial_c p \frac{\partial_d p}{p} \right) + 3 \left( \frac{\partial_a p}{p} \frac{\partial_b p}{p} \partial_c p \frac{\partial_d p}{p} \right) + 4 \left( \frac{\partial_a p}{p} \frac{\partial_b p}{p} \partial_c p \frac{\partial_d p}{p} \right) \right\} dy.
\]
Therefore the Kullback–Leibler risk from \( p(y; u) \) to \( p_{\alpha, \beta}(y; \hat{u}_\text{MLE}) \) is expanded as

\[
E[D(p(y; u), p_{\alpha, \beta}(y; \hat{u}_\text{MLE}))] = \frac{1}{2} g_{ab} E[\tilde{u}^a \tilde{u}^b] + \frac{1}{2n^2} g_{\kappa \lambda} E[\tilde{\beta}^\kappa \tilde{\beta}^\lambda] + \left( \frac{1}{2} \Gamma_{abc} - \frac{1}{3} T_{abc} \right) E[\tilde{u}^a \tilde{u}^b \tilde{u}^c]
\]

\[+ \frac{1}{n} \left( \frac{1}{2} (\Gamma_{abc} + \Gamma_{acb} + \Gamma_{cab}) - T_{abc} \right) E[\tilde{u}^a \tilde{u}^b \tilde{u}^c]
\]

+ (terms independent of \( \alpha, \beta \)) + o(n^{-2}).

Because \( \hat{\beta} \) is a smooth function of \( O_p(1) \) and \( \hat{\beta} = \beta + o_p(1) \),

\[E[\tilde{\beta}^\kappa \tilde{\beta}^\lambda] = \beta^\kappa \beta^\lambda + o(1),
\]

\[E[\tilde{u}^a \tilde{u}^b \tilde{u}^c] = \frac{1}{n} g^{ab} \beta^c + o(n^{-1})
\]

hold and

\[E[\tilde{u}^a \tilde{u}^b \tilde{u}^c] = (\alpha^a E[\tilde{u}^b \tilde{u}^c] + \alpha^b E[\tilde{u}^c \tilde{u}^d] + \alpha^c E[\tilde{u}^a \tilde{u}^d]) + o(n^{-2})
\]

\[= (\alpha^a g^{bc} + \alpha^b g^{ca} + \alpha^c g^{ab})/n^2 + o(n^{-2}).
\]

Lastly we derive \( E[\tilde{u}^a \tilde{u}^b] \). It can be expanded as follows (Efron (1975)):

\[E[\tilde{u}^a \tilde{u}^b] = \frac{1}{n} g^{ab} + \frac{1}{n} (g^{ca} \partial_c E[\tilde{u}^b] + g^{cb} \partial_c E[\tilde{u}^a]) + E \left[ (\tilde{u}^a - g^{ac} \partial_c L)(\tilde{u}^b - g^{bd} \partial_d L) \right].
\]

From the likelihood equation,

\[\partial_a L(\tilde{u}_\text{MLE}) = 0,
\]

\[\partial_a L + \tilde{u}^b_{\text{MLE}} \partial_{ab} L + \frac{1}{2} \tilde{u}^c_{\text{MLE}} \tilde{u}^d_{\text{MLE}} \partial_{acd} L + o_p(n^{-1}) = 0,
\]

\[g_{ab} \tilde{u}^b_{\text{MLE}} = \partial_a L + \tilde{u}^c_{\text{MLE}} (\partial_{ab} L + g_{ab}) + \frac{1}{2} \tilde{u}^c_{\text{MLE}} \tilde{u}^d_{\text{MLE}} \partial_{acd} L + o_p(n^{-1}),
\]

\[\tilde{u}^b = \frac{\alpha^b}{n} + g^{ab} \partial_a L + g^{ab} g^{cd} \partial_d L (\partial_{ac} L + g_{ac}) + \frac{1}{2} g^{ab} \tilde{u}^c_{\text{MLE}} \tilde{u}^d_{\text{MLE}} \partial_{acd} L + o_p(n^{-1}).
\]

Thus

\[E[\tilde{u}^b] = \frac{\alpha^b}{n} + (\text{terms independent of } \alpha, \beta) + o(n^{-1})
\]

and

\[E[(\tilde{u}^a - g^{ac} \partial_c L)(\tilde{u}^b - g^{bd} \partial_d L)]
\]

\[= \frac{\alpha^a \alpha^b}{n^2} + \frac{\alpha^a g^{be} g^{cd} E[\tilde{u}^c_{\text{MLE}} + \partial_{ecd} L]}{2n^2} + \frac{\alpha^b g^{ac} g^{cd} E[\tilde{u}^c_{\text{MLE}} + \partial_{ecd} L]}{2n^2}
\]

\[+ (\text{terms independent of } \alpha, \beta) + o(n^{-2})
\]

\[= \frac{\alpha^a \alpha^b}{n^2} - \frac{\alpha^a g^{be} g^{cd} \Gamma_{ecd}}{2n^2} - \frac{\alpha^b g^{ac} g^{cd} \Gamma_{ecd}}{2n^2} + (\text{terms independent of } \alpha, \beta) + o(n^{-2}),
\]
hence we obtain

$$E[\tilde{u}^a \tilde{u}^b] = \frac{1}{n} g^{ab} + \frac{1}{n^2} \left( g^{ca} \partial_c \alpha^b + g^{cb} \partial_c \alpha^a \right) + \frac{\alpha^a \alpha^b}{n^2} - \frac{\alpha^a g^{be} g^{cd} \Gamma_{cde}^m}{2n^2} - \frac{\alpha^b g^{ae} g^{cd} \Gamma_{cde}^m}{2n^2} + (\text{terms independent of } \alpha, \beta) + o(n^{-2}).$$

Here,

$$m \Gamma_{abc} = H_{abc},$$

and

$$-\Gamma_{bca} + T_{abc} = \frac{m}{H_{abc}}$$

hold. The first is from the definition and the second is from the relation

$$\partial_b g_{\alpha \kappa} = \int \partial_b \partial_{\alpha \kappa} p \frac{\partial \kappa}{p} dy + \int \partial_b \partial_{\alpha \kappa} p \frac{\partial a}{p} dy - \int \partial_a p \partial_{\alpha \kappa} p \frac{\partial b}{p^2} dy$$

$$= \frac{m}{\Gamma_{abc}} + \frac{m}{\Gamma_{bca}} - T_{abc}$$

and $$g_{\alpha \kappa} = 0.$$  

Therefore the risk is expanded as follows:

$$E[D(p(y; u), p_{\alpha, \beta}(y; \hat{u}_{\text{MLE}}))]$$

$$= \frac{d}{2n} + \frac{g_{ab}}{2n^2} \left( g^{ca} \partial_c \alpha^b + g^{cb} \partial_c \alpha^a \right) + \frac{g_{ab} \alpha^a \alpha^b}{2n^2} - \frac{g_{ab} \alpha^a g^{be} g^{cd} \Gamma_{cde}^m}{2n^2} + \frac{g_{bc}}{2n^2} \left( \frac{m}{\Gamma_{abc}} + \frac{m}{\Gamma_{bca}} + \frac{m}{\Gamma_{cab}} - 2T_{abc} \right) + g_{\kappa \lambda} \frac{g^{ab}}{2n^2} \left( \Gamma_{\kappa ab} + \Gamma_{bca} + \Gamma_{cab} - 2T_{abc} \right) + (\text{terms independent of } \alpha, \beta) + o(n^{-2})$$

$$= \frac{d}{2n} + \frac{g_{ab}}{2n^2} \alpha^a \alpha^b + \frac{1}{n^2} \left( \alpha^a \Gamma_{abc} + \partial_a \alpha^a \right) + \frac{g_{bc}}{2n^2} \beta^\kappa \beta^\lambda + \frac{g_{\kappa \lambda}}{2n^2} \left( \Gamma_{\kappa ab} + \Gamma_{bca} + \Gamma_{cab} - 2T_{abc} \right) + (\text{terms independent of } \alpha, \beta) + o(n^{-2}).$$

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